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# Synthesis and photophysical properties of novel oxadiazole substituted BODIPY fluorophores

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# **Supporting Information**

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## 1. General information

Reagents were purchased from commercial sources and were used without any additional purification. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded in Chloroform-*d* solutions at 25°C, using a 600 MHz NMR spectrometer; peak positions are given in parts per million ( $\delta$ ) referenced to the appropriate solvent residual peak. High-resolution mass spectra were recorded on Bruker maXis QTOF (tandem quarrupole/time-of-flight mass analyzer), equipped with an ESI source. The m/z scanning range was 50–3000. External calibration of the mass scale was carried out using a low-concentration calibration solution "Tuning mix" (Agilent Technologies). Samples were injected using a 500 µL Hamilton RN 1750 syringe (Switzerland). The measurements were carried out in the positive ion mode (+) (grounded spray needle, 4500-V high-voltage capillary; HV End Plate Offset: –500 V). The flow rate during injection was controlled with a syringe pump (3 µL/min). Nitrogen was used as a nebulizer gas (1.0 bar) and dry gas (4.0 L/min, 200°C). The data were processed using the Bruker Data Analysis 4.0 software. The reaction progress was monitored by TLC and the spots were visualized under UV light (254 or 365 nm). Melting points (not corrected) were determined on a SMP-10 apparatus. Solvents were distilled and dried according to standard procedures. The photoluminescence spectra were obtained using Camlin Modular Fluorescence Spectrometer FluoroSENS Pro-11. The concentration of the solutions for photoluminescence study was 1µM in all experiments. The quantum yield was estimated by direct method using an integrating sphere.

### 2. General procedure for the synthesis of BODIPY dyes:

In 25 mL 2 neck round bottom flask 3-phenyl-5-(5-phenyl-1*H*-pyrrol-3-yl)-1,2,4-oxadiazole (1 equiv.) was degassed by argon for 10 min. Then aldehyde (0.5 equiv.) was added and again purged by argon for 10 min. Then few drops of TFA was added and stirred at 120°C for 2 hours. The reaction progress was controlled by TLC (Sorbfil, 1:3, EtOAc – hexane). After completion of the reaction, the dark green mass was cooled and to the resulting paste, DCM (10.0 mL) was added, followed immediately by the addition of DDQ (1 equiv.). The deep red/purple solution was stirred overnight. After that, DIPEA (10 equiv.) was added and stirred for 30 minutes. Subsequently, reaction mixture was cooled in ice bath and BF<sub>3</sub>·OEt<sub>2</sub> (20 equiv.) was added slowly, dropwise, and the mixture was again stirred overnight. Then, the reaction mixture was transferred to a separation funnel, and washed with saturated Na<sub>2</sub>CO<sub>3</sub> (3 × 20 mL) followed by brine (2 × 20 mL). The organic solvent was removed in vacuo, and the residue was subjected to column chromatography (silica gel, 1:6, EtOAc – hexane) to give the desired product.

Entry	Solvent	Catalyst	Temp (°C)	Base	Time	Yield (%) <sup>a</sup>
1	DCM	TFA	25	-	-	NR
2	DCM	TFA	reflux	Et <sub>3</sub> N	10 days	Trace
3	DCE	TFA	25	-	-	NR
4	DCE	TFA	reflux	Et <sub>3</sub> N	7 days	Trace
5	DCE	5 mol% PPTS	25	-	-	NR [1]
6	DCE	10 mol% PPTS	reflux	-	7 days	trace <sup>b</sup>
7	toluene	10% mol I <sub>2</sub>	reflux	-	8 days	trace <sup>[2]b</sup>
8	Solv. free	TFA	120	Et <sub>3</sub> N	2h	32
9	Solv. free	TFA	150	Et <sub>3</sub> N	2h	17
10	Solv. free	TFA	200	Et <sub>3</sub> N	2h	Trace
11	Solv. free	TFA	120	DIPEA	2h	37

Table S1. Optimization of reaction conditions.

<sup>a</sup> Isolated yield, after column chromatography <sup>b</sup> After acid-condensation reaction

<sup>b</sup> 1 equiv. pyrrole, 0.5 equiv. aldehyde, a few drops of TFA, 1 equiv. DDQ, 10 equiv. DIPEA, 20 equiv. BF<sub>3</sub>OEt<sub>2</sub>. DCM = dichloromethane; DCE = 1,2-dichloroethane; TFA = trifluoroacetic acid; PPTS = pyridinium *p*-toluenesulfonate; DDQ = 2,3-dichloro-5,6-dicyano-1,4-benzoquinone; DIPEA = *N*,*N*-diisopropylethylamine; NR = no reaction.

### 3. NMR and HRMS characterization data



**5,5'-(5,5-Difluoro-3,7,10-triphenyl-5***H***-4λ<sup>4</sup>,5λ<sup>4</sup>-dipyrrolo[1,2-***c***:2',1'***f***][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3a). (262 mg, 0.37 mmol, 37%) dark purple solid, mp = 261–263 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-***d***) δ 7.91–7.89 (m, 4H), 7.80–7.79 (m, 4H), 7.50–7.47 (m, 6H), 7.46–7.45 (m, 1H), 7.45–7.44 (m, 1H), 7.42–7.39 (m, 4H), 7.32–7.31 (m, 2H), 7.09 (s, 2H), 6.97 (t,** *J* **= 7.7 Hz, 2H), 6.82 (t,** *J* **= 7.7 Hz, 1H). <sup>13</sup>C NMR (151 MHz, Chloroform-***d***) δ 171.3, 168.3, 158.9, 146.3, 134.35-134.34 (m), 132.3, 131.34, 131.3, 130.7, 130.6, 130.2, 129.8 (t,** *J* **= 3.7 Hz), 128.8, 128.7, 127.9, 127.5, 126.4, 125.59–125.58 (m). <sup>19</sup>F NMR (565 MHz, Chloroform-***d***) δ -132.21 (q,** *J***<sub>F-B</sub> = 30.2 Hz). HRMS (ESI) m/z calcd for C<sub>43</sub>H<sub>27</sub>BF<sub>2</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 709.2337 found 709.2333.** 

**5,5'-(5,5-Difluoro-3,7-diphenyl-10-(***o***-tolyl)-5***H***-4λ<sup>4</sup>,5λ<sup>4</sup>-dipyrrolo[1,2***c***:<b>2'**,1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3b). (217 mg, 0.30 mmol, 30%)burgundy solid, mp > 300 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*) δ 7.92–7.90 (m, 4H), 7.81–7.79 (m, 4H), 7.50– 7.48 (m, 6H), 7.47–7.46 (m, 1H), 7.45–7.44 (m, 1H), 7.42–7.40 (m, 4H), 7.14 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.02 (s, 2H), 6.81 (t, *J* = 7.6 Hz, 1H), 6.74 (d, *J* = 7.7 Hz, 1H), 6.62 (td, *J* = 7.6, 1.3 Hz, 1H), 2.38 (s, 3H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*) δ 170.9, 168.2, 158.8, 145.8, 137.8, 134.31– 134.30 (m), 131.4, 131.3, 130.8, 130.7, 130.4, 130.3, 129.9, 129.8 (t, *J* = 3.7 Hz), 128.8, 128.7, 127.5, 126.4, 125.35–125.33 (m), 125.2, 20.2. <sup>19</sup>F NMR (565 MHz, Chloroform-*d*) δ -131.53–131.85 (m), -133.41-133.73 (m). HRMS (ESI) m/z calcd for C<sub>44</sub>H<sub>29</sub>BF<sub>2</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 723.2493 found 723.2490.



**5,5'-(5,5-Difluoro-3,7-diphenyl-10-**(*p*-tolyl)-5*H*-4λ<sup>4</sup>,5λ<sup>4</sup>-dipyrrolo[1,2*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3c). (310 mg, 0.43 mmol, 43%) burgundy solid, mp = 240–242 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*) δ 7.90–7.88 (m, 4H), 7.78 (d, *J* = 8.0 Hz, 4H), 7.49–7.46 (m, 6H), 7.46–7.44 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 4H), 7.14 (d, *J* = 6.8 Hz, 2H), 7.07 (s, 2H), 6.70 (d, *J* = 7.4 Hz, 2H), 1.49 (s, 3H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*) δ 171.2, 168.2, 158.7, 146.7, 141.3, 134.48–134.47 (m), 131.4, 131.3, 130.6, 130.1, 129.8 (t, *J* = 3.6 Hz), 129.75, 128.8, 128.7, 128.6, 128.16–128.13 (m), 127.4, 126.4, 125.24-125.21 (m), 20.5.<sup>19</sup>F NMR (565 MHz, Chloroform-*d*) δ -132.24 (q, *J*<sub>F-B</sub>= 30.3 Hz). HRMS (ESI) m/z calcd for C<sub>44</sub>H<sub>29</sub>BF<sub>2</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 723.2493

found 723.2506. 5,5'-(5,5-Difluoro-10-(3-methoxyphenyl)-3,7-diphenyl-5*H*-4 $\lambda$ <sup>4</sup>,5 $\lambda$ <sup>4</sup>-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-

**1,2,4-oxadiazole)** (3d). (303 mg, 0.41 mmol, 41%) dark purple solid, mp = 228–230 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*)  $\delta$  7.90–7.89 (m, 4H), 7.81 (d, *J* = 7.3 Hz, 4H), 7.46–7.44 (m, 2H), 7.40 (t, *J* = 7.5 Hz, 4H), 7.07 (s, 2H), 6.86–6.84 (m, 3H), 6.25–6.24 (m, 1H), 3.37 (s, 3H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*)  $\delta$  171.3, 168.3, 158.9, 158.89, 145.9, 134.2, 133.4, 131.34, 131.3, 130.7, 129.8 (t, *J* = 4.2 Hz), 129.1, 128.8, 128.7, 128.25–128.24 (m), 127.5, 126.4, 125.40–125.35 (m), 122.7, 116.0, 54.9. <sup>19</sup>F NMR (565 MHz, Chloroform-*d*)  $\delta$  -132.22 (q, *J*<sub>F-B</sub> = 30.4 Hz). HRMS (ESI) m/z calcd for C<sub>44</sub>H<sub>29</sub>BF<sub>2</sub>N<sub>6</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 739.2442 found 739.2440.

# **5,5'-(5,5-Difluoro-10-(4-methoxyphenyl)-3,7-diphenyl-5***H*-4λ<sup>4</sup>,**5**λ<sup>4</sup>**dipyrrolo**[**1**,**2**-*c*:**2'**,**1'-f**][**1,3,2**]**diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole**) (3e). (413 mg, 0.56 mmol, 56%) amorphous mass. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*) δ 7.89–7.88 (m, 4H), 7.81 (d, *J* = 7.9 Hz, 4H), 7.48–7.47 (m, 6H), 7.45–7.44 (m, 2H), 7.42–7.39 (m, 4H), 7.20 (d, *J* = 8.2 Hz, 2H), 7.09 (s, 2H), 6.41 (d, *J* = 8.2 Hz, 2H), 3.05 (s, 3H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*) δ 171.4, 168.3, 161.6, 158.5, 146.5, 134.53–134.51 (m), 131.8, 131.4, 131.3, 130.5, 129.8 (t, *J* = 4.1 Hz), 128.8, 128.6, 127.4, 126.4, 125.19–125.16 (m), 125.1, 113.7, 54.7. <sup>19</sup>F NMR (565 MHz, Chloroform-*d*) δ -132.11 (q, *J*<sub>F-B</sub> = 30.4 Hz). HRMS (ESI) m/z calcd for C<sub>44</sub>H<sub>29</sub>BF<sub>2</sub>N<sub>6</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 739.2442 found 739.2447. **5,5'-(10-(2-bromophenyl)-5,5-difluoro-3,7-diphenyl-5***H***-4λ<sup>4</sup>,<b>5**λ<sup>4</sup>-

dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-

**1,2,4-oxadiazole**) (3f). (228 mg, 0.29 mmol, 29%) dark blue solid, mp = 158–160 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*)  $\delta$  7.93–7.91 (m, 4H), 7.83 (d, *J* = 7.2 Hz, 4H), 7.50–7.49 (m, 6H), 7.46–7.45 (m, 2H), 7.41 (t, *J* = 7.4 Hz, 4H), 7.31 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 7.09 (s, 2H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.62 (t, *J* = 7.6 Hz, 1H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*)  $\delta$  170.9, 168.3, 159.3, 134.06–134.05 (m), 132.8, 132.6, 132.0, 131.6, 131.4, 131.3, 130.8, 129.8 (t, *J* = 3.7 Hz), 128.9, 128.7, 127.5, 126.8, 126.3, 125.84–125.82 (m), 124.8. <sup>19</sup>F NMR (565 MHz, Chloroform-*d*)  $\delta$  -132.16–132.91 (m). HRMS (ESI) m/z calcd for C<sub>43</sub>H<sub>26</sub>BBrF<sub>2</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 787.1442 found 787.1448.

