Avenue to Phosphaalkenes from Ph$_3$GePCO

Kevin M. Szkop, Andrew R. Jupp, Hlib Razumkov, Douglas W. Stephan*

Supplemental Information
Table of Contents

Spectra of (Z)-2 ........................................................................................................................................ 3
Spectra of (E)-2 ........................................................................................................................................ 5
Thermal isomerization of (Z)-2 and (E)-2 .................................................................................................. 8
Photolysis of (Z)-2 .................................................................................................................................... 9
Photolysis of (E)-2 .................................................................................................................................... 10
Reaction of (E)-2 with t-Bu$_3$P-SiMe$_3$ .................................................................................................. 11
Independent in-situ syntheses and characterization of (E)-3/(Z)-3 .............................................................. 12
Reaction of (E)-2 with Ph$_2$P-SiPh$_3$ ...................................................................................................... 13
Independent in-situ syntheses and characterization of (E)-4/(Z)-4 .............................................................. 14
Reaction of (E)-2 with Ph$_2$P-SiMe$_3$ ...................................................................................................... 15
Independent in-situ syntheses and characterization of (E)-5/(Z)-5 .............................................................. 16
Computational details ................................................................................................................................ 17
REFERENCES ............................................................................................................................................. 31

List of Figures

Figure 1. $^1$H NMR spectrum of (Z)-2 (C$_6$D$_6$) .................................................................................... 3
Figure 2. $^{13}$C($^1$H) NMR spectrum of (Z)-2 (C$_6$D$_6$) ........................................................................... 3
Figure 3. $^{31}$P($^1$H) NMR spectrum of (Z)-2 (C$_6$D$_6$) ........................................................................... 4
Figure 4. $^{29}$Si-$^1$H HMBC NMR spectrum of (Z)-2 (C$_6$D$_6$) ............................................................... 4
Figure 5. ATR IR spectrum of (Z)-2 ........................................................................................................... 5
Figure 6. $^1$H NMR spectrum of (E)-2 (C$_6$D$_6$) .................................................................................... 5
Figure 7. $^{13}$C($^1$H) NMR spectrum of (E)-2 (C$_6$D$_6$) ........................................................................... 6
Figure 8. $^{31}$P($^1$H) NMR spectrum of (E)-2 (C$_6$D$_6$) ........................................................................... 6
Figure 9. $^{29}$Si-$^1$H HMBC NMR spectrum of (E)-2 (C$_6$D$_6$) ............................................................... 7
Figure 10. ATR IR spectrum of (E)-2 ........................................................................................................ 7
Figure 11. $^{31}$P($^1$H) NMR spectra of heated solutions of (Z)-2 (THF) ...................................................... 8
Figure 12. $^{31}$P($^1$H) NMR spectra of heated solutions of (E)-2 (THF) ...................................................... 8
Figure 13. Stacked $^{31}$P($^1$H) NMR spectra of photolysis of (Z)-2 (C$_6$D$_6$) ............................................ 9
Figure 14. Stacked $^{31}$P($^1$H) NMR spectra of photolysis of (E)-2 (C$_6$D$_6$) ............................................ 10
Figure 15. Stacked $^{31}$P($^1$H) NMR spectra of displaying silane exchange (THF) ...................................... 11
Figure 16. Stacked $^{31}$P($^1$H) NMR spectra of in-situ formation of (E)-3/(Z)-3 (THF) ............................ 12
Figure 17. Stacked $^{31}$P($^1$H) NMR spectra of displaying phosphine exchange (THF) ............................ 13
Figure 18. Stacked $^{31}$P($^1$H) NMR spectra of in-situ formation of (E)-4/(Z)-4 (THF) ............................ 14
Figure 19. Stacked $^{31}$P($^1$H) NMR spectra of displaying silylphosphine exchange (THF) ..................... 15
Figure 20. $^{31}$P($^1$H) NMR spectrum of in-situ formation of (E)-5/(Z)-5 (THF) ......................................... 16
Figure 21. Optimised structures of (E)-2 (left) and (Z)-2 (right) (ωB97X-D/6-31G*). .............................. 17
Spectra of (Z)-2

\[
\begin{align*}
&\text{[K]} \\
&\text{[K] (t-Bu)}_2\text{PGePh}_3 + \text{Ph}_3\text{SiCl} \\
&\text{THF 23 }^\circ\text{C, 5 min} \\
&\Rightarrow \text{(t-Bu)}_2\text{P} = \text{SiPh}_3
\end{align*}
\]

\[\text{f1 (ppm)} \]

\[\begin{align*}
8.04 & \quad 7.82 & \quad 7.24 & \quad 7.16 \\
6.47 & \quad 6.54 & \quad 9.75 & \quad 9.20 \\
18.00 & \quad 9.20 & \quad 9.75 & \quad 6.54 \\
6.47 & \quad 6.54 & \quad 9.75 & \quad 9.20 \\
18.00 & \quad 9.20 & \quad 9.75 & \quad 6.54 \\
\end{align*}\]

Figure 1. \(^1\text{H}\) NMR spectrum of (Z)-2 (C\(_6\)D\(_6\))

\[\text{f1 (ppm)} \]

\[\begin{align*}
228.78 & \quad 229.37 & \quad 229.6 \quad 229.37 \\
130.23 & \quad 136.20 & \quad 136.18 & \quad 136.31 \\
136.20 & \quad 136.31 & \quad 136.31 & \quad 136.20 \\
130.23 & \quad 136.31 & \quad 136.31 & \quad 136.20 \\
30.27 & \quad 30.38 & \quad 30.38 & \quad 30.27 \\
\end{align*}\]