5,5'-(10-(4-bromophenyl)-5,5-difluoro-3,7-diphenyl-5H-4 $\lambda$ <sup>4</sup>,5 $\lambda$ <sup>4</sup>-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-

**1,2,4-oxadiazole**) (3g). (126 mg, 0.16 mmol, 16%) dark blue solid, mp = 197–198 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*)  $\delta$  7.90–7.89 (m, 4H), 7.83–7.81 (m, 4H), 7.50–7.49 (m, 6H), 7.48–7.47 (m, 2H), 7.43 (t, *J* = 7.4 Hz, 4H), 7.14 (d, *J* = 8.3 Hz, 2H), 7.11 (s, 2H), 7.09 (d, *J* = 8.3 Hz, 2H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*)  $\delta$  171.4, 168.2, 158.4, 154.1, 152.7, 151.5, 149.7, 142.9, 134.6, 131.5, 131.2, 131.0, 130.5, 129.78–129.74 (m), 128.8, 128.6, 128.0, 127.5, 126.5, 125.0, 121.0, 117.5, 116.9. <sup>19</sup>F NMR (565 MHz, Chloroform-*d*)  $\delta$  -132.18 (q, *J*<sub>F-B</sub> = 30.1 Hz). HRMS (ESI) m/z calcd for C<sub>43</sub>H<sub>26</sub>BBrF<sub>2</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 787.1442 found 787.1449.



# 5,5'-(10-(4-chlorophenyl)-5,5-difluoro-3,7-diphenyl-5H-4 $\lambda$ <sup>4</sup>,5 $\lambda$ <sup>4</sup>-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-

**1,2,4-oxadiazole**) (3h). (215 mg, 0.29 mmol, 29%) dark blue solid, mp = 276–277 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*)  $\delta$  7.90–7.89 (m, 4H), 7.83–7.81 (m, 4H), 7.50–7.47 (m, 8H), 7.44–7.42 (m, 4H), 7.22 (d, *J* = 8.3 Hz, 2H), 7.11 (s, 2H), 6.93 (d, J = 8.3 Hz, 2H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*)  $\delta$  171.1, 168.5, 159.2, 151.2, 144.59–144.57 (m), 137.4, 134.20–134.18 (m), 131.4 13C NMR (151 MHz, Chloroform-d)  $\delta$  144.60 –144.55 (m), 131.41 (d, *J* = 2.9 Hz), 131.2, 130.84, 130.8, 129.8 (t, *J* = 4.2 Hz), 128.9, 128.7, 128.3, 128.08–128.05 (m), 127.5, 126.1, 125.69–125.66 (m). <sup>19</sup>F NMR (565 MHz, Chloroform-*d*)  $\delta$  -132.17 (q, *J*<sub>F-B</sub> = 30.9 Hz). HRMS (ESI) m/z calcd for C<sub>43</sub>H<sub>26</sub>BClF<sub>2</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 743.1947 found 743.1953.

# 5,5'-(5,5-difluoro-10-(3-fluorophenyl)-3,7-diphenyl-5*H*-4 $\lambda^4$ ,5 $\lambda^4$ -

dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-1,2,4-oxadiazole) (3i). (225 mg, 0.31 mmol, 31%) burgundy solid, mp = 260–262 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*)  $\delta$  7.90–7.89 (m, 4H), 7.83–7.81 (m, 4H), 7.50–7.48 (m, 6H), 7.47–7.46 (m, 2H), 7.42 (t, *J* = 7.5 Hz, 4H), 7.10 (s, 2H), 7.08–7.07 (m, 2H), 6.94–6.90 (m, 1H), 6.47 (td, *J* = 8.5, 2.4 Hz, 1H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*)  $\delta$  171.1, 168.4, 162.9, 161.2, 159.3, 144.0, 134.2, 134.16, 134.05–134.04 (m), 131.4, 131.2, 130.8, 129.8 (t, *J* = 3.8 Hz), 129.7, 128.9, 128.7, 128.14–128.12 (m), 127.5, 126.2, 126.0 (d, *J* = 3.1 Hz), 125.88–125.79 (m), 117.7, 117.6, 117.4. <sup>19</sup>F NMR (565 MHz, Chloroform-*d*)  $\delta$  -112.38–112.42 (m), -131.71–132.04 (m), -132.31–132.63 (m). HRMS (ESI) m/z calcd for C<sub>43</sub>H<sub>26</sub>BF<sub>3</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 727.2242 found 727.2241.

# 5,5'-(5,5-difluoro-10-(4-fluorophenyl)-3,7-diphenyl-5H-4 $\lambda$ <sup>4</sup>,5 $\lambda$ <sup>4</sup>-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine-1,9-diyl)bis(3-phenyl-

**1,2,4-oxadiazole)** (3j). (174 mg, 0.24 mmol, 24%) purple solid, mp = 248–250 °C. <sup>1</sup>H NMR (600 MHz, Chloroform-*d*)  $\delta$  7.90–7.89 (m, 4H), 7.83–7.82 (m, 4H), 7.50–7.47 (m, 8H), 7.44–7.42 (m, 4H), 7.30–7.28 (m, 2H), 7.12 (s, 2H), 6.66 (t, *J* = 8.5 Hz, 1H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*)  $\delta$  13C NMR (151 MHz, Chloroform-*d*)  $\delta$  171.2, 168.5, 159.2, 144.9, 134.37–134.32 (m), 132.3, 132.28, 131.5, 131.2, 130.8, 129.8 (t, *J* = 4.2 Hz), 129.0, 128.7, 128.13–128.08 (m), 127.4, 126.1, 125.75–125.72 (m), 115.5, 115.3. <sup>19</sup>F NMR (565 MHz, Chloroform-*d*)  $\delta$  -108.80–108.85 (m), -132.17 (q, *J*<sub>F-B</sub> = 30.3 Hz). HRMS (ESI) m/z calcd for C<sub>43</sub>H<sub>26</sub>BF<sub>3</sub>N<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 727.2242 found 727.2250.

4. Photoluminescence data





#### 5. Quantum-chemical calculations

DFT and time-dependent density functional theory (TD-DFT) calculations to obtain minimum energy structures in both the ground and excited states for the structures **3a** and **4** were performed by using Gaussian09 set of programs.<sup>3</sup> The ground state was optimized at B3LYP level<sup>4</sup> with 6-31G(d,p) basis set and stationary points were characterized using vibrational analysis - to confirm the minimum nature of the optimized geometries. The effect of dispersion correction<sup>5</sup> was also evaluated on the optimized geometries (empiricaldispersion=gd3bj) and found to be negligible (see Table S2). The excitation spectra for **3a** and **4** structures were simulated by using TD-DFT calculations with a range-separated versions CAM-B3LYP<sup>6</sup> and 6-311+G(d,p) and TZVP basis sets. Solvent effects were treated by the conductor-like polarizable continuum model (CPCM) model<sup>7</sup> adopted in the linear response formalism when used with TD-DFT. According to a general trend of TD-DFT methods<sup>8</sup> we found an overestimation of **3a** and **4** absorption band peaks of about 0.3 eV, (compare the simulated spectra of Fig. S11 with the experimental one of Fig. 3); nevertheless, the yellow-light shift going from **4** to **3a** is well reproduced and the solvent effect was found to be negligible (see Table S2) in agreement with our experimental results. Finally, our TD-DFT analysis revealed that the

maximum of absorption for the S0  $\leftarrow$ -S1 transition corresponds to the HOMO and LUMO difference and the MO contributions are reported in Fig. 4 and Fig. S12 for **3a** and **4**, respectively. The near-UV region with maximum at about 360 nm (see Fig. S11) can be attributed to the S0  $\leftarrow$ -S2 and S0  $\leftarrow$ -S3 transitions with the former more relevant for **3a** and the latter for **4** complexes. DFT and TD-DFT calculations of the structures reported in Table S3 were carried out with B3LYP hybrid functional combined with 6-31G(d) basis set by using ORCA 4.1.1. package programs.<sup>9</sup> Input files and molecular orbital plots were prepared with Gabedit 2.4.7 software.<sup>10</sup> In the case of compounds containing boronic atom, the def2-TZVP basis set<sup>11</sup> was used in combination with CPCM to take into account the effect of the solvent.

Table S2. Variability of simulation spectra depending on the computational approach for compounds 3a and 4 (in parenthesis) compared with the experimental data. Wavelengths in nm.

Geo	Methods	Calc. $\lambda_{ex}$ <b>3a</b> and (4) <sup>a</sup>	$\Delta \lambda_{ex}{}^{b}$	Calc. $\Delta\lambda_{ex(3a-4)}$ shift <sup>c</sup>
B3LYP/631G(d,p)	CAM-	537 (510)	51 (51)	26
	B3LYP/6311G(d,p)			
	CAM-	534 (508)	53 (53)	26
	B3LYP/TZVP			
D3-	CAM-	533 (513)	55 (48)	20
B3LYP/631G(d,p)	B3LYP/6311G(d,p)			
	CAM-	531 (511)	57 (50)	20
	B3LYP/TZVP			
B3LYP/631G(d,p)	CAM-	538 (510) <sup>d</sup>	-	-
	B3LYP/6311G(d,p)			

a) Calculated  $\lambda_{ex}$  values for **3a** and **4** (in parenthesis) to be compared with the experimental  $\lambda_{ex}$  of 588 and 561 nm for **3a** and **4**, respectively (see Fig. 3 of the text).

b) Variation between experimental and calculated  $\lambda_{ex}$  for **3a** and **4** (in parenthesis).

c) Calculated shift going from 4 to 3a. Values to be compared with the experimental shift of 27 nm.

d) Calculated values using  $CH_2Cl_2$  as solvent in a place of THF.



Fig. S11 TD-DFT (CAM-B3LYP/6311+G(d,p)) simulated spectra for 3a (A) and 4 (B) in THF as solvent (CPCM model). Wavelenghts in nm.



Fig. S12 HOMO (A) and LUMO (B) countours calculated at the TD-DFT level for compound 4 corresponding to the  $S0 \leftarrow -S1$  transition.



**Fig. S13** TD-DFT analysis (CAM-B3LYP/6311+G(d,p)) of MO contributions for S0  $\leftarrow$ -S2 and S0  $\leftarrow$ -S3 transitions to the near-UV region (maximum at about 360 nm, see Fig. S11) for complexes **3a** (A, B) and **4** (C, D).



**Fig. S14** TD-DFT (CAM-B3LYP/6311+G(d,p)) simulated spectra for absorption (A) and emission (B) of selected oxadiazole compounds (**3a**, **3d**, **3e**, **3g**) in THF as solvent. Compound 4 (dotted line) is also reported for comparison.

**Table S3.** Calculated main assignments (coefficient), excitation energies *E* (in eV), maximum absorption wavelengths  $\lambda_{abs}$  (in nm), the oscillator strength *f*, for selected compounds at the TD-CAM-B3LYP/6-311+G(d,p)//B3LYP/6-31G(d,p) level, by using THF as solvent (CPCM).

Compounds	Main assignment	E	$\lambda_{abs}$	f
3a	$H \rightarrow L (0.696)$	2.3104	536.62	0.8027
3a	$H_{-1} \to L (0.593)$	3.3502	370.09	0.1473
3a	$H_{-10} \rightarrow L (0.586)$	3.7130	333.92	0.0476
3d	$H \rightarrow L (0.696)$	2.2954	540.14	0.7878
3d	$H_{-1} \rightarrow L (0.6976)$	3.0240	410.00	0.0414
3d	$H_{-4} \rightarrow L (0.5909)$	3.4189	362.64	0.1038
3e	$H \rightarrow L (0.6954)$	2.3218	534.00	0.7907
3e	$H_{-1} \rightarrow L (0.6905)$	2.8373	436.98	0.1766
3e	$H_{-10} \rightarrow L (0.5745)$	3.7068	334.48	0.0535
3g	$H \rightarrow L (0.6956)$	2.2846	542.69	0.8073
3g	$H_{-1} \rightarrow L (0.6732)$	3.2707	379.08	0.1591
3g	$H_{-10} \rightarrow L (0.5169)$	3.6422	340.41	0.0529
4	$H \rightarrow L (0.6965)$	2.4287	510.49	0.8634
4	$H_{-1} \rightarrow L (0.6886)$	3.3556	369.49	0.0039
4	$H_{-11} \rightarrow L (0.14859)$	3.5117	353.06	0.0420

**Table S4.** Calculated main assignments (coefficient), excitation energies *E* (in eV), maximum emission wavelengths  $\lambda_{em}$  (in nm), the oscillator strength *f*, for selected compounds at the TD-CAM-B3LYP/6-311+G(d,p)//TD-CAM-B3LYP/6-31G(d,p) level, by using THF as solvent (CPCM).

Compounds	Main assignment	E	λ <sub>em</sub>	f
3a	$H \leftarrow L (0.6969)$	2.1620	573.48	0.7815
3d	$H \leftarrow L (0.6969)$	2.1540	575.60	0.7723
3e	$H \leftarrow L (0.6967)$	2.1720	570.83	0.7768
3g	$H \leftarrow L (0.6969)$	2.1402	579.32	0.7957
4	$H \leftarrow L (0.6977)$	2.2775	544.40	0.8385

# Table S5. DFT/TD-DFT calculations for 3a-3j compounds.

Compound	HOMO-1 / eV	HOMO / eV	LUMO / eV	LUMO+1 / eV
3a				
	-6.59	-5.74	-3.24	-1.41
3b				
	-6.50	-5.74	-3.24	-1.39
Зс				
	-6.41	-5.73	-3.22	-1.40
3d	-6.06	-572	-3.24	-1 40

3e	-6.00	-572	-3.20	-1.41
3f				
3g	-6.53	-5.76	-3.34	-1.45 -1.45
3h	-0.59	-5.77	-3.33	-1.45
3i	-6.63	-5.76	-3.30	-1.43



Table S6. Cartesian coordinates for the optimized compounds 3, calculated at B3LYP/31G(d,p)/CPCM(CCl<sub>2</sub>H<sub>2</sub>).