Figure 2. \(^{13}\text{C}(\text{H})\) NMR spectrum of (Z)-2 (C\(_6\)D\(_6\))
Figure 3. $^{31}\text{P}^1\text{H}$ NMR spectrum of (Z)-2 (C$_6$D$_6$)

Figure 4. $^{29}\text{Si}^1\text{H}$ HMBC NMR spectrum of (Z)-2 (C$_6$D$_6$)
Figure 5. ATR IR spectrum of (Z)-2

Spectra of (E)-2

\[
\text{Ph}_3\text{GePO} \xrightarrow{\text{Ph}_3\text{Si-P(t-Bu)_2}} \text{Ph}_3\text{Si-P(t-Bu)_2}\text{GePh}_3
\]

THF
23 °C, 5 min

Figure 6. \textsuperscript{1}H NMR spectrum of (E)-2 (C\textsubscript{6}D\textsubscript{6})
Figure 7. $^{13}$C($^1$H) NMR spectrum of (E)-2 (C$_6$D$_6$)

Figure 8. $^{31}$P($^1$H) NMR spectrum of (E)-2 (C$_6$D$_6$)
Figure 9. $^{29}$Si-$^1$H HMBC NMR spectrum of (E)-2 (C$_6$D$_6$)

Figure 10. ATR IR spectrum of (E)-2
Thermal isomerization of (Z)-2 and (E)-2

In the glovebox, solutions of (Z)-2 and (E)-2 (ca. 0.10 M) in tetrahydrofuran were charged into separate NMR tubes. Both solutions were maintained at ambient temperature for 24 hours, then heated in the same oil bath set to 55 °C for a total of 78 hours. The solutions were periodically removed from the oil bath and analyzed by $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy.

Figure 11. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of heated solutions of (Z)-2 (THF)

Figure 12. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of heated solutions of (E)-2 (THF)

Time points (bottom to top): 1 h (23 °C), 24 h (23 °C), 1 h (55 °C), 4.5 h (55 °C), 30 h (55 °C), 55 h (55 °C), 78 h (55 °C)
Photolysis of (Z)-2

A solution of (Z)-2 (13.8 mg, 0.018 mmol) in C₆D₆ was transferred to a J-Young NMR tube and irradiated for 1 hour. Analysis by ³¹P{¹H} NMR spectroscopy revealed isomerization to (E)-2.

![NMR spectra](image)

Figure 13. Stacked ³¹P{¹H} NMR spectra of photolysis of (Z)-2 (C₆D₆)

Reaction mixture before photolysis (bottom) and after 1 hour of irradiation (top)
**Photolysis of (E)-2**

A solution of (E)-2 (18.6 mg, 0.024 mmol) in C₆D₆ was transferred to a J-Young NMR tube and irradiated for 1 hour. Analysis by ³¹P{¹H} NMR spectroscopy revealed isomerization to (Z)-2.

![Diagram of (E)-2 and (Z)-2](attachment:image.png)

**Figure 14. Stacked ³¹P{¹H} NMR spectra of photolysis of (E)-2 (C₆D₆)**

Reaction mixture before photolysis (bottom) and after 1 hour of irradiation (top)
Reaction of \((E)-2\) with \(t\text{-}Bu_2P\text{-SiMe}_3\)

\[
\text{Ph}_3\text{Si}O\]
\[
(t\text{-}Bu)_2\text{P}O\text{GePh}_3
\]
\[
\xrightarrow{\text{Me}_3\text{Si-P}(t\text{-}Bu)_2}
\]
\[
\text{Ph}_3\text{Si-P}(t\text{-}Bu)_2
\]
\[
\text{Me}_3\text{Si}O\]
\[
(t\text{-}Bu)_2\text{P}O\text{GePh}_3
\]

A solution of \((E)-2\) (18.3 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL) was combined with a solution of \(t\text{-}Bu_2P\text{-SiMe}_3\) (5.2 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL). The homogenous yellow solution was transferred to an NMR tube and analyzed by \(^{31}\text{P}\{^1\text{H}\}\) NMR spectroscopy. Analysis after 30 minutes at ambient temperature shows a small amount of silane exchange as evidenced by the formation of \((E)-3\). The lack of signal attributed \((Z)-2\) or \((Z)-3\) implied that silane exchange occurred without thermal isomerization. Heating the reaction mixture to 85 °C for 1.5 h showed increased silane exchange and the formation of \((Z)-2\) or \((Z)-3\).

---

Figure 15. Stacked \(^{31}\text{P}\{^1\text{H}\}\) NMR spectra of displaying silane exchange (THF)

Bottom: 23 °C, 30 min. Middle: 85 °C, 1 h. Top: 85 °C, 2 h.

\(\text{Ph}_3\text{Si-P}(t\text{-}Bu)_2\) \(\text{Me}_3\text{Si-P}(t\text{-}Bu)_2\) \((E)-2\) \((Z)-2\) \((E)-3\) \((Z)-3\)
Independent *in-situ* syntheses and characterization of \((E)-3/(Z)-3\)

\[
\text{Ph}_3\text{GePCO} \xrightarrow{\text{Me}_3\text{Si-P(t-Bu)}_2 / \text{THF}} (E)-3 + (Z)-3
\]

70 °C, 1 h

Equimolar solutions of \(\text{Ph}_3\text{GePCO} (20.4 \text{ mg}, 0.06 \text{ mmol, 1 equiv.})\) and \((\text{t-Bu})_2\text{P-SiMe}_3 (12.3 \text{ mg}, 0.06 \text{ mmol, 1 equiv.})\) were combined in tetrahydrofuran \((\text{ca. 0.6 mL})\). The pale-yellow reaction mixture was transferred to an NMR tube and analyzed by \(^{31}\text{P}(^1\text{H})\) NMR spectroscopy, which showed complete conversion to \((E)-3\) \((\delta 159 \text{ ppm, 55 ppm, } ^2J_{PP} = 20 \text{ Hz})\) and a small amount of \((Z)-3\) \((\delta 234 \text{ ppm, 59 ppm, } ^2J_{PP} = 33 \text{ Hz})\). Heating to 70 °C for 1 hour leads to increased isomerization.

Figure 16. Stacked \(^{31}\text{P}(^1\text{H})\) NMR spectra of *in-situ* formation of \((E)-3/(Z)-3\) (THF)

Bottom: 23 °C, 30 min. Top: 70 °C, 1 h.
Reaction of (E)-2 with Ph₂P-SiPh₃

A solution of (E)-2 (18.3 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL) was combined with a solution of Ph₂P-SiPh₃ (9.6 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL). The homogenous yellow solution was transferred to an NMR tube and analyzed by ³¹P{¹H} NMR spectroscopy. Analysis after 30 minutes at ambient temperature showed a mixture of exclusively starting materials. Heating the reaction mixture to 85 ºC for 1.5 h showed both phosphine exchange and thermal isomerization, both characterized by the formation of (Z)-2, (E)-4 and (Z)-4.

Figure 17. Stacked ³¹P{¹H} NMR spectra of displaying phosphine exchange (THF)

Bottom: 23 ºC, 30 min. Middle: 85 ºC, 1 h. Top: 85 ºC, 2 h.

Ph₃Si-P(t-Bu)₂ Ph₃Si-PPPh₂ (E)-2 (Z)-2 (E)-4 (Z)-4
Independent *in-situ* syntheses and characterization of \((E)-4/(Z)-4\)

\[
\begin{align*}
\text{Ph}_3\text{GePCO} & \underset{\text{Ph}_3\text{SiPPh}_2}{\xrightarrow{\text{THF}}} (E)-4 + (Z)-4 \\
85 \, ^\circ\text{C}, 1 \, \text{h}
\end{align*}
\]

Equimolar solutions of \(\text{Ph}_3\text{GePCO} (7.1 \, \text{mg}, 0.02 \, \text{mmol}, 1 \, \text{equiv.})\) and \(\text{Ph}_3\text{P}-\text{SiPh}_3 (8.7 \, \text{mg}, 0.02 \, \text{mmol}, 1 \, \text{equiv.})\) were combined in tetrahydrofuran (ca. 0.6 mL). The pale-yellow reaction mixture was transferred to an NMR tube and analyzed by \(^{31}\text{P}\{\text{1H}\} \text{NMR}\) spectroscopy, which showed trace amounts of \((E)-4\) (\(\delta 171 \, \text{ppm}, 11 \, \text{ppm}, ^2J_{PP} = 16 \, \text{Hz}\)). Heating to 85 °C for 1 hour is accompanied by a colour change to bright yellow and increased formation of both \((E)-4\) and \((Z)-4\) (\(\delta 244 \, \text{ppm}, 19 \, \text{ppm}, ^2J_{PP} = 33 \, \text{Hz}\)), consistent with thermal isomerization.

![Figure 18](image_url)

Figure 18. Stacked \(^{31}\text{P}\{\text{1H}\} \text{NMR}\) spectra of \(*in-situ*\) formation of \((E)-4/(Z)-4\) (THF)

Bottom: 23 °C, 30 min. Top: 85 °C, 1 h.
Reaction of \((E)-2\) with \(\text{Ph}_2\text{P-SiMe}_3\)

A solution of \((E)-2\) (24.0 mg, 0.031 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL) was combined with a solution of \(\text{Ph}_2\text{P-SiMe}_3\) (8.1 mg, 0.031 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL). The homogenous yellow solution was transferred to an NMR tube and analyzed by \(^{31}\text{P}\{^1\text{H}\}\) NMR spectroscopy. Analysis after 30 minutes at ambient temperature showed the formation of \((Z)-2\), small amounts of \((E)-5\) (\(\delta 225\) ppm, 17 ppm, \(^2J_{\text{PP}} = 31\) Hz) and \((Z)-5\) (\(\delta 159\) ppm, 11 ppm, \(^2J_{\text{PP}} = 28\) Hz) and \(\text{t-Bu}_2\text{P-SiPh}_3\).

Figure 19. Stacked \(^{31}\text{P}\{^1\text{H}\}\) NMR spectra of displaying silylphosphine exchange (THF)

Bottom: 23 °C, 30 min. Top: 85 °C, 1.5 h.
Independent *in-situ* syntheses and characterization of \((E)-5/(Z)-5\)

![Chemical Reaction](image)

Equimolar solutions of Ph₃GeCO (17.0 mg, 0.047 mmol, 1 equiv.) and Ph₂P-SiMe₃ (12.1 mg, 0.047 mmol, 1 equiv.) were combined in tetrahydrofuran (ca. 0.6 mL). The pale-yellow reaction mixture was transferred to an NMR tube and analyzed by \(^{31}\text{P}\{\text{H}\}\) NMR spectroscopy, which showed the formation of \((E)-5\) and \((Z)-5\). Heating to 85 °C for 1 hour is accompanied by the appearance of multiple unidentified products.

![NMR Spectrum](image)

Figure 20. \(^{31}\text{P}\{\text{H}\}\) NMR spectrum of *in-situ* formation of \((E)-5/(Z)-5\) (THF)
Computational details

Electronic structure calculations, including geometry optimizations and frequency calculations, were performed using Gaussian 09\textsuperscript{3} using an ultrafine grid.\textsuperscript{4} The structures of (\textit{E})-2 and (\textit{Z})-2 were optimized at multiple levels of theory (see below), using the coordinates from the crystal structures as a starting point. All structures were confirmed as minima on the potential energy hypersurface by the absence of any imaginary frequencies.