		3a				3b	
C	1.69997	1.65547	1.26782	C	1.64032	1.59904	1.34395
C	0.86618	0.58968	1.57618	C	0.80065	0.53237	1.62821
C	1.55103	-0.60683	1.25950	C	1.48063	-0.66158	1.28889
N	2.78775	-0.28682	0.78321	N	2.72024	-0.33936	0.82387
C	2.94136	1.09808	0.82192	C	2.87814	1.04523	0.88311
C	4.19550	1.70199	0.60817	C	4.13244	1.65089	0.68739
C	5.30679	0.92162	0.23436	C	5.25422	0.87043	0.35025
N	5.17501	-0.43745	-0.04784	N	5.14070	-0.49634	0.09611
В	3.88517	-1.27060	0.25500	В	3.83760	-1.32665	0.34571
C	6.33174	-0.88441	-0.61420	C	6.31181	-0.94405	-0.43804
C	7.25274	0.18709	-0.66446	C	7.22141	0.13740	-0.50095
C	6.64629	1.30145	-0.10081	C	6.59225	1.25816	0.02194
C	7.37800	2.53346	0.17022	C	7.29243	2.52383	0.22289
C	6.62627	-2.23322	-1.12579	C	6.63149	-2.30227	-0.90708
C	0.97729	-1.94826	1.45598	C	0.89790	-2.00318	1.44915
C	4.34635	3.17070	0.77650	C	4.27878	3.12494	0.86925
C	0.15653	-2.14110	2.58707	C	0.05822	-2.21794	2.56211
C	-0.45452	-3.37067	2.82343	C	-0.56242	-3.44957	2.75946
C	-0.26969	-4.42847	1.92856	C	-0.36871	-4.48691	1.84269
C	0.53116	-4.24426	0.79813	C	0.45116	-4.28047	0.72977
C	1.15152	-3.01870	0.55890	C	1.08142	-3.05299	0.52985
C	6.23641	-3.42236	-0.48192	C	6.23459	-3.47752	-0.24231
C	6.60555	-4.65955	-1.00864	C	6.62897	-4.72481	-0.72503
C	7.36388	-4.73745	-2.17979	C	7.41979	-4.82671	-1.87259
C	7.76032	-3.56288	-2.82547	C	7.82294	-3.66605	-2.53897
C	7.40163	-2.32306	-2.30099	C	7.43917	-2.41614	-2.05820
C	4.18871	3.75639	2.04190	C	4.28995	3.63252	2.17602
C	4.64659	3.98023	-0.32975	C	4.39508	3.99310	-0.23841
C	4.78018	5.35936	-0.17081	C	4.54933	5.36150	0.01790
C	4.33699	5.13436	2.19750	C	4.43828	4.99985	2.40501
C	4.62957	5.93829	1.09230	C	4.57575	5.86572	1.31969
F	3.47540	-1.87119	-0.93465	F	3.48201	-1.93228	-0.85847
F	4.12843	-2.21338	1.25249	F	4.03419	-2.26534	1.35760
H	-0.15615	0.65219	1.91860	H	8.24837	0.07219	-0.82913
Н	4.22431	5.57923	3.18202	H	-0.22057	0.59289	1.97426

Ц	2 07257	2 12070	2 00281	Ц	4 45082	5 38120	3 12186
	5.97237	5.00000	2.90261		4.43082	2.04(00	2.01294
н	5.00094	5.98088	-1.03367	Н	4.20026	2.94699	3.01384
H	4.75295	3.53195	-1.31333	H	4.63596	6.04461	-0.82341
H	0.01842	-1.32894	3.29440	H	-0.08748	-1.42234	3.28653
Н	-0.74736	-5.38709	2.10960	Н	-0.85402	-5.44696	1.99338
н	-1 07128	-3 50257	3 70788	н	-1 19395	-3 59914	3 63060
11	-1.07120	-3.30257	0.22(00	11	1 70405	2,00202	0.24150
П	1./5/55	-2.88550	-0.32088	Н	1./0405	-2.90282	-0.34130
H	0.67071	-5.05826	0.09197	H	0.59819	-5.07835	0.00691
Н	5.66091	-3.37607	0.43219	H	5.63167	-3.41208	0.65271
Н	7.70216	-1.41553	-2.81523	Н	7.74555	-1.52021	-2.58897
н	8 34528	-3 61076	-3 73932	н	8 43286	-3 73285	-3 43523
11	7 64652	5 70500	2 59425		7 72210	5 20101	2 24204
п	/.04033	-3.70300	-2.36423		1.12210	-3.80191	-2.24504
H	6.30307	-5.56791	-0.49569	H	6.32048	-5.62190	-0.19606
N	8.86181	4.10473	-0.28192	N	8.66614	4.14731	-0.37184
C	1.24847	3.04244	1.30810	C	1.20820	2.98924	1.44928
н	4 74015	7.01206	1 21523	Н	4 69561	6 93325	1 48326
N	1.77448	3 05000	0.27521	N	1 20443	3 02000	0.54808
	1.2/440	3.93099	0.37331		1.20443	3.92990	0.54696
0	0.59198	3.44599	2.41699	0	0.60524	3.36003	2.59950
N	0.16298	4.75937	2.17271	N N	0.18201	4.68516	2.42059
C	0.59520	5.00474	0.95176	C	0.56392	4.97004	1.19151
N	7.49242	3.20688	1.27959	N	7.47138	3.21773	1.30998
C	8 42016	4 17596	0.95811	C	8 32863	4 21896	0.90029
	0.42010	6 29105	0.95011		0.32603	4.21090	0.90029
Č	0.30330	0.28105	0.20004	C	0.51090	0.2/318	0.33835
C	8.88833	5.18641	1.91771	C	8.83481	5.26092	1.80515
C	8.27406	5.28387	3.17569	C	8.31913	5.35953	3.10657
C	8.71454	6.23497	4.09644	C	8.79578	6.34256	3.97413
C	9 76899	7 09225	3 77037	C	9 78891	7 23032	3 55147
	10 28 280	6 00916	2 51626		10 20521	7 12/12	2 25440
	0.41027	0.99610	2.31030		0.20049	7.13413	2.23449
C	-0.4102/	7.29140	0.85696		-0.38048	1.28313	1.24303
C	-0.62193	8.49411	0.18617	C	-0.60794	8.51247	0.62819
C	-0.06742	8.69953	-1.08196	C	-0.14499	8.74564	-0.67151
C	0.70301	7.69668	-1.67704	C	0.54844	7.74313	-1.35513
Ċ	0.02018	6 49072	-1.01008	C C	0 78061	6 51036	-0.74457
	1 22100	0.49072	-1.01000		1.14725	0.51050	-0.7++37
н	-1.22109	9.2/1/4	0.03118	Н	-1.14/23	9.28969	1.1019/
H	-0.84258	7.12984	1.83903	H	-0.74070	7.10050	2.25017
H	1.52140	5.70892	-1.46167	H	1.32025	5.72785	-1.26701
Н	1.13498	7.85262	-2.66102	Н	0.90893	7.92049	-2.36398
н	-0 23671	9 63746	-1 60347	н	-0 32573	9 70487	-1 14844
и 11	8 23/1/	6 30500	5.06703	и 11 11	8 30101	6 /1511	1.11011
	0.23414	0.30390	2.41700		0.39101	0.41311	4.97932
Н	/.45288	4.61/69	3.41/98	Н	/.54488	4.66933	3.42445
Н	10.11262	7.83012	4.49001	H	10.16088	7.99367	4.22923
C	9.94737	6.05091	1.59189	C	9.83295	6.15535	1.38264
Н	11.20508	7.66076	2.26142	Н	11.08019	7.82034	1.92443
н	10 42755	5 97335	0.62157	н	10 23766	6.07608	0 37869
0	8 17200	3 00/04	-0.81462		7 08108	3 01274	-0.83156
	0.17290	0.11(00	-0.01402		1.90190	3.01274	-0.63130
н	8.2/486	0.11680	-1.00638	C	4.29158	3.495/8	-1.001/9
				Н	3.32073	3.01689	-1.83478
				H	5.06343	2.75886	-1.90617
				Н	4.38709	4.32621	-2.36575
		30				3d	
C	1 67137	1 66482	1 53703	C	1 66/37	1 71215	1.64164
	1.0/13/	1.00402	1.03703		1.00437	1./1313	1.04104
C	0.84540	0.58838	1.8514/		0.82687	0.62945	1.8033/
C	1.53526	-0.59812	1.49126	C	1.51932	-0.54418	1.48506
N	2.76799	-0.26254	1.01463	N	2.76340	-0.19365	1.05086
C	2.91392	1.12231	1.07619	C	2.91361	1.18579	1.18141
C	4,16363	1.73659	0.86223	C	4,16899	1.80399	1.02821
	5 27571	0.06685	0.46752		5 28827	1.05382	0.62210
	5.27571	0.20003	0.1(220		5.2003/	1.03303	0.02210
	5.14958	-0.38//1	0.10339		3.10//2	-0.28/09	0.2391/
В	3.86617	-1.23172	0.46086	В	3.87678	-1.14172	0.49111
C	6.30660	-0.81917	-0.41513	C	6.33440	-0.69424	-0.31654
C	7.22180	0.25760	-0.45060	C	7.24930	0.38399	-0.29348
C	6.61148	1.35917	0.13428	C	6.62884	1.46022	0.32524
	7 22676	2 50075	0.42588		7 2//71	2 68210	0.67025
	1.55020	2.370/3	0.42300		1.344/1	2.00319	0.07023