Calculations were initially carried out by carrying out a geometry optimization and frequency analysis using the ωB97X-D functional and the 6-31G* basis set. Single point energy calculations were subsequently carried out at the ωB97X-D/6-311+G** level of theory. These calculations showed that (\textit{E})-2 is lower in energy (Table 1).

![Figure 21. Optimised structures of (\textit{E})-2 (left) and (\textit{Z})-2 (right) (ωB97X-D/6-31G*).](image)

<table>
<thead>
<tr>
<th></th>
<th>(\textit{E})-2</th>
<th>(\textit{Z})-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electronic energy (Hartrees)</td>
<td>-4868.104533</td>
<td>-4868.097513</td>
</tr>
<tr>
<td>Electronic energy (kcal/mol)</td>
<td>-3054779.407</td>
<td>-3054775.002</td>
</tr>
<tr>
<td>Relative electronic energy (kcal/mol)</td>
<td>0</td>
<td>+4.4</td>
</tr>
<tr>
<td>Thermal correction to Gibbs free energy (Hartrees)</td>
<td>0.734237</td>
<td>0.732010</td>
</tr>
<tr>
<td>Thermal correction to Gibbs free energy (kcal/mol)</td>
<td>460.740</td>
<td>459.343</td>
</tr>
<tr>
<td>Gibbs free energy (kcal/mol)</td>
<td>-3054318.667</td>
<td>-3054315.659</td>
</tr>
<tr>
<td>Relative Gibbs free energy (kcal/mol)</td>
<td>0</td>
<td>+3.0</td>
</tr>
</tbody>
</table>

The calculations were subsequently carried at alternative and higher levels of theory. In all cases below the geometry optimizations, frequency calculations and single point energies were determined using the following methods:

A) ωB97X-D/6-311+G**
B) ωB97X-D/6-31+G** with solvent correction (THF)

C) M06-2x/6-311+G** with solvent correction (THF) and Grimme’s D3 dispersion correction

The results of these are tabulated in Table 2. Again, in all cases, the Z-isomer is slightly higher in energy than the E-isomer.

Table 2. Electronic energies and Gibbs free energy of (E)-2 and (Z)-2 using methods A, B and C.

<table>
<thead>
<tr>
<th></th>
<th>Method A</th>
<th></th>
<th>Method B</th>
<th></th>
<th>Method C</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(E)-2</td>
<td>(Z)-2</td>
<td>(E)-2</td>
<td>(Z)-2</td>
<td>(E)-2</td>
<td>(Z)-2</td>
</tr>
<tr>
<td>Electronic energy (Hartrees)</td>
<td>-4868.105011</td>
<td>-4868.097988</td>
<td>-4868.114859</td>
<td>-4868.109711</td>
<td>-4867.85354</td>
<td>-4867.850797</td>
</tr>
<tr>
<td>Electronic energy (kcal/mol)</td>
<td>-3054779.707</td>
<td>-3054775.300</td>
<td>-3054785.887</td>
<td>-3054782.656</td>
<td>-3054621.907</td>
<td>-3054620.186</td>
</tr>
<tr>
<td>Relative electronic energy (kcal/mol)</td>
<td>0</td>
<td>+4.4</td>
<td>0</td>
<td>+3.2</td>
<td>0</td>
<td>+1.7</td>
</tr>
<tr>
<td>Gibbs free energy (Hartrees)</td>
<td>-4867.379895</td>
<td>-4867.375553</td>
<td>-4867.391276</td>
<td>-4867.386510</td>
<td>-4867.13016</td>
<td>-4867.128092</td>
</tr>
<tr>
<td>Gibbs free energy (kcal/mol)</td>
<td>-3054324.691</td>
<td>-3054321.966</td>
<td>-3054331.832</td>
<td>-3054328.842</td>
<td>-3054167.98</td>
<td>-3054166.682</td>
</tr>
<tr>
<td>Relative Gibbs free energy (kcal/mol)</td>
<td>0</td>
<td>+2.7</td>
<td>0</td>
<td>+3.0</td>
<td>0</td>
<td>+1.30</td>
</tr>
</tbody>
</table>

Table 3. Cartesian coordinates of optimised structure of (E)-2 (ωB97X-D/6-31G*).

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>1</td>
<td>32</td>
<td>5.869114</td>
<td>5.386343</td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>6.663494</td>
<td>9.865631</td>
</tr>
<tr>
<td>3</td>
<td>14</td>
<td>4.962580</td>
<td>9.785579</td>
</tr>
<tr>
<td>4</td>
<td>15</td>
<td>6.774570</td>
<td>6.728057</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>5.329540</td>
<td>8.444896</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>6.208132</td>
<td>8.267644</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>8.527564</td>
<td>9.824771</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>5.629886</td>
<td>9.783913</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>4.221804</td>
<td>9.302919</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>9.157645</td>
<td>8.664730</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>8.839827</td>
<td>11.138725</td>
</tr>
<tr>
<td>12</td>
<td>6</td>
<td>9.181615</td>
<td>9.890267</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>6.174287</td>
<td>8.877034</td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>5.498678</td>
<td>11.224393</td>
</tr>
<tr>
<td>15</td>
<td>1</td>
<td>3.799359</td>
<td>9.885733</td>
</tr>
<tr>
<td>16</td>
<td>1</td>
<td>4.225728</td>
<td>8.246823</td>
</tr>
<tr>
<td>17</td>
<td>1</td>
<td>3.554020</td>
<td>9.414296</td>
</tr>
<tr>
<td>18</td>
<td>1</td>
<td>10.235494</td>
<td>8.854821</td>
</tr>
<tr>
<td>19</td>
<td>1</td>
<td>9.031199</td>
<td>7.711288</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>8.752754</td>
<td>8.559341</td>
</tr>
<tr>
<td>21</td>
<td>1</td>
<td>8.370588</td>
<td>12.007663</td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>9.924891</td>
<td>11.302161</td>
</tr>
<tr>
<td>23</td>
<td>1</td>
<td>8.516123</td>
<td>11.097207</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
<td>8.822495</td>
<td>10.741929</td>
</tr>
<tr>
<td>25</td>
<td>1</td>
<td>10.269019</td>
<td>9.988008</td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>8.987269</td>
<td>8.978412</td>
</tr>
<tr>
<td>27</td>
<td>1</td>
<td>6.388857</td>
<td>7.867366</td>
</tr>
<tr>
<td>28</td>
<td>1</td>
<td>5.427881</td>
<td>8.793816</td>
</tr>
</tbody>
</table>
Table 4. Cartesian coordinates of optimised structure of (Z)-2 (ωB97X-D/6-31G*).

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>1</td>
<td>32</td>
<td>0</td>
<td>2.509873</td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>0</td>
<td>1.595891</td>
</tr>
<tr>
<td>3</td>
<td>15</td>
<td>0</td>
<td>1.115233</td>
</tr>
<tr>
<td>4</td>
<td>14</td>
<td>0</td>
<td>0.733367</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>0</td>
<td>0.723222</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>2.649166</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0</td>
<td>2.510573</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>0</td>
<td>0.484740</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>0</td>
<td>1.858696</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>0</td>
<td>-0.696363</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>0</td>
<td>-0.613181</td>
</tr>
<tr>
<td>12</td>
<td>1</td>
<td>0</td>
<td>-1.270434</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>0</td>
<td>1.145595</td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>0</td>
<td>2.379689</td>
</tr>
<tr>
<td>15</td>
<td>6</td>
<td>0</td>
<td>4.309384</td>
</tr>
<tr>
<td>16</td>
<td>6</td>
<td>0</td>
<td>2.541406</td>
</tr>
<tr>
<td>17</td>
<td>1</td>
<td>0</td>
<td>1.681560</td>
</tr>
<tr>
<td>18</td>
<td>6</td>
<td>0</td>
<td>-0.147891</td>
</tr>
<tr>
<td>19</td>
<td>6</td>
<td>0</td>
<td>-0.367326</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>0</td>
<td>-0.839453</td>
</tr>
<tr>
<td>21</td>
<td>6</td>
<td>0</td>
<td>0.790376</td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>0</td>
<td>0.367175</td>
</tr>
<tr>
<td>23</td>
<td>6</td>
<td>0</td>
<td>3.513340</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
<td>0</td>
<td>3.420824</td>
</tr>
<tr>
<td>25</td>
<td>6</td>
<td>0</td>
<td>2.369915</td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>0</td>
<td>3.173178</td>
</tr>
<tr>
<td>27</td>
<td>6</td>
<td>0</td>
<td>3.625560</td>
</tr>
<tr>
<td>28</td>
<td>1</td>
<td>0</td>
<td>4.265230</td>
</tr>
<tr>
<td>29</td>
<td>6</td>
<td>0</td>
<td>3.224993</td>
</tr>
<tr>
<td>30</td>
<td>1</td>
<td>0</td>
<td>4.256856</td>
</tr>
<tr>
<td>31</td>
<td>6</td>
<td>0</td>
<td>-1.751178</td>
</tr>
<tr>
<td>32</td>
<td>1</td>
<td>0</td>
<td>-1.714112</td>
</tr>
<tr>
<td>33</td>
<td>6</td>
<td>0</td>
<td>4.738683</td>
</tr>
<tr>
<td>34</td>
<td>1</td>
<td>0</td>
<td>4.044603</td>
</tr>
<tr>
<td>35</td>
<td>6</td>
<td>0</td>
<td>3.791096</td>
</tr>
<tr>
<td>36</td>
<td>1</td>
<td>0</td>
<td>3.896894</td>
</tr>
<tr>
<td>37</td>
<td>6</td>
<td>0</td>
<td>0.004927</td>
</tr>
<tr>
<td>38</td>
<td>1</td>
<td>0</td>
<td>0.747733</td>
</tr>
<tr>
<td>39</td>
<td>6</td>
<td>0</td>
<td>0.288535</td>
</tr>
<tr>
<td>40</td>
<td>1</td>
<td>0</td>
<td>-0.955654</td>
</tr>
<tr>
<td>41</td>
<td>6</td>
<td>0</td>
<td>1.838980</td>
</tr>
<tr>
<td>42</td>
<td>1</td>
<td>0</td>
<td>2.251065</td>
</tr>
<tr>
<td>43</td>
<td>6</td>
<td>0</td>
<td>-0.016530</td>
</tr>
<tr>
<td>44</td>
<td>1</td>
<td>0</td>
<td>-0.206684</td>
</tr>
<tr>
<td>45</td>
<td>6</td>
<td>0</td>
<td>3.193052</td>
</tr>
<tr>
<td>46</td>
<td>1</td>
<td>0</td>
<td>3.795476</td>
</tr>
<tr>
<td>47</td>
<td>1</td>
<td>0</td>
<td>3.862814</td>
</tr>
<tr>
<td>48</td>
<td>1</td>
<td>0</td>
<td>2.477055</td>
</tr>
<tr>
<td>49</td>
<td>6</td>
<td>0</td>
<td>-0.722055</td>
</tr>
<tr>
<td>50</td>
<td>1</td>
<td>0</td>
<td>-0.123537</td>
</tr>
<tr>
<td>51</td>
<td>1</td>
<td>0</td>
<td>-1.740569</td>
</tr>
<tr>
<td>52</td>
<td>1</td>
<td>0</td>
<td>-0.778125</td>
</tr>
<tr>
<td>53</td>
<td>6</td>
<td>0</td>
<td>-0.769950</td>
</tr>
<tr>
<td>54</td>
<td>1</td>
<td>0</td>
<td>0.034944</td>
</tr>
<tr>
<td>55</td>
<td>6</td>
<td>0</td>
<td>1.710935</td>
</tr>
<tr>
<td>56</td>
<td>1</td>
<td>0</td>
<td>1.214037</td>
</tr>
<tr>
<td>57</td>
<td>1</td>
<td>0</td>
<td>0.959399</td>
</tr>
<tr>
<td>58</td>
<td>1</td>
<td>0</td>
<td>2.394616</td>
</tr>
<tr>
<td>59</td>
<td>6</td>
<td>0</td>
<td>0.247708</td>
</tr>
<tr>
<td>60</td>
<td>1</td>
<td>0</td>
<td>-0.587044</td>
</tr>
<tr>
<td>61</td>
<td>6</td>
<td>0</td>
<td>2.903023</td>
</tr>
<tr>
<td>62</td>
<td>1</td>
<td>0</td>
<td>3.105167</td>
</tr>
<tr>
<td>Center Number</td>
<td>Atomic Number</td>
<td>Atomic Type</td>
<td>Coordinates (Angstroms)</td>
</tr>
<tr>
<td>---------------</td>
<td>---------------</td>
<td>-------------</td>
<td>-------------------------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>1</td>
<td>32</td>
<td>0</td>
<td>5.856353</td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>0</td>
<td>6.672232</td>
</tr>
<tr>
<td>3</td>
<td>14</td>
<td>0</td>
<td>4.968539</td>
</tr>
<tr>
<td>4</td>
<td>15</td>
<td>0</td>
<td>6.745306</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>0</td>
<td>5.352214</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>6.204752</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0</td>
<td>8.538945</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>0</td>
<td>5.658396</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>0</td>
<td>4.243078</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>0</td>
<td>9.165798</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>0</td>
<td>8.867038</td>
</tr>
<tr>
<td>12</td>
<td>6</td>
<td>0</td>
<td>9.176237</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>0</td>
<td>6.206236</td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>0</td>
<td>5.550529</td>
</tr>
<tr>
<td>15</td>
<td>1</td>
<td>0</td>
<td>3.821015</td>
</tr>
<tr>
<td>16</td>
<td>1</td>
<td>0</td>
<td>4.233779</td>
</tr>
<tr>
<td>17</td>
<td>1</td>
<td>0</td>
<td>3.586380</td>
</tr>
<tr>
<td>18</td>
<td>1</td>
<td>0</td>
<td>10.243610</td>
</tr>
<tr>
<td>19</td>
<td>1</td>
<td>0</td>
<td>9.030514</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>0</td>
<td>8.769911</td>
</tr>
<tr>
<td>21</td>
<td>1</td>
<td>0</td>
<td>8.396478</td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>0</td>
<td>9.950953</td>
</tr>
<tr>
<td>23</td>
<td>1</td>
<td>0</td>
<td>8.557460</td>
</tr>
</tbody>
</table>