$ \begin{array}{c} c & 0.07031 & -1.04621 & 1.6826 & C & 0.94638 & -1.88620 & 1.5890 \\ c & 0.15803 & -2.16278 & 2.80116 & C & 0.10454 & -2.15879 & 2.69027 \\ c & -0.04484 & -3.39952 & 3.02079 & C & -0.50543 & -3.40224 & 2.84142 \\ c & -0.26008 & -4.44132 & 2.10730 & C & -0.29839 & -4.4091 & 1.88868 \\ c & 0.53254 & +2.3354 & 0.97515 & C & 0.52354 & -4.15111 & 0.78817 \\ c & 1.14856 & -3.00058 & 0.75255 & C & 1.14267 & -2.91130 & 0.63397 \\ c & 6.22231 & -3.35982 & -0.32864 & C & 6.24651 & -3.23664 & -0.3379 \\ c & 6.22234 & -4.63898 & -2.05396 & C & 7.4148 & -4.4729 & -2.08193 \\ c & 7.34954 & -4.63898 & -2.05396 & C & 7.4148 & -4.4729 & -2.08193 \\ c & 7.37700 & -2.22264 & -2.13098 & C & 7.44290 & -2.02989 & -2.06521 \\ c & 4.16322 & -3.2525 & -0.12349 & C & 4.16451 & -3.24564 & -0.37210 \\ c & 4.16322 & -3.2525 & -0.12349 & C & 4.16451 & -3.74588 & -0.49774 \\ c & 4.61231 & -4.0739 & -0.04813 & C & 4.57747 & 4.13984 & 0.25427 \\ c & 4.3226 & 5.15980 & 2.47527 & C & 4.26883 & 5.11212 & 2.84747 \\ c & 4.57181 & 5.99450 & 1.38713 & C & 4.57747 & 4.13984 & 0.25427 \\ c & 4.3269 & 5.15980 & -0.73616 & F & 3.49357 & -1.67324 & -0.73723 \\ F & 3.40944 & -1.81305 & -0.73616 & F & 3.49357 & -1.67324 & -0.73723 \\ F & 3.40944 & -1.81305 & -0.73708 & H & 4.10616 & -2.13616 & 1.40486 \\ H & 8.24305 & 0.19803 & -0.79708 & H & 8.27567 & 0.33968 & -0.62676 \\ H & -0.1763 & 0.63923 & 2.17953 & H & -0.0118 & 0.66919 & 2.19418 \\ H & -0.5763 & 0.63923 & 2.7724 & H & -0.0118 & 0.66919 & 2.19418 \\ H & -0.5727 & -5.03469 & 0.25446 & H & 5.6363 & -3.24422 & 0.03798 \\ H & 0.6727 & -5.03469 & 0.25446 & H & 5.6363 & -3.24727 & 2.00454 \\ H & 0.6727 & -5.03469 & -0.25764 & H & 0.68160 & -3.59718 & -0.47011 \\ H & 0.9738 & -5.03725 & -5.3790 & H & -0.05127 & -2.72471 & -0.23020 \\ H & 1.74395 & -2.48964 & -0.13479 & H & 0.68116 & -3.215711 \\ H & 0.07278 & -5.03469 & 0.25446 & H & 5.65363 & -3.24422 & 0.57990 \\ H & 7.63481 & -5.9773 & -2.47710 & H & 6.33095 & -3.37611 & -0.47061 \\ H & 0.0738 & 3.7172 & -2.04248 & 1.07378 & H & -0.05127 & -2.338815 & -3.00118 \\ H & 0.07$	С	6.60518	-2.15748	-0.95178	С	6.64445	-2.01009	-0.89928	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Ċ	0 97031	-1 94621	1 66826	Ċ	0 94638	-1 89620	1 58900	
$ \begin{array}{c} C & 0.15803 & 2.16278 & 2.20116 & C & 0.10454 & 2.15879 & 2.69027 \\ C & 0.404484 & -3.3952 & 3.02079 & C & 0.50543 & -3.40224 & 2.84142 \\ C & 0.2608 & -4.4132 & 2.10730 & C & 0.22334 & -4.15111 & 0.78817 \\ C & 0.33254 & +2.3354 & 0.97515 & C & 0.22344 & -4.15111 & 0.78817 \\ C & 0.14456 & -3.00058 & 0.75255 & C & 1.14267 & -2.91130 & 0.63397 \\ C & 6.22231 & -3.35982 & -0.32864 & C & 6.24651 & -3.23664 & -0.33319 \\ C & 6.22846 & -4.8598 & -2.05396 & C & 7.4148 & -4.4729 & -2.08193 \\ C & 7.34954 & -4.63898 & -2.05396 & C & 7.4148 & -4.4729 & -2.08193 \\ C & 7.37700 & -2.22264 & -2.13098 & C & 7.44290 & -2.02989 & -2.06521 \\ C & 4.14323 & 3.78221 & 2.31130 & C & 4.1645 & 3.24563 & -2.05041 \\ C & 4.1211 & 4.02739 & -0.04813 & C & 4.57747 & 4.13984 & 0.25427 \\ C & 4.67352 & 5.00255 & 0.12349 & C & 4.67575 & 5.51738 & 0.49974 \\ C & 4.23269 & 5.15980 & 2.47527 & C & 4.26883 & 5.11212 & 2.84747 \\ C & 4.27181 & 5.9946 & 1.37813 & C & 4.57747 & 4.13984 & 0.25427 \\ F & 3.44944 & -1.81305 & -0.73016 & F & 3.49357 & -1.67824 & -0.73723 \\ F & 3.1201 & -2.19086 & 1.43980 & F & 4.10616 & F & 3.49357 & 1.67824 & -0.73723 \\ F & 4.12031 & -2.19086 & 1.43980 & F & 4.10616 & 7.033968 & -0.62676 \\ H & 6.07301 & 1.6286 & 5.32213 & 3.46603 & H & 4.15897 & 3.45221 \\ H & 4.05303 & 6.02291 & -0.73728 & H & -0.05127 & -1.39114 & 3.44220 \\ H & 0.01973 & -1.36666 & 3.52318 & H & -0.77488 & -5.37427 & 2.00454 \\ H & -0.1320 & -3.05692 & 2.7524 & H & -1.33818 & -3.70418 \\ H & -1.05506 & -3.54942 & 3.90691 & H & 1.76527 & -2.72471 & -0.23020 \\ H & 1.74395 & -2.84986 & -0.13479 & H & 0.68106 & -3.54942 & 3.00518 \\ H & 7.67244 & -1.33124 & 3.29563 & 3.25721 \\ H & 7.63481 & 5.9773 & 2.47710 & H & 6.8106 & -3.54942 & 3.00618 \\ H & 7.05248 & -0.5773 & 2.47710 & H & 6.83095 & -5.3761 & -0.47001 \\ H & 0.7277 & -5.03469 & 0.25446 & H & 5.65363 & -3.24422 & 0.57099 \\ H & 7.67448 & -5.37275 & 0.57790 & H & 7.7562 & -2.39841 & -2.37211 \\ H & 0.07278 & 3.54977 & -3.5986 & H & 7.75529 & -3.39901 \\ H & 7.67248 & 7.067573 & -2.07241 & H & 8.8090 & 0.305$	Č	4 30879	3 20171	1.04657	C C	4 30570	3 25934	1 30230	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C C	0.15803	-2 16278	2 80116		0.10454	-2 15870	2 60027	
$ \begin{array}{c} \mathbf{C} & 0.3033 \\ \mathbf{C} & 0.3024 \\ \mathbf{C} & 0.3028 \\ \mathbf{C} & 0.3225 \\ \mathbf{C} & 0.3225 \\ \mathbf{C} & 1.1426 \\ \mathbf{C} & 1.0058 \\ \mathbf{C} & 0.3225 \\ \mathbf{C} & 1.1426 \\ \mathbf{C} & 1.0058 \\ \mathbf{C} & 0.3225 \\ \mathbf{C} & 1.1426 \\ \mathbf{C} & 1.0058 \\ \mathbf{C} & 0.3225 \\ \mathbf{C} & 1.1426 \\ \mathbf{C} & 1.0058 \\ \mathbf{C} & 0.3295 \\ \mathbf{C} & 0.32854 \\ \mathbf{C} & 0.32854 \\ \mathbf{C} & 0.32854 \\ \mathbf{C} & 0.22310 \\ \mathbf{C} & 0.32854 \\ \mathbf{C} & 0.32852 \\ \mathbf{C} & 7.34954 \\ \mathbf{C} & 4.3528 \\ \mathbf{C} & 2.0113 \\ \mathbf{C} & 1.148 \\ \mathbf{C} & 4.44729 \\ \mathbf{C} & 2.02389 \\ \mathbf{C} & 7.37100 \\ \mathbf{C} & 2.22264 \\ \mathbf{C} & 2.13098 \\ \mathbf{C} & 7.44290 \\ \mathbf{C} & 4.148 \\ \mathbf{C} & 4.46121 \\ \mathbf{C} & 4.02739 \\ \mathbf{C} & 0.04813 \\ \mathbf{C} & 4.57747 \\ \mathbf{C} & 4.13984 \\ \mathbf{C} & 2.84747 \\ \mathbf{C} & 4.5260 \\ \mathbf{S} & 5.1718 \\ \mathbf{C} & 4.07322 \\ \mathbf{C} & 4.1305 \\ \mathbf{C} & 7.37100 \\ \mathbf{C} & 4.1305 \\ \mathbf{C} & 7.3720 \\ \mathbf{C} & 4.26883 \\ \mathbf{S} & 5.11212 \\ \mathbf{C} & 2.84747 \\ \mathbf{C} & 4.5261 \\ \mathbf{C} & 4.0327 \\ \mathbf{C} & 4.57181 \\ \mathbf{S} & 5.9450 \\ \mathbf{C} & 7.3723 \\ \mathbf{F} & 4.1031 \\ \mathbf{C} & 4.52620 \\ \mathbf{C} & 0.0701 \\ \mathbf{B} & 8.2767 \\ \mathbf{C} & 3.3375 \\ \mathbf{C} & 4.52620 \\ \mathbf{C} & 0.0701 \\ \mathbf{B} & 8.2767 \\ \mathbf{C} & 3.3372 \\ \mathbf{F} & 4.1031 \\ \mathbf{C} & 4.5265 \\ \mathbf{C} & 0.33968 \\ \mathbf{C} & 0.74723 \\ \mathbf{H} & 8.2757 \\ \mathbf{C} & 4.26883 \\ \mathbf{S} & 5.11212 \\ \mathbf{C} & 4.9747 \\ \mathbf{C} & 4.5261 \\ \mathbf{C} & 0.3723 \\ \mathbf{H} & 4.02108 \\ \mathbf{C} & 0.0701 \\ \mathbf{B} & 8.2767 \\ \mathbf{C} & 3.3712 \\ \mathbf{H} & 4.0530 \\ \mathbf{C} & 0.0329 \\ \mathbf{H} & 5.4387 \\ \mathbf{C} & 0.3723 \\ \mathbf{H} & 4.0517 \\ \mathbf{H} & 4.0563 \\ \mathbf{C} & 0.35897 \\ \mathbf{H} & 4.10616 \\ \mathbf{C} & 2.13616 \\ \mathbf{H} & 4.0463 \\ \mathbf{A} & 3.3275 \\ \mathbf{H} & 4.02108 \\ \mathbf{H} & 4.0566 \\ \mathbf{A} & 3.35712 \\ \mathbf{H} & 4.0550 \\ \mathbf{A} & 3.53712 \\ \mathbf{H} & 4.0556 \\ \mathbf{A} & 3.35712 \\ \mathbf{H} & 4.0556 \\ \mathbf{A} & 3.3275 \\ \mathbf{H} & 0.05127 \\ \mathbf{A} & -3.54815 \\ \mathbf{A} & -3.7427 \\ \mathbf{A} & 0.0578 \\ \mathbf{H} & 7.0528 \\ \mathbf{A} & 3.38275 \\ \mathbf{A} & 0.0578 \\ \mathbf{H} & 7.0548 \\ \mathbf{A} & 0.05781 \\ \mathbf{A} & 3.05978 \\ \mathbf{H} & 1.00378 \\ \mathbf{A} & 3.05978 \\ \mathbf{H} & 1.00568 \\ \mathbf{A} & 3.3277 \\ \mathbf{A} & 3.38915 \\ $	C C	0.13803	2.10278	2.00110		0.10434	2.13879	2.09027	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-0.44464	-3.39932	3.02079		-0.30343	-3.40224	2.04142	
C         0.53254         -4.2334         0.97515         C         0.52354         -4.1311         0.63397           C         6.12231         -3.33982         -0.32864         C         6.24651         -3.23564         -0.33319           C         6.52054         -4.53898         -0.79910         C         6.63022         -4.4320         -0.92336           C         7.3494         -4.68898         -2.05396         C         7.41148         -4.44729         -2.08190           C         7.73710         -2.22264         -2.13098         C         7.44290         -2.02989         -2.06221           C         4.1432         3.7821         2.31130         C         4.45445         3.74588         2.61114           C         4.61221         4.02739         -0.04813         C         4.57747         4.13984         0.25427           C         4.2269         5.13690         2.47527         C         4.26683         5.11212         2.84747           C         4.5260         5.13980         F         4.10616         2.13616         1.44089           F         4.12031         -2.19086         1.43737         C         4.25686         3.55772	C	-0.26008	-4.44132	2.10/30	C	-0.29839	-4.40491	1.88968	
C         1.14456         -3.00038         0.7525         C         1.14267         -2.91130         0.05397           C         6.52464         -4.58564         -0.87930         C         6.63022         -4.43920         -0.92336           C         7.34954         -4.63898         -2.03596         C         7.4148         -4.4729         -2.08193           C         7.34954         -4.63898         -2.03596         C         7.4148         -4.4729         -2.03898         -2.06221           C         7.3700         -2.2244         -2.13098         C         4.67747         -1.13984         -2.6724           C         4.14322         3.78221         -2.31130         C         4.16455         3.74588         2.61114           C         4.61221         4.02739         -0.04813         C         4.57747         4.13984         0.23427           C         4.73252         5.44295         0.13713         C         4.26260         6.00701         1.80420           F         3.44944         -1.81305         -0.73616         F         3.49357         1.67824         -0.73723           F         4.1031         2.109086         1.43980         F         4.106	C	0.53254	-4.23354	0.97515	C	0.52354	-4.15111	0.78817	
C         6.22231         -3.33982         -0.32864         C         6.24651         -3.23564         -0.33319           C         6.59464         -4.58864         -0.87930         C         6.22051         -4.44729         -0.20336           C         7.34913         -4.618898         -2.05396         C         7.41148         -4.44729         -2.02889         -2.65041           C         7.37700         -2.22264         -2.13098         C         7.44290         -2.02889         -2.06211           C         4.14332         3.78221         -2.31100         C         4.14645         -3.74588         2.61114           C         4.61221         4.02739         -0.04813         C         4.5777         4.13984         0.23427           C         4.23269         5.13980         2.47572         C         4.2688         5.11212         2.84747           C         4.57891         -2.01080         0.60701         1.80420           F         3.44944         -1.81305         -0.737616         F         3.40397         1.67824         -0.73723           F         4.12031         -2.19086         1.43980         F         4.10616         -2.13616         1.44086	С	1.14456	-3.00058	0.75255	C	1.14267	-2.91130	0.63397	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	6.22231	-3.35982	-0.32864	C	6.24651	-3.23564	-0.33319	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	6.59464	-4.58564	-0.87930	C	6.63022	-4.43920	-0.92336	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	7.34954	-4.63898	-2.05396	C	7.41148	-4.44729	-2.08193	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	7.73913	-3.45113	-2.67921	C	7.81628	-3.23623	-2.65041	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	7.37700	-2.22264	-2.13098	C	7.44290	-2.02989	-2.06221	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	4.14332	3.78221	2.31130	C	4.14645	3.74588	2.61114	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	4.61221	4.02739	-0.04813	C	4.57747	4.13984	0.25427	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Ċ	4 73252	5 40295	0 12349	Ċ	4 67575	5 51738	0 49974	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Č	4 28269	5 1 5 9 8 0	2 47527	C C	4 26883	5 11212	2 84747	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C C	4.57181	5 99/50	1 38713		4.52620	6.00701	1 80420	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	E	4.57161	1 91205	0.72616		4.32020	1 67824	0.72722	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	г Б	5.44944	-1.81303	-0./3010		5.49557	-1.0/624	-0.73723	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	F	4.12031	-2.19086	1.43980	F H	4.10010	-2.13010	1.44080	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	H	8.24305	0.19803	-0./9/08	H	8.2/56/	0.33968	-0.62676	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	-0.17563	0.63929	2.17953	H	-0.20108	0.66919	2.19418	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	4.16286	5.59251	3.46503	Н	4.15897	5.49568	3.85772	
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Н	3.92799	3.15421	3.17082	H	3.95266	3.05897	3.42821	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	4.95303	6.02931	-0.73728	H	-0.05127	-1.39114	3.44220	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	0.01973	-1.36366	3.52318	H	-0.77488	-5.37427	2.00454	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-0.73129	-5.40550	2.27524	H	-1.13882	-3.58815	3.70418	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	-1.05506	-3.54942	3.90691	H	1.76527	-2.72471	-0.23020	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	1.74395	-2.84986	-0.13479	Н	0.68106	-4.92128	0.03798	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н	0.67227	-5.03469	0.25446	Н	5.65363	-3.24422	0.57099	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	5 64948	-3 33275	0 58790	Н	7 75062	-1 09348	-2 51711	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	7 67204	-1.30454	-2 62941	Н	8 41921	-3 22950	-3 55377	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	н	8 32121	-3 47997	-3 59568	н	7 70529	-5 38904	-2 53621	
H $7.03461$ $-2.47710$ H $0.2033$ $-5.37031$ $-0.47001$ H $6.29738$ $-5.50438$ $-0.38201$ N $8.80069$ $4.3032$ $0.31274$ N $8.79914$ $4.18737$ $-0.00568$ C $1.21490$ $3.09578$ $1.76810$ C $1.20997$ $3.04698$ $1.60936$ N $1.26160$ $4.06690$ $0.90114$ N $1.23977$ $3.98443$ $0.70548$ O $0.53694$ $3.42433$ $2.88884$ O $0.53666$ $3.41163$ $2.72212$ N $0.11925$ $4.75426$ $2.72902$ N $0.10118$ $4.72894$ $2.51354$ C $0.57710$ $5.08172$ $1.53695$ C $0.54625$ $5.01481$ $1.30603$ N $7.45490$ $3.28561$ $1.81999$ N $7.45720$ $3.23858$ $1.54965$ C $8.36492$ $4.28859$ $1.55678$ C $8.37127$ $4.22453$ $1.24065$ C $0.36899$ $6.40656$ $0.93491$ C $0.31643$ $6.31248$ $0.65513$ C $8.22296$ $5.24012$ $3.84633$ C $8.22834$ $5.28973$ $3.47939$ C $8.65500$ $6.13611$ $4.82463$ C $9.72489$ $7.08570$ $4.10682$ C $10.28345$ $7.03809$ $4.54532$ C $9.03631$ $7.01645$ $2.84994$ C $-0.42357$ $7.37133$ $1.57967$ C $-0.51529$ $7.27669$ $1.24953$ C $-0.61089$ $8.62280$ $0.99644$ </td <td>и П</td> <td>7 63481</td> <td>5 50773</td> <td>-5.55500</td> <td></td> <td>6 3 2 0 0 5</td> <td>5 37651</td> <td>0.47001</td> <td></td>	и П	7 63481	5 50773	-5.55500		6 3 2 0 0 5	5 37651	0.47001	
H         0.29733         -0.30236         -0.32211         N         8.80009         4.30382         0.31274           N         8.79914         4.18737         -0.00568         C         1.21490         3.09578         1.76810           N         1.23977         3.98443         0.70548         O         0.53694         3.42433         2.88884           O         0.53666         3.41163         2.72212         N         0.111925         4.75426         2.72902           N         0.10118         4.72894         2.51354         C         0.57710         5.08172         1.53695           C         0.54625         5.01481         1.30603         N         7.45490         3.28561         1.81999           N         7.45720         3.23858         1.54965         C         8.36492         4.28859         1.55678           C         0.31643         6.31248         0.65513         C         8.82215         5.24296         2.57726           C         8.84046         5.21682         2.21869         C         9.68550         7.03809         4.54532           C         9.72489         7.82670         4.10682         C         10.68357         7.37133		6 20728	-5.59775	-2.4//10	II N	0.32093	-3.37031	-0.47001	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	П N	0.29730	-3.30436	-0.36201		0.00009	4.30362	1 76910	
C       1.20997       3.04698       1.60936       N       1.26160       4.06690       0.90114         N       1.23977       3.98443       0.70548       O       N       0.11925       4.75426       2.72902         N       0.10118       4.72894       2.51354       C       0.57710       5.08172       1.53695         C       0.54625       5.01481       1.30603       N       7.45490       3.28561       1.81999         N       7.45720       3.23858       1.54965       C       8.36492       4.28859       1.55678         C       8.37127       4.22453       1.24065       C       0.36899       6.40656       0.93491         C       0.31643       6.31248       0.65513       C       8.2215       5.24296       2.57726         C       8.84046       5.21682       2.21869       C       8.65500       6.13611       4.82463         C       9.72489       7.08570       4.10682       C       10.28345       7.04472       3.28008         C       -0.51529       7.27669       1.24953       C       -0.61089       8.62280       0.99644         C       -0.72253       8.50193       0.61943 <td< td=""><td>N C</td><td>8./9914</td><td>4.18/3/</td><td>-0.00368</td><td></td><td>1.21490</td><td>3.09578</td><td>1./0810</td><td></td></td<>	N C	8./9914	4.18/3/	-0.00368		1.21490	3.09578	1./0810	
N         1.2397/7         3.98443         0.70548         O         0.36694         3.42433         2.88884           O         0.53666         3.41163         2.72212         N         0.11925         4.75426         2.72902           N         0.10118         4.72894         2.51354         C         0.57710         5.08172         1.53695           C         0.54625         5.01481         1.30603         N         7.45490         3.28561         1.81999           N         7.45720         3.23858         1.54965         C         8.36492         4.28859         1.55678           C         0.31643         6.31248         0.65513         C         8.2215         5.24296         2.57726           C         8.84046         5.21682         2.21869         C         8.65500         6.13611         4.82463           C         8.67072         6.22248         4.41776         C         9.68550         7.03809         4.54532           C         9.72489         7.08570         4.10682         C         10.28345         7.04472         3.28008           C         -0.0133         8.77615         -0.60588         C         0.77604         7.96563	C	1.20997	3.04698	1.60936	N	1.26160	4.06690	0.90114	
O         0.53666         3.41163         2.72212         N         0.11925         4.75426         2.72902           N         0.10118         4.72894         2.51354         C         0.57710         5.08172         1.53695           C         0.54625         5.01481         1.30603         N         7.45790         3.28561         1.81999           N         7.45720         3.23858         1.54965         C         8.36492         4.28859         1.55678           C         0.31643         6.31248         0.65513         C         8.82215         5.24296         2.57726           C         8.84046         5.21682         2.21869         C         8.65500         6.13611         4.82463           C         8.22834         5.28973         3.47939         C         8.65500         6.13611         4.82463           C         9.72489         7.08570         4.10682         C         10.28345         7.04472         3.28008           C         -0.51529         7.27669         1.24953         C         -0.61089         8.62280         0.99644           C         -0.72253         8.50193         0.61943         C         -0.01312         8.92294	N	1.23977	3.98443	0.70548	0	0.53694	3.42433	2.88884	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	0	0.53666	3.41163	2.72212	N	0.11925	4.75426	2.72902	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Ν	0.10118	4.72894	2.51354	C	0.57710	5.08172	1.53695	
N $7.45720$ $3.23858$ $1.54965$ C $8.36492$ $4.28859$ $1.55678$ C $8.37127$ $4.22453$ $1.24065$ C $0.36899$ $6.40656$ $0.93491$ C $0.31643$ $6.31248$ $0.65513$ C $8.82215$ $5.24296$ $2.57726$ C $8.84046$ $5.21682$ $2.21869$ C $8.22296$ $5.24012$ $3.84633$ C $8.22834$ $5.28973$ $3.47939$ C $8.65500$ $6.13611$ $4.82463$ C $8.67072$ $6.22248$ $4.41776$ C $9.68550$ $7.03809$ $4.54532$ C $9.72489$ $7.08570$ $4.10682$ C $10.28345$ $7.04472$ $3.28008$ C $10.33631$ $7.01645$ $2.84994$ C $-0.61089$ $8.62280$ $0.99644$ C $-0.72253$ $8.50193$ $0.61943$ C $-0.61089$ $8.62280$ $0.99644$ C $-0.72253$ $8.50193$ $0.61943$ C $-0.01312$ $8.92294$ $-0.23238$ C $0.72325$ $7.81948$ $-1.19889$ C $0.96923$ $6.71106$ $-0.29663$ C $0.93526$ $6.59068$ $-0.57309$ H $-1.22522$ $9.36434$ $1.49900$ H $-1.36778$ $9.24313$ $1.08233$ H $-0.88923$ $7.13645$ $2.53126$ H $1.02310$ $8.02856$ $-2.15033$ H $-0.16413$ $9.89834$ $-0.68612$ H $1.20310$ $8.02856$ $-2.15033$ H $-0.16413$	С	0.54625	5.01481	1.30603	N	7.45490	3.28561	1.81999	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ν	7.45720	3.23858	1.54965	C	8.36492	4.28859	1.55678	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	8.37127	4.22453	1.24065	C	0.36899	6.40656	0.93491	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	0.31643	6.31248	0.65513	C	8.82215	5.24296	2.57726	
C8.228345.289733.47939C8.655006.136114.82463C8.670726.222484.41776C9.685507.038094.54532C9.724897.085704.10682C10.283457.044723.28008C10.336317.016452.84994C-0.423577.371331.57967C-0.515297.276691.24953C-0.610898.622800.99644C-0.722538.501930.61943C-0.013128.92294-0.23238C-0.105338.77615-0.60588C0.776047.96563-0.87615C0.723257.81948-1.19889C0.969236.71106-0.29663C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C <td>С</td> <td>8.84046</td> <td>5.21682</td> <td>2.21869</td> <td>C</td> <td>8.22296</td> <td>5.24012</td> <td>3.84633</td> <td></td>	С	8.84046	5.21682	2.21869	C	8.22296	5.24012	3.84633	
C8.670726.222484.41776C9.685507.038094.54532C9.724897.085704.10682C10.283457.044723.28008C10.336317.016452.84994C-0.423577.371331.57967C-0.515297.276691.24953C-0.610898.622800.99644C-0.722538.501930.61943C-0.013128.92294-0.23238C-0.105338.77615-0.60588C0.776047.96563-0.87615C0.723257.81948-1.19889C0.969236.71106-0.29663C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051 <td>С</td> <td>8.22834</td> <td>5.28973</td> <td>3.47939</td> <td>C</td> <td>8.65500</td> <td>6.13611</td> <td>4.82463</td> <td></td>	С	8.22834	5.28973	3.47939	C	8.65500	6.13611	4.82463	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	8.67072	6.22248	4.41776	C	9.68550	7.03809	4.54532	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ċ	9.72489	7.08570	4.10682	Ċ	10.28345	7.04472	3.28008	
C10.10101.010101.010101.010101.010101.01010C-0.515297.276691.24953C-0.610898.622800.99644C-0.722538.501930.61943C-0.013128.92294-0.23238C-0.105338.77615-0.60588C0.776047.96563-0.87615C0.723257.81948-1.19889C0.969236.71106-0.29663C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Č	10 33631	7 01645	2 84994	C C	-0.42357	7 37133	1 57967	
C-0.313251.24933C-0.010338.022800.99044C-0.722538.501930.61943C-0.013128.92294-0.23238C-0.105338.77615-0.60588C0.776047.96563-0.87615C0.723257.81948-1.19889C0.969236.71106-0.29663C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	C C	-0.51529	7 27660	1 2/053		-0.61089	8 62280	0.00644	
C-0.722338.301930.01943C-0.013128.92294-0.23238C-0.105338.77615-0.60588C0.776047.96563-0.87615C0.723257.81948-1.19889C0.969236.71106-0.29663C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	C C	-0.31323	7.27009 8 50103	0.61042		-0.01089	8.02280	0.22228	
C-0.103338.7/813-0.60388C0.7/6047.96363-0.8/813C0.723257.81948-1.19889C0.969236.71106-0.29663C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H1.203108.02856-2.15033H-0.164139.89834-0.68612H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	C	-0.72233	0.30195	0.01945		-0.01312	0.92294	-0.23236	
C0.723257.81948-1.19889C0.969236.71106-0.29663C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H1.203108.02856-2.15033H-0.164139.89834-0.68612H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	C	-0.10555	8.//015	-0.00388		0.77604	/.90303	-0.8/615	
C0.935266.59068-0.57309H-1.225229.364341.49900H-1.367789.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H1.203108.02856-2.15033H-0.164139.89834-0.68612H8.192146.274505.39139H7.400504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	C	0.72325	/.81948	-1.19889		0.96923	6./1106	-0.29663	
H-1.367/89.243131.08233H-0.889237.136452.53126H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H1.203108.02856-2.15033H-0.164139.89834-0.68612H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	C	0.93526	6.59068	-0.5/309	H	-1.22522	9.36434	1.49900	
H-0.996357.061452.19813H1.584245.96477-0.78826H1.581195.84459-1.02347H1.238798.19397-1.83162H1.203108.02856-2.15033H-0.164139.89834-0.68612H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Н	-1.36778	9.24313	1.08233	H	-0.88923	7.13645	2.53126	
H1.581195.84459-1.02347H1.238798.19397-1.83162H1.203108.02856-2.15033H-0.164139.89834-0.68612H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Н	-0.99635	7.06145	2.19813	H	1.58424	5.96477	-0.78826	
H1.203108.02856-2.15033H-0.164139.89834-0.68612H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Н	1.58119	5.84459	-1.02347	Н	1.23879	8.19397	-1.83162	
H-0.271379.73135-1.09601H8.186996.129295.80476H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Н	1.20310	8.02856	-2.15033	H	-0.16413	9.89834	-0.68612	
H8.192146.274505.39139H7.420504.539794.05260H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Н	-0.27137	9.73135	-1.09601	H	8.18699	6.12929	5.80476	
H7.407344.619123.70988H10.023187.732105.30993H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Н	8.19214	6.27450	5.39139	H	7.42050	4.53979	4.05260	
H10.070587.808654.84049C9.856366.152812.29834C9.898826.087621.90785H11.086637.742403.06051	Н	7.40734	4.61912	3.70988	Н	10.02318	7.73210	5.30993	
С 9.89882 6.08762 1.90785 Н 11.08663 7.74240 3.06051	Н	10.07058	7.80865	4.84049	C	9.85636	6.15281	2.29834	
	С	9.89882	6.08762	1.90785	Н	11.08663	7.74240	3.06051	