Table 5. Cartesian coordinates of optimised structure of \((\text{E})-2\) (ωB97X-D/6-311+G**; Method A).
<table>
<thead>
<tr>
<th>Row</th>
<th>Type</th>
<th>Value</th>
<th>Value</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>1</td>
<td>8.814447</td>
<td>10.73257</td>
<td>3.842374</td>
</tr>
<tr>
<td>25</td>
<td>1</td>
<td>10.263232</td>
<td>9.971708</td>
<td>3.158988</td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>8.970575</td>
<td>8.971398</td>
<td>3.833644</td>
</tr>
<tr>
<td>27</td>
<td>1</td>
<td>6.401301</td>
<td>7.873365</td>
<td>-0.143969</td>
</tr>
<tr>
<td>28</td>
<td>1</td>
<td>5.470361</td>
<td>8.814227</td>
<td>-1.318971</td>
</tr>
<tr>
<td>29</td>
<td>1</td>
<td>7.126407</td>
<td>9.284509</td>
<td>-0.940818</td>
</tr>
<tr>
<td>30</td>
<td>1</td>
<td>5.089357</td>
<td>11.896220</td>
<td>0.797849</td>
</tr>
<tr>
<td>31</td>
<td>1</td>
<td>4.920112</td>
<td>11.242076</td>
<td>-0.836740</td>
</tr>
<tr>
<td>32</td>
<td>1</td>
<td>6.519569</td>
<td>11.654351</td>
<td>-0.218052</td>
</tr>
<tr>
<td>33</td>
<td>6</td>
<td>6.622093</td>
<td>5.863109</td>
<td>5.986975</td>
</tr>
<tr>
<td>34</td>
<td>6</td>
<td>5.848090</td>
<td>6.190219</td>
<td>7.100346</td>
</tr>
<tr>
<td>35</td>
<td>6</td>
<td>8.016440</td>
<td>5.874852</td>
<td>6.116738</td>
</tr>
<tr>
<td>36</td>
<td>6</td>
<td>6.450002</td>
<td>6.526767</td>
<td>8.310077</td>
</tr>
<tr>
<td>37</td>
<td>1</td>
<td>4.765874</td>
<td>6.204639</td>
<td>7.030179</td>
</tr>
<tr>
<td>38</td>
<td>6</td>
<td>8.619536</td>
<td>6.205019</td>
<td>7.323765</td>
</tr>
<tr>
<td>39</td>
<td>1</td>
<td>8.642289</td>
<td>5.624025</td>
<td>5.264634</td>
</tr>
<tr>
<td>40</td>
<td>6</td>
<td>7.833849</td>
<td>6.534718</td>
<td>8.424086</td>
</tr>
<tr>
<td>41</td>
<td>1</td>
<td>5.829645</td>
<td>6.790916</td>
<td>9.158519</td>
</tr>
<tr>
<td>42</td>
<td>1</td>
<td>9.701360</td>
<td>6.207290</td>
<td>7.405160</td>
</tr>
<tr>
<td>43</td>
<td>1</td>
<td>8.300741</td>
<td>6.800672</td>
<td>9.366189</td>
</tr>
<tr>
<td>44</td>
<td>6</td>
<td>6.453152</td>
<td>3.564142</td>
<td>3.837778</td>
</tr>
<tr>
<td>45</td>
<td>6</td>
<td>6.201165</td>
<td>3.025499</td>
<td>2.572307</td>
</tr>
<tr>
<td>46</td>
<td>6</td>
<td>7.092698</td>
<td>2.761777</td>
<td>4.784705</td>
</tr>
<tr>
<td>47</td>
<td>6</td>
<td>5.784882</td>
<td>1.725379</td>
<td>2.259916</td>
</tr>
<tr>
<td>48</td>
<td>1</td>
<td>7.700794</td>
<td>3.625086</td>
<td>1.816402</td>
</tr>
<tr>
<td>49</td>
<td>6</td>
<td>7.471239</td>
<td>1.458230</td>
<td>4.476662</td>
</tr>
<tr>
<td>50</td>
<td>1</td>
<td>7.300949</td>
<td>3.153789</td>
<td>5.775111</td>
</tr>
<tr>
<td>51</td>
<td>6</td>
<td>7.215617</td>
<td>0.938570</td>
<td>3.213916</td>
</tr>
<tr>
<td>52</td>
<td>1</td>
<td>6.375739</td>
<td>1.325003</td>
<td>1.272462</td>
</tr>
<tr>
<td>53</td>
<td>1</td>
<td>7.966351</td>
<td>0.848652</td>
<td>5.225034</td>
</tr>
<tr>
<td>54</td>
<td>1</td>
<td>7.511269</td>
<td>-0.076592</td>
<td>2.972459</td>
</tr>
<tr>
<td>55</td>
<td>6</td>
<td>3.903346</td>
<td>5.346045</td>
<td>4.261874</td>
</tr>
<tr>
<td>56</td>
<td>6</td>
<td>3.225769</td>
<td>4.562754</td>
<td>5.198815</td>
</tr>
<tr>
<td>57</td>
<td>6</td>
<td>3.157028</td>
<td>6.042473</td>
<td>3.311213</td>
</tr>
<tr>
<td>58</td>
<td>6</td>
<td>1.837208</td>
<td>4.494970</td>
<td>5.199906</td>
</tr>
<tr>
<td>59</td>
<td>1</td>
<td>3.782776</td>
<td>3.996015</td>
<td>5.939549</td>
</tr>
<tr>
<td>60</td>
<td>6</td>
<td>1.768231</td>
<td>5.972955</td>
<td>3.302023</td>
</tr>
<tr>
<td>61</td>
<td>1</td>
<td>3.664347</td>
<td>6.660090</td>
<td>2.577757</td>
</tr>
<tr>
<td>62</td>
<td>6</td>
<td>1.105556</td>
<td>5.203185</td>
<td>4.251832</td>
</tr>
<tr>
<td>63</td>
<td>1</td>
<td>3.258143</td>
<td>3.886605</td>
<td>5.937362</td>
</tr>
<tr>
<td>64</td>
<td>1</td>
<td>1.204111</td>
<td>6.523536</td>
<td>2.556838</td>
</tr>
<tr>
<td>65</td>
<td>1</td>
<td>0.022257</td>
<td>5.149567</td>
<td>4.249574</td>
</tr>
<tr>
<td>66</td>
<td>6</td>
<td>6.553370</td>
<td>10.455820</td>
<td>5.798616</td>
</tr>
<tr>
<td>67</td>
<td>6</td>
<td>6.825965</td>
<td>11.816939</td>
<td>5.970836</td>
</tr>
<tr>
<td>68</td>
<td>6</td>
<td>7.498201</td>
<td>9.529264</td>
<td>6.259698</td>
</tr>
<tr>
<td>69</td>
<td>6</td>
<td>8.013769</td>
<td>12.238766</td>
<td>6.558253</td>
</tr>
<tr>
<td>70</td>
<td>6</td>
<td>7.994403</td>
<td>12.605080</td>
<td>6.491585</td>
</tr>
<tr>
<td>71</td>
<td>6</td>
<td>8.681900</td>
<td>9.946268</td>
<td>6.852473</td>
</tr>
<tr>
<td>72</td>
<td>6</td>
<td>7.310733</td>
<td>8.460019</td>
<td>6.152587</td>
</tr>
<tr>
<td>73</td>
<td>6</td>
<td>8.945346</td>
<td>11.303678</td>
<td>6.995689</td>
</tr>
<tr>
<td>74</td>
<td>6</td>
<td>8.210381</td>
<td>13.298597</td>
<td>6.678151</td>
</tr>
<tr>
<td>75</td>
<td>6</td>
<td>9.395842</td>
<td>9.207081</td>
<td>7.198505</td>
</tr>
<tr>
<td>76</td>
<td>6</td>
<td>9.871871</td>
<td>11.633689</td>
<td>7.452965</td>
</tr>
<tr>
<td>77</td>
<td>6</td>
<td>3.889386</td>
<td>11.076901</td>
<td>4.239124</td>
</tr>
<tr>
<td>78</td>
<td>6</td>
<td>4.413132</td>
<td>12.169884</td>
<td>3.555597</td>
</tr>
<tr>
<td>79</td>
<td>6</td>
<td>2.495467</td>
<td>10.970342</td>
<td>3.428170</td>
</tr>
<tr>
<td>80</td>
<td>6</td>
<td>3.582344</td>
<td>13.110442</td>
<td>2.941841</td>
</tr>
<tr>
<td>81</td>
<td>6</td>
<td>5.486224</td>
<td>12.266096</td>
<td>3.421976</td>
</tr>
<tr>
<td>82</td>
<td>6</td>
<td>1.658871</td>
<td>11.898051</td>
<td>3.716705</td>
</tr>
<tr>
<td>83</td>
<td>6</td>
<td>2.047609</td>
<td>10.156124</td>
<td>4.886850</td>
</tr>
<tr>
<td>84</td>
<td>6</td>
<td>2.200976</td>
<td>12.971579</td>
<td>3.022781</td>
</tr>
<tr>
<td>85</td>
<td>6</td>
<td>4.013941</td>
<td>13.948452</td>
<td>2.405009</td>
</tr>
<tr>
<td>86</td>
<td>6</td>
<td>0.582995</td>
<td>11.784627</td>
<td>3.791313</td>
</tr>
<tr>
<td>87</td>
<td>6</td>
<td>1.551130</td>
<td>13.699854</td>
<td>2.549911</td>
</tr>
<tr>
<td>88</td>
<td>6</td>
<td>3.978915</td>
<td>8.982716</td>
<td>6.451302</td>
</tr>
<tr>
<td>89</td>
<td>6</td>
<td>4.257213</td>
<td>9.302143</td>
<td>7.784432</td>
</tr>
<tr>
<td>90</td>
<td>6</td>
<td>2.936539</td>
<td>8.084521</td>
<td>6.194530</td>
</tr>
<tr>
<td>91</td>
<td>6</td>
<td>3.527399</td>
<td>8.738614</td>
<td>8.825065</td>
</tr>
<tr>
<td>92</td>
<td>1</td>
<td>5.067655</td>
<td>9.985061</td>
<td>8.018773</td>
</tr>
<tr>
<td>93</td>
<td>6</td>
<td>2.204372</td>
<td>7.518546</td>
<td>7.230385</td>
</tr>
<tr>
<td>94</td>
<td>1</td>
<td>2.701894</td>
<td>7.798791</td>
<td>5.175687</td>
</tr>
</tbody>
</table>
Table 6. Cartesian coordinates of optimised structure of (Z)-2 (ωB97X-D/6-311+G**; Method A).