Н	11.15849	7.68348	2.60673	Н	10.32394	6.15290	1.31884
Н	10.37757	6.02848	0.93551	0	8.12649	3.22938	-0.28599
0	8.11521	3.09325	-0.55644	Н	4.68201	3.78329	-0.76556
н	4.72835	3.59241	-1.03668	н	4.60395	7.06700	2.01564
C	4,70173	7.48873	1.55623	0	4.91031	6.29240	-0.59616
н	4.58809	7.78467	2.60240	C	5.01255	7.70552	-0.41574
Н	3.94040	8.01613	0.96954	Н	4.07890	8.12450	-0.02316
Н	5 67800	7 84322	1 20609	Н	5 20808	8 11928	-1 40568
	5.07000	7.01522	1.2000)	н	5 83919	7 96408	0 25644
		36			5.05717	3f	0.23011
C	1 70938	1 72615	1 67331	C	1 66142	1 66800	1.61106
	0.86462	0.65093	1.0755		0.81075	0.59572	1 83587
	1 54624	-0 53196	1 55089		1 48828	-0.58835	1 45997
	2 70201	0.10610	1.07/3		2 72724	0.25460	1.02757
	2.75201	1 18200	1.10745		2.75754	1 1 2 3 8 8	1.02757
	2.93331	1.18233	1.21975		2.90495	1.12366	1.14050
	5 3 1 8 0 6	1.79070	0.62750		5 20477	0.04330	0.66068
	5 17424	0.21205	0.02759		5 15750	0.94339	0.00008
	2 88077	-0.51295	0.23493		2 84210	-0.39/11	0.29974
B C	6 2 2 2 0 0	-1.13401	0.31099		6 2 2 8 6 7	-1.22400	0.49301
	0.33300	-0.73381	-0.32777		7 26457	-0.83111	-0.24338
	6 66622	0.52474	-0.29392		6 65120	1 22105	-0.20231
	0.00023	2.60466	0.33393		7 28745	1.52195	0.39179
	7.40625	2.00400	0.70977		7.30743	2.33792	0.71202
	0.01003	-2.03032	-0.92/81		0.02333	-2.13093	-0.82438
	0.90307	-1.0/0/5	1.07392		0.90094	-1.95209	1.30776
	4.5/405	2.12108	1.29971		4.32770	3.17123	1.30287
	0.15551	-2.12190	2.79032		0.03330	-2.1/339	2.03388
	-0.48308	-3.33817	2.90200		-0.36441	-3.41410	2.80900
	-0.29930	-4.3/31/	2.02003		-0.33939	-4.43133	1.0////
	0.51115	-4.13809	0.90592		0.48/83	-4.19/33	0./909/
	1.13903	-2.90007	0.75010		6 16020	-2.90229	0.03130
	0.20455	-3.27030	-0.5/541		0.10029	-5.5/011	-0.29005
	0.30204	-4.4/8/2	-0.96246		0.33174	-4.3/811	-0.88432
	7.35262	-4.48300	-2.1403/		7.30049	-4.39613	-2.00490
	7.73203	-3.2/300	-2.70351		7.03/40	-3.3943/	-2.33000
	/.40330	-2.00887	-2.09639		1.4/004	-2.165/9	-1.94975
	4.13/09	3.//33/	2.38397		4.28302	3.00128	2.03921
	4.73341	4.10691	0.20039		4.30330	4.14033	0.30424
	4.30007	5.00062	2.01/51		4.42490	5 20224	2.90300
	4.03937	1 69224	0.70297		4.01214	3.89234	1.93443
Г Б	5.45005 4.12420	-1.06234	-0.70265	Г Б	3.40110	-1.74900	-0.74332
	4.12450	-2.13439	1.430/4		4.02878	-2.22540	1.44000
	0.16220	0.20434	-0.02931		0.29/08	0.10402	-0.31023
	-0.10220	0.70310	2.24620		-0.21309	0.04913	2.10/01
	4.14838	3.34912	3.80809	П	4.38992	3.23/12	4.00362
	3.89900	5.11551	5.4004/		4.13023	2.80083	5.42245 2.20157
П	-0.00610	-1.34430	5.55540 2.15140		-0.13422	-1.39009	5.59157
П	-0./82/1	-5.55/01	2.15149		-0.84120	-3.39///	1.99034
	-1.10993	-3.52867	3.83544		-1.236/2	-3.58591	3.00109
	1./5162	-2./344/	-0.14424		1./5522	-2./901/	-0.22183
H	0.65270	-4.91846	0.16242	H	0.66000	-4.98007	0.05724
	5.62064	-3.28/05	0.53661		5.52/19	-3.3/32/	0.58057
	1.12214	-1.13183	-2.34409		/.83501	-1.25388	-2.3/930
	8.34668	-3.26502	-3.01413		8.48204	-3.39601	-5.41095
	/.6068/	-5.42566	-2.01/21		/.65019	-5.54336	-2.45840
	6.24216	-5.41648	-0.53786		0.17064	-5.50995	-0.45918
N a	8.91780	4.18/30	0.40340		8.94138	4.06410	0.34793
	1.26531	3.11271	1.76492		1.22568	3.05167	1.75808
N O	1.33297	4.06617	0.8/9/6		1.31906	4.05135	0.92834
	0.57491	3.46972	2.86926		0.50242	3.34966	2.85955
	0.16959	4.79948	2.6/636		0.09848	4.68596	2.72456
	0.64820	5.09930	1.48519		0.60996	5.04959	1.56519
L N	7.50909	3.19253	1.86830	N	7.44996	3.21663	1.82304

C	8 4 5 3 0 2	4 17133	1 63690	C	8 42712	4 15478	1 55824	
	0.46267	4.17133	0.05400		0.42/12	4.13478	0.00422	
C	0.46367	0.41440	0.83480	C	0.42692	0.39142	0.99422	
C	8.91250	5.10213	2.67801	C	8.86979	5.15141	2.54392	
C	8.27981	5.10736	3.93070	C	8.20951	5.24595	3.77869	
C	8.71358	5.98063	4.92850	C	8.62829	6.18181	4.72492	
C	9 77901	6 85182	4 68512	C	9 70628	7 02685	4 44742	
	10 41046	6 85055	2 42610		10 26601	6.02569	2 21657	
	10.41040	0.83033	5.45019		10.30001	0.95308	5.21057	
C	-0.30545	7.41007	1.48058	C	-0.36597	7.34840	1.65044	
C	-0.46880	8.65155	0.86949	C	-0.53347	8.61443	1.09358	
C	0.13012	8.91093	-0.36804	C	0.08396	8.93671	-0.12001	
C	0.89595	7.92272	-0.99292	C	0.87300	7.98715	-0.77482	
Ċ	1.06442	6 67779	-0.38577	C C	1 0/651	6 71825	-0.22165	
	1.00442	0.07777	1 25747		1.04051	0.71025	-0.22103	
П	-1.064/1	9.41/40	1.33/4/	П	-1.14//8	9.33014	1.00403	
H	-0.77108	7.20749	2.43959	H	-0.84646	7.09666	2.59030	
H	1.66009	5.90636	-0.86172	H	1.65893	5.97606	-0.72261	
Н	1.35950	8.11932	-1.95507	H	1.35226	8.23304	-1.71773	
Н	-0.00186	9.87896	-0.84321	Н	-0.05083	9,92405	-0.55257	
н	8 21948	5 98022	5 89579	н	8 11225	6 25059	5 67814	
11	7 45040	4 42122	4 10042		7 27127	4 59956	2.09226	
н	/.43049	4.43123	4.10942	н	/.3/12/	4.38830	5.98520	
Н	10.11/95	7.52790	5.46509	Н	10.03295	7.75262	5.18/01	
C	9.98185	5.98115	2.43513	C	9.95275	6.00341	2.26701	
Н	11.24096	7.52401	3.24473	H	11.20641	7.58857	2.99933	
н	10.47532	5.97465	1.46841	Н	10.46777	5.92847	1.31456	
0	8 22664	3 13863	-0.22256	0	8 25/170	2 08308	_0.22205	
	4 72254	7 21 402	-0.22250		4 ( 1955	5 40079	-0.222)3	
0	4./3234	7.31492	2.08033		4.04833	5.49078	0.01/92	
C	5.01905	8.25358	1.04675	Н	4.77700	6.22049	-0.1/36/	
Н	5.02949	9.23350	1.52484	H	4.72417	6.94468	2.19763	
Н	4.24455	8.23224	0.27110	Br	4.47714	3.65656	-1.55228	
Н	5.99714	8.05942	0.59215					
C	4 85586	5 48040	0.47780					
	5 11095	6 12701	0.77700					
п	5.11065	0.12/91	-0.55202					
11	4 00707	2 71725	0.740(1					
H	4.88707	3.71725	-0.74061					
H	4.88707	3.71725 <b>3</b> g	-0.74061			3h		
H C	4.88707	3.71725 3g 1.68634	-0.74061 1.68238	C	1.68293	<b>3h</b> 1.69153	1.68816	
H C C	4.88707 1.68041 0.83375	3.71725 3g 1.68634 0.61250	-0.74061 1.68238 1.91858	C C	1.68293 0.83710	<b>3h</b> 1.69153 0.61763	1.68816 1.92688	
H C C C	4.88707 1.68041 0.83375 1.51129	3.71725 3g 1.68634 0.61250 -0.57044	-0.74061 1.68238 1.91858 1.54068	C C C	1.68293 0.83710 1.51443	<b>3h</b> 1.69153 0.61763 -0.56538	1.68816 1.92688 1.54865	
H C C C N	4.88707 1.68041 0.83375 1.51129 2.75623	3.71725 3g 1.68634 0.61250 -0.57044 -0.23533	-0.74061 1.68238 1.91858 1.54068 1.09738	C C C N	1.68293 0.83710 1.51443 2.75858	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027	1.68816 1.92688 1.54865 1.10331	
H C C C N	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277	3.71725 3g 1.68634 0.61250 -0.57044 -0.23533 1.14214	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21801	C C C N	1.68293 0.83710 1.51443 2.75858 2.02465	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847	1.68816 1.92688 1.54865 1.10331 1.22338	
H C C C C N C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.19620	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74212	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05672	C C C N C	1.68293 0.83710 1.51443 2.75858 2.92465	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847	1.68816 1.92688 1.54865 1.10331 1.22338	
H C C C C N C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972	C C C N C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049	
H C C C C N C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835	C C C C N C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725	
H C C C C N C C C N	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633	C C C C N C C C N	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482	
H C C C C N C C C N B	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275	C C C C N C C C N B	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381	
H C C C C N C C C N B C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015	C C C C N C C C N B C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330	
H C C C C N C C C N B C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656	C C C C N C C C C N B C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991	
H C C C C N C C C N B C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.4540	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.25704	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.26282	C C C N C C C C N B C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64406	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.26288	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.26093	
H C C C C N C C C C N B C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.2463	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71410	C C C C N C C C C N B C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.5552	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71570	
H C C C C N C C C C N B C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418	C C C N C C C C N B C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418	C C C N C C C C N B C C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283	C C C C N C C C C C C C C C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093 0.92669	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826	C C C C N C C C C C C C C C C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093 0.92669 4.35230	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2 16308	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023	C C C C N C C C C C C C C C C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093 0.92669 4.35230 0.08958	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2 15790	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 0.53936	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 <b>3</b> 39832	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.01922	C C C C N C C C C C C C C C C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093 0.92669 4.35230 0.08958 0.53460	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 3.39312	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 2.5120	3.71725 <b>3g</b> 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 4.40(15)	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.0001	C C C C N C C C C C C C C C C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093 0.92669 4.35230 0.08958 -0.53460	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 4.40120	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98255	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.65120	C C C C N C C C C C C C C C C C C C C C	1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093 0.92669 4.35230 0.08958 -0.53460 -0.34737	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.86138	C C C C N C C C C C C C C C C C C C C C	$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ \end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.86138 0.69957	C C C C N C C C C C C C C C C C C C C C	$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.86138 0.69957 -0.29833	C C C C N C C C C C C C C C C C C C C C	$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ \end{array}$	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401	
H C C C C N C C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53968	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.86138 0.69957 -0.29833 -0.89047	C C C C N C C C C C C C C C C C C C C C	$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\end{array}$	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820	
H C C C C N C C C N B C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53968 -4.55849	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.86138 0.69957 -0.29833 -0.89047 -2.05080		1.68293 0.83710 1.51443 2.75858 2.92465 4.18792 5.29680 5.15463 3.85315 6.31344 7.24620 6.64496 7.38939 6.60093 0.92669 4.35230 0.08958 -0.53460 -0.34737 0.46940 1.10336 6.18660 6.54992 7.32639	3h 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988	
H C C C C N C C C N C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870 7.75110	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53968 -4.55849 3.25231	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.86138 0.69957 -0.29833 -0.89047 -2.05080 -2.61901		$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\\ 7.32639\\ 7.74725\end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976 3.24284	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988 2.62755	
H C C C C N C C C N C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870 7.75110 7.2575	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53968 -4.55849 -3.35331 2.14197	-0.74061 1.68238 1.91858 1.54068 1.09738 1.21891 1.05972 0.65835 0.29633 0.53275 -0.28015 -0.25656 0.36282 0.71418 -0.86418 1.65283 1.31826 2.76023 2.91922 1.96901 0.86138 0.69957 -0.29833 -0.29833 -0.89047 -2.05080 -2.61901 2.05070		$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\\ 7.32639\\ 7.74735\\ 7.20490\end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976 -3.34384 -3.34384	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988 -2.05988 -2.62755 2.92528	
H C C C C C N C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870 7.75110 7.39795	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53849 -3.35331 -2.14197	$\begin{array}{r} -0.74061 \\ \hline \\ 1.68238 \\ 1.91858 \\ 1.54068 \\ 1.09738 \\ 1.21891 \\ 1.05972 \\ 0.65835 \\ 0.29633 \\ 0.53275 \\ -0.28015 \\ -0.25656 \\ 0.36282 \\ 0.71418 \\ -0.86418 \\ 1.65283 \\ 1.31826 \\ 2.76023 \\ 2.91922 \\ 1.96901 \\ 0.86138 \\ 0.69957 \\ -0.29833 \\ -0.89047 \\ -2.05080 \\ -2.61901 \\ -2.02870 \\ -2.02870 \\ \hline \end{array}$		$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\\ 7.32639\\ 7.74735\\ 7.39480\\ 7.39480\\ \end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976 -3.34384 -2.13327	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988 -2.62755 -2.03528	
H C C C C C N C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870 7.75110 7.39795 4.19479	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53968 -4.55849 -3.35331 -2.14197 3.70649	$\begin{array}{r} -0.74061 \\ \hline \\ 1.68238 \\ 1.91858 \\ 1.54068 \\ 1.09738 \\ 1.21891 \\ 1.05972 \\ 0.65835 \\ 0.29633 \\ 0.53275 \\ -0.28015 \\ -0.25656 \\ 0.36282 \\ 0.71418 \\ -0.86418 \\ 1.65283 \\ 1.31826 \\ 2.76023 \\ 2.91922 \\ 1.96901 \\ 0.86138 \\ 0.69957 \\ -0.29833 \\ -0.89047 \\ -2.05080 \\ -2.61901 \\ -2.02870 \\ 2.61542 \end{array}$	C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\\ 7.32639\\ 7.74735\\ 7.39480\\ 4.19712\end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976 -3.34384 -2.13327 3.71856	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988 -2.62755 -2.03528 2.60956	
H C C C C C N C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870 7.75110 7.39795 4.19479 4.66056	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53968 -4.55849 -3.35331 -2.14197 3.70649 4.07195	$\begin{array}{c} -0.74061 \\ \hline \\ 1.68238 \\ 1.91858 \\ 1.54068 \\ 1.09738 \\ 1.21891 \\ 1.05972 \\ 0.65835 \\ 0.29633 \\ 0.53275 \\ -0.28015 \\ -0.25656 \\ 0.36282 \\ 0.71418 \\ -0.86418 \\ 1.65283 \\ 1.31826 \\ 2.76023 \\ 2.91922 \\ 1.96901 \\ 0.86138 \\ 0.69957 \\ -0.29833 \\ -0.89047 \\ -2.05080 \\ -2.61901 \\ -2.02870 \\ 2.61542 \\ 0.26715 \end{array}$	C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\\ 7.32639\\ 7.74735\\ 7.39480\\ 4.19712\\ 4.66394 \end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976 -3.34384 -2.13327 3.71856 4.07410	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988 -2.62755 -2.03528 2.60956 0.26017	
H C C C C C N C C C C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870 7.75110 7.39795 4.19479 4.66056 4.35118	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53968 -4.55849 -3.35331 -2.14197 3.70649 4.07195 5.06915	$\begin{array}{c} -0.74061 \\ \hline \\ 1.68238 \\ 1.91858 \\ 1.54068 \\ 1.09738 \\ 1.21891 \\ 1.05972 \\ 0.65835 \\ 0.29633 \\ 0.53275 \\ -0.28015 \\ -0.25656 \\ 0.36282 \\ 0.71418 \\ -0.86418 \\ 1.65283 \\ 1.31826 \\ 2.76023 \\ 2.91922 \\ 1.96901 \\ 0.86138 \\ 0.69957 \\ -0.29833 \\ -0.89047 \\ -2.05080 \\ -2.61901 \\ -2.02870 \\ 2.61542 \\ 0.26715 \\ 2.86562 \\ \end{array}$	C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\\ 7.32639\\ 7.74735\\ 7.39480\\ 4.19712\\ 4.66394\\ 4.35572\end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976 -3.34384 -2.13327 3.71856 4.07410 5.08150	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988 -2.62755 -2.03528 2.60956 0.26017 2.85417	
H C C C C N C C C N B C C C C C C C C C C	4.88707 1.68041 0.83375 1.51129 2.75623 2.92277 4.18689 5.29664 5.15467 3.85256 6.31390 7.24683 6.64549 7.39124 6.60203 0.92322 4.35047 0.08498 -0.53936 -0.35120 0.46667 1.10082 6.18630 6.55021 7.32870 7.75110 7.39795 4.19479 4.66056 4.35118 4.65463	3.71725 <b>3</b> g 1.68634 0.61250 -0.57044 -0.23533 1.14314 1.74213 0.97447 -0.36450 -1.20012 -0.79123 0.27116 1.35794 2.56012 -2.11123 -1.91497 3.19726 -2.16308 -3.39832 -4.40615 -4.16629 -2.93516 -3.33100 -4.53849 -3.35331 -2.14197 3.70649 4.07195 5.06915 5.91886	$\begin{array}{c} -0.74061 \\ \hline \\ 1.68238 \\ 1.91858 \\ 1.54068 \\ 1.09738 \\ 1.21891 \\ 1.05972 \\ 0.65835 \\ 0.29633 \\ 0.53275 \\ -0.28015 \\ -0.25656 \\ 0.36282 \\ 0.71418 \\ -0.86418 \\ 1.65283 \\ 1.31826 \\ 2.76023 \\ 2.91922 \\ 1.96901 \\ 0.86138 \\ 0.69957 \\ -0.29833 \\ -0.89047 \\ -2.05080 \\ -2.61901 \\ -2.02870 \\ 2.61542 \\ 0.26715 \\ 2.86562 \\ 1.80210 \end{array}$		$\begin{array}{c} 1.68293\\ 0.83710\\ 1.51443\\ 2.75858\\ 2.92465\\ 4.18792\\ 5.29680\\ 5.15463\\ 3.85315\\ 6.31344\\ 7.24620\\ 6.64496\\ 7.38939\\ 6.60093\\ 0.92669\\ 4.35230\\ 0.08958\\ -0.53460\\ -0.34737\\ 0.46940\\ 1.10336\\ 6.18660\\ 6.54992\\ 7.32639\\ 7.74735\\ 7.39480\\ 4.19712\\ 4.66394\\ 4.35572\\ 4.65989\end{array}$	<b>3h</b> 1.69153 0.61763 -0.56538 -0.23027 1.14847 1.74807 0.97993 -0.35885 -1.19449 -0.78476 0.27785 1.36388 2.56605 -2.10413 -1.90997 3.20364 -2.15790 -3.39312 -4.40130 -4.16164 -2.93048 -3.32461 -4.53252 -4.54976 -3.34384 -2.13327 3.71856 4.07410 5.08150 5.92780	1.68816 1.92688 1.54865 1.10331 1.22338 1.06049 0.65725 0.29482 0.53381 -0.28330 -0.25991 0.36093 0.71578 -0.86932 1.66211 1.31451 2.77036 2.93029 1.98025 0.87178 0.70906 -0.30401 -0.89820 -2.05988 -2.62755 -2.03528 2.60956 0.26017 2.85417 1.78781	

F	3 45563	-1 72986	-0 69390	F	3 4 5 1 9 6	-1 72218	-0 69249
F	4 07138	-2 19736	1 48154	F	4 07438	-2 19339	1 48026
л Ц	8 27280	0.20002	0 50700	и 1	9.07450 9.27101	0.21580	0.50240
	0.27209	0.20882	-0.38788		0.2/191	0.21369	-0.39240
H	-0.19221	0.66527	2.25152	H	-0.1883/	0.67045	2.20130
H	4.23929	5.45/48	3.8/158	H	4.24610	5.4//22	3.85/83
H	3.96990	3.03647	3.43921	Н	3.97162	3.05182	3.43575
Н	-0.05645	-1.39111	3.51062	H	-0.05155	-1.38578	3.52065
Н	-0.83942	-5.36895	2.08977	H	-0.83542	-5.36409	2.10176
Н	-1.16931	-3.57377	3.78665	Н	-1.16390	-3.56815	3.79826
Н	1.71997	-2.75887	-0.16925	Н	1.72131	-2.75473	-0.16073
Н	0.60891	-4.94053	0.11233	Н	0.61114	-4.93587	0.12261
н	5 59593	-3 33143	0 60746	н	5 59759	-3 32612	0.60266
н	7 71934	-1 20995	-2 48314	н	7 71499	-1 20050	-2 48903
н	8 35222	-3 35517	-3 52357	н	8 34684	-3 34446	-3 53319
и П	7 60707	5 50/18	2 50660	и П	7 60430	5 40487	2 51716
	( 22775	-5.50418	-2.30000		( 22957	-3.49407	-2.31/10
	0.22773	-3.4/201	-0.43/30		0.22837	-3.40003	-0.44352
N	8.93053	4.10859	0.3860/	N	8.91909	4.12433	0.39001
C	1.23587	3.07069	1.79666	C	1.23826	3.07615	1.79996
N	1.31218	4.04333	0.93344	N	1.30682	4.04391	0.93066
0	0.52581	3.39955	2.89708	0	0.53687	3.41063	2.90420
N	0.11085	4.72853	2.72406	N	0.11942	4.73835	2.72696
C	0.60470	5.05738	1.54670	C	0.60356	5.06087	1.54385
N	7.47754	3.18529	1.85420	N	7.48219	3.18055	1.86100
C	8.44261	4.14105	1.61038	C	8.44102	4.14289	1.61847
C	0.40649	6.37882	0.93490	C	0.39918	6.37848	0.92580
C	8.90010	5.09565	2.63021	C	8.90321	5.08896	2.64412
C	8.26755	5.12808	3.88248	C	8.28609	5.10042	3.90439
C	8.70065	6.02347	4.86071	C	8.72426	5.98661	4.88865
C	9.76587	6.88916	4.59819	C	9.77903	6.86438	4.62404
C	10.39783	6.86013	3.34988	C	10.39532	6.85663	3.36759
C	-0.37385	7.35654	1.57531	С	-0.36889	7.36278	1.57090
Ċ	-0.55761	8.60181	0.97850	Ċ	-0.55849	8.60424	0.96798
Ċ	0.03171	8 88270	-0.25907	Ċ	0.01269	8 87470	-0.28039
Ċ	0.80898	7 91274	-0.89768	C C	0 77762	7 89810	-0.92376
	0.000000	6 66428	-0.30/01		0.97273	6 65350	-0.32484
Ц	-1.16206	0.35303	1 47731	н Н	-1.15311	0.05550	1 47057
	-1.10200	7 12666	2 52280		-1.15511	7 15107	2 52708
	-0.83244	5.00677	2.33369		-0.81321	7.13107 5.80101	2.33798
	1.00211	3.900//	-0./9291		1.30///	5.89101 9.10451	-0.81002
п	1.20084	8.12/11	-1.858/0	П	1.22108	8.10451	-1.89290
H	-0.11622	9.85379	-0./2308	Н	-0.1396/	9.84292	-0./489/
H	8.206/5	6.04390	5.82785	H	8.24230	5.99081	5.86201
Н	7.44047	4.45358	4.07730	Н	7.46655	4.41/07	4.10023
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C	9.96957	5.96904	2.36811	C	9.96210	5.97452	2.37990
Н	11.22814	7.52949	3.14381	Н	11.21729	7.53567	3.15964
Н	10.46289	5.94212	1.40169	H	10.44331	5.96405	1.40708
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C	4.80885	5.43833	0.50205	C	4.81320	5.44070	0.48984
Н	5.03819	6.11271	-0.31509	Н	5.04297	6.11462	-0.32801
Н	4.76702	3.69125	-0.74398	Н	4.77005	3.68908	-0.74929
Br	4.86509	7.79337	2.13643	Cl	4.85540	7.65184	2.08719
		3i				3ј	
С	1.72598	1.68891	1.70110	С	1.68177	1.69052	1.68535
C	0.87421	0.61975	1.93915	C	0.83530	0.61674	1.92370
C	1.53988	-0.56575	1.54795	C	1.51333	-0.56651	1.54818
N	2.78351	-0.23725	1.09682	Ň	2.75840	-0.23166	1.10458
C	2.95938	1.14000	1.22134	C	2,92406	1.14705	1.22347
C C	4,22502	1.73066	1.05222	Č Č	4.18698	1.74837	1.06010
C C	5.33131	0.95524	0.65832	Č	5.29548	0.97988	0.65499
N N	5 18510	-0 38585	0 30589	Ň	5 1 5 3 3 5	-0 35856	0 29164
R	3 87348	-1 20977	0.53196	R	3 85273	-1 19488	0 53317
	6 34535	-0.82141	-0 26178		6 31317	-0 78486	-0 28462
	7 78222	0 23674	-0 23994		7 24600	0 27717	-0.25905
	1.20000	0.20074	0.43777		7.27007	0.2//1/	0.20700

С	6 68333	1 33138	0 36682	C	6 64412	1 36336	0 36147
C C	7 42001	2 52564	0.30062		7 20762	2 56644	0.71520
C	7.43001	2.55504	0.70937	C a	1.38/02	2.30044	0./1559
С	6.62970	-2.14565	-0.83825	C	6.60093	-2.10400	-0.8/160
С	0.94217	-1.90645	1.65297	C	0.92611	-1.91142	1.66342
С	4.40324	3.18940	1.28730	C	4.35019	3.20232	1.31631
С	0 10820	-2 15826	2 76261	C	0.08860	-2 15790	2 77168
C C	0.52502	2.15020	2.70201		0.52467	2.15790	2.77100
C	-0.32303	-3.39003	2.91343		-0.33407	-3.39333	2.95562
C	-0.35026	-4.39030	1.95273	C	-0.34583	-4.40343	1.98619
С	0.46342	-4.14649	0.84284	C	0.47148	-4.16534	0.87779
С	1.10649	-2.91895	0.68921	C	1.10424	-2.93384	0.71272
С	6 20663	-3 36071	-0 26782	C	6 18601	-3 32508	-0.30813
Ċ	6 56761	-1 57397	-0.85252	Ċ	6 5/1027	-1 53244	-0.90356
C	7.25024	4 (0102	-0.03232		7 22(52	4 5 4 9 6 6	-0.90330
C	7.35034	-4.60192	-2.009/6	C	7.32653	-4.54866	-2.06470
С	7.77985	-3.40145	-2.58256	C	7.74820	-3.34214	-2.63056
С	7.42967	-2.18562	-1.99974	C	7.39544	-2.13216	-2.03713
С	4.31812	3.70017	2.58874	C	4.17892	3.71600	2.61131
Ċ	4 67389	4 04745	0 21131	Ċ	4 67523	4 07329	0 26464
C C	4 52275	5.05061	2 77805		1 22 4 92	5.07921	2 25250
C	4.32373	5.05901	2.77893		4.55465	5.07821	2.83839
С	4.78514	5.93412	1./3024	C	4.65099	5.91447	1.79281
F	3.47730	-1.73104	-0.69858	F	3.44950	-1.72308	-0.69241
F	4.07795	-2.21256	1.47811	F	4.07648	-2.19381	1.47914
Н	8.31085	0.16687	-0.56523	н	8.27226	0.21514	-0.59016
н	-0 14749	0.67762	2 28/16	н	-0.19059	0.66080	2 25690
11	-0.14/49	2.05(0)	2.20410		-0.19039	5 40112	2.25090
Н	4.13268	3.05696	3.44207	Н	4.21/31	5.49113	3.85467
Н	-0.02310	-1.39236	3.52104	Н	3.94353	3.04675	3.43264
Н	-0.84545	-5.35031	2.06711	H	-0.05356	-1.38433	3.52027
Н	-1.15162	-3.56861	3.78266	Н	-0.83295	-5.36646	2.10951
н	1 72264	-2 73962	-0 18120	н	-1 16433	-3 56706	3 80181
и Ц	0.50544	4 01/66	0.08560	11 11	1 72270	2 75034	0.15605
11	0.39344	-4.91400	0.08509		1.72270	-2.73934	-0.13095
Н	5.61232	-3.35383	0.63531	Н	0.61464	-4.94116	0.13054
Н	7.75647	-1.25719	-2.45766	Н	5.59652	-3.32758	0.59821
Н	8.38415	-3.41043	-3.48496	H	7.71607	-1.19899	-2.48975
Н	7.62644	-5.55109	-2.45970	Н	8.34831	-3.34179	-3.53580
н	6 23947	-5 50318	-0 39587	н	7 60444	-5 49331	-2 52294
N	0.23747	4 07052	0.37507	11	6 22722	5 16620	0.45221
IN C	0.90234	4.07033	0.5/09/		0.22/22	-3.40038	-0.43221
С	1.29832	3.07612	1.84327	N	8.91442	4.12/21	0.38594
Ν	1.36146	4.05883	0.99074	C	1.23961	3.07602	1.79811
Ο	0.62372	3.39915	2.96787	N	1.30739	4.04427	0.92930
Ν	0.22089	4.73491	2.82392	0	0.54602	3.41290	2.90673
C	0.68512	5 07322	1 63726	N	0 13538	4 74330	2 73392
	7.50011	2 1 9 2 7 9	1.03720		0.13330	5.06456	1 5 4 9 6 1
IN C	7.30011	5.16576	1.03013		0.01464	3.00430	1.34801
С	8.47245	4.13059	1.59126	N	7.47853	3.18483	1.858/5
С	0.48835	6.40580	1.04933	C	8.43436	4.14913	1.61351
С	8.91160	5.11008	2.59606	C	0.41867	6.38598	0.93575
С	8.20947	5.22820	3.80582	C	8.88978	5,10309	2.63505
Ċ	8 62169	6 15360	4 76516	Ċ	8 26816	5 12011	3 80310
C C	0.72422	6 06 49 4	4.70510		0.20010 9.60940	6 01550	1 07200
C	9.73433	0.90484	4.32034		8.09840	0.01550	4.07200
C	10.43546	6.850/4	3.32060	C	9./4948	6.89/02	4.60564
С	-0.24948	7.38925	1.73009	C	10.37016	6.88365	3.35138
С	-0.43024	8.64593	1.15644	C	-0.33625	7.37538	1.58864
С	0.11956	8.93253	-0.09795	C	-0.51598	8.62136	0.99191
Ċ	0.85426	7 95668	0.77608	Ċ	0.05107	8 80138	-0.25806
C	1.04074	(	-0.77098		0.00177	7.000(9	-0.23800
C	1.04074	6.69690	-0.20/39		0.803/1	/.90968	-0.90930
Н	-1.00116	9.40263	1.686/3		0.98915	6.66055	-0.31651
Н	-0.67692	7.16513	2.70194	H	-1.10020	9.38269	1.50069
Н	1.61323	5.93508	-0.72561	Н	-0.77779	7.16419	2.55709
Н	1.28159	8,17563	-1.75093	н	1.57435	5.89438	-0.81373
и П	_0.02509	9 01 259	-0 54348	U 11	1 2/521	8 11569	_1 87075
11	-0.02370	2.91230 6 0406E	5 600/1		0.00250	0.11300	0.70170
H	8.0/299	0.24005	3.09841		-0.09239	9.80313	-0./21/2
Н	7.34369	4.59975	3.98348	H	8.21302	6.02400	5.84441
Н	10.05527	7.68237	5.27639	H	7.45110	4.43433	4.09098
С	10.02876	5.92899	2.35791	H	10.08542	7.59089	5.37114
Н	11.30290	7.47703	3.13354	C	9.94496	5.99238	2.36838

Н	10.57593	5.83546	1.42521	Н	11.18904	7.56576	3.14136	
0	8.29406	3.00318	-0.21757	Н	10.42924	5.97798	1.39715	
C	4.85337	5.41294	0.43649	0	8.22189	3.06897	-0.22038	
Н	5.05281	6.07640	-0.39924	C	4.82165	5,43933	0.49657	
н	4.72592	3.64971	-0.79711	Н	5.05959	6.12873	-0.30623	
F	4.48264	5.54616	4.04136	Н	4.79237	3.68633	-0.74280	
Н	4 93534	6 98958	1 93180	F	4 79754	7 23691	2 02551	
		0.00000	100100	4		,	2102001	
		С	1 69346	2.61036	0 77729			
		C	0 79981	1 55218	0.90447			
		C	1 50734	0.33818	0.78225			
		N	2 82646	0.62149	0.59134			
		C	2.02040	2 01284	0.63836			
		C	4 28994	2.57278	0.71081			
		C	5 44098	1 76056	0.61964			
		N N	5 32203	0 39059	0.34559			
		R	3 98143	-0.39672	0.37011			
		D C	6 55905	-0.10515	0.06211			
		C	7 50213	0.03480	0.19697			
		C C	6 8/100	2 00577	0.19097			
		C C	6 01080	-1 47846	-0 3/231			
		C C	0.91089	-0.08881	0.88142			
		C C	0.87270	4 04554	0.80142			
		C C	0.18474	1 1 2 2 5 2	1 80/27			
		C C	-0.184/4	-1.13233	1.00437			
		C C	0.51014	2.34231	1.93219			
		C C	0.52826	2 20002	0.20707			
		C C	1 21541	-3.29992	0.20797			
		C C	6 3/32/	-2.09297	0.07807			
		C C	6 77576	-3.90066	-0.18563			
		C C	7 77665	-4.03633	-0.18505			
		C C	8 35108	-7 89268	-1.71267			
		C C	7 92743	-1.62804	-1.30898			
		C C	4 04522	4 65510	2 08984			
		C	4 98662	4 83328	-0 13329			
		C C	5 12456	6 21049	0.03684			
		C	4 19819	6 03034	2 26306			
		C	4 73503	6 81136	1 23659			
		F	3 84256	-1.05134	-0.86025			
		F	3 95815	-1 31221	1 43026			
		Н	-0 27399	1.63743	0.99561			
		Н	3 89531	6 49152	3 19904			
		Н	3 62570	4 04892	2 88718			
		Н	5 53893	6 81297	-0 76669			
		Н	5.29187	4.36624	-1.06479			
		Н	-0.45732	-0.29509	2.43914			
		Н	-1.03845	-4.37787	1.23124			
		Н	-1.66785	-2.43340	2.65806			
		Н	2.01161	-2.00121	-0.64732			
		Н	0.80478	-4.14001	-0.42333			
		Н	5.57355	-2.54685	0.97253			
		Н	8.36985	-0.74523	-1.75990			
		Н	9.12712	-2.98428	-2.46767			
		Н	8.10712	-5.02319	-1.46244			
		Н	6.33023	-4.78414	0.26270			
		Н	4.84983	7.88361	1.37132			
		С	1.23801	4.01631	0.72269			
		С	7.57179	3.33133	0.93976			
		С	7.40370	3.95372	2.18833			
		С	8.17728	5.05918	2.53969			
		С	9.13663	5.55940	1.65424			
		С	9.32197	4.94075	0.41527			
		C	0.34643	4.49292	1.70022			

С	-0.18063	5.78233	1.61711	
С	0.16550	6.61417	0.54897	
С	1.04064	6.14557	-0.43573	
С	1.56981	4.85817	-0.35258	
Η	-0.86234	6.13544	2.38655	
Н	0.07771	3.84988	2.53388	
Н	-0.24611	7.61728	0.48182	
Н	8.03513	5.52735	3.50978	
Н	6.67060	3.56273	2.88609	
Н	9.73654	6.42272	1.92916	
С	8.55074	3.83236	0.06364	
Н	10.06720	5.31999	-0.27902	
Н	8.69416	3.35570	-0.90207	
Н	8.57230	0.81785	0.09898	
Н	1.30570	6.78173	-1.27603	
Н	2.23500	4.49607	-1.12960	

Table S7.Total energies for the optimized compounds 3, calculated at B3LYP/31G(d,p)/CPCM(CCl<sub>2</sub>H<sub>2</sub>).

Compound	Total energy /				
	Hatree				
3a	-2357.12876368				
3b	-2416.65709432				
3c	-2471.59658013				
3d	-2396.42014345				
3e	-2440.35730430				
3f	-2456.32922605				
3g	-2440.25152207				
3h	-2471.59519117				
3i	-2456.32849846				
3j	-2396.41715296				
4	-1835.57217178				

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# 8. NMR spectra for products

<sup>1</sup>H NMR spectrum for **3a** -7.31 -7.26 Chloroform-d -6.99 -6.99 -6.95 -6.83 -6.83 -6.83 -6.83 -6.83 -6.81 -6.82 -6.5 -6.0 5 88 -5 -5.5 7.90 -3 -5.0 -2 -1 -4.5 -0 7 52 11 12 23 28 24 F -1 -4.0 8.5 7.5 f1 (мд) 7.0 6.5 8.0 -3.5 -3.0 -2.5 -2.0 -1.5 -1.0 -0.5 -0.0 80 80 212 212 111 --0.5 15 14 13 12 11 10 7 f1 (мд) 9 8 5 3 2 0 6 4 1

 $^{13}$ C NMR spectrum for **3a** 









<sup>13</sup>C NMR spectrum for **3b** 



<sup>19</sup>F NMR spectrum for **3b** 





<sup>1</sup>H NMR spectrum for **3c** 

<sup>13</sup>C NMR spectrum for **3c** 



<sup>19</sup>F NMR spectrum for **3c** 



<sup>1</sup>H NMR spectrum for 3d



<sup>13</sup>C NMR spectrum for **3d** 



<sup>19</sup>F NMR spectrum for **3d** 



<sup>1</sup>H NMR spectrum for 3eoroform-d -5.0 5 -3.05 \$ \$ 888666668 28 68 68 8 2 LUNDER LUN -4.5 Chloroform-d -2 5 -4.0 6.40 6.40 7.89 -1 -3.5 -0 4.10.4 T- 56'T -3.0 8.0 7.5 7.0 f1 (мд) 6.5 -2.5 -2.0 -1.5 -1.0 -0.5 -0.0 4.10 5.86 1.75 1.93 1.89 1.89 1.95-1 3.00-1 -0.5 15 7 f1 (мд) o 14 13 12 11 10 9 8 4 3 2 6 5 1

<sup>13</sup>C NMR spectrum for **3e** 



<sup>19</sup>F NMR spectrum for **3e** 







 $^{13}\mathrm{C}$  NMR spectrum for **3f** 



<sup>19</sup>F NMR spectrum for **3f** 



<sup>1</sup>H NMR spectrum for 3g



 $^{13}$ C NMR spectrum for **3g** 



<sup>19</sup>F NMR spectrum for **3g** 



<sup>1</sup>H NMR spectrum for **3h** 



<sup>13</sup>C NMR spectrum for **3h** 







<sup>1</sup>H NMR spectrum for **3i** 



<sup>13</sup>C NMR spectrum for **3i** 



<sup>19</sup>F NMR spectrum for **3i** 







<sup>13</sup>C NMR spectrum for 3j



<sup>19</sup>F NMR spectrum for **3**j