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Ångstroms)</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>32</td>
<td>0</td>
<td>2.511761</td>
<td>8.930367</td>
<td>2.700652</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>0</td>
<td>1.594793</td>
<td>5.585849</td>
<td>2.759065</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>15</td>
<td>0</td>
<td>1.142659</td>
<td>8.186174</td>
<td>4.443384</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>14</td>
<td>0</td>
<td>0.737791</td>
<td>6.064188</td>
<td>7.019586</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>0</td>
<td>0.743475</td>
<td>5.727156</td>
<td>5.350906</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>2.647002</td>
<td>10.859320</td>
<td>3.069098</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0</td>
<td>2.523289</td>
<td>4.032311</td>
<td>3.327823</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>0</td>
<td>0.482810</td>
<td>4.368332</td>
<td>7.758663</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>0</td>
<td>1.854466</td>
<td>8.730632</td>
<td>0.872593</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>0</td>
<td>-0.698418</td>
<td>7.180209</td>
<td>7.438225</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>0</td>
<td>-0.631474</td>
<td>2.213006</td>
<td>7.691761</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>1</td>
<td>0</td>
<td>-1.295395</td>
<td>1.518797</td>
<td>7.188492</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>0</td>
<td>1.162906</td>
<td>6.485921</td>
<td>4.314615</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>0</td>
<td>2.382020</td>
<td>6.800436</td>
<td>7.522773</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>6</td>
<td>0</td>
<td>4.323615</td>
<td>8.218546</td>
<td>2.960000</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>6</td>
<td>0</td>
<td>2.541744</td>
<td>8.179403</td>
<td>7.708179</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>1</td>
<td>0</td>
<td>1.682338</td>
<td>8.835711</td>
<td>7.620418</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>6</td>
<td>0</td>
<td>-0.154886</td>
<td>5.125273</td>
<td>2.150924</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>6</td>
<td>0</td>
<td>-0.376480</td>
<td>3.457621</td>
<td>7.131873</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>0</td>
<td>-0.846542</td>
<td>3.722973</td>
<td>6.199779</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>6</td>
<td>0</td>
<td>0.804224</td>
<td>9.542111</td>
<td>0.442514</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>0</td>
<td>0.400439</td>
<td>10.304960</td>
<td>1.105537</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>6</td>
<td>0</td>
<td>3.514364</td>
<td>5.984447</td>
<td>7.632937</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>1</td>
<td>0</td>
<td>3.422946</td>
<td>4.910610</td>
<td>7.500102</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>6</td>
<td>0</td>
<td>2.346652</td>
<td>7.762478</td>
<td>-0.005375</td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>0</td>
<td>3.134326</td>
<td>7.091440</td>
<td>0.317369</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>6</td>
<td>0</td>
<td>3.656447</td>
<td>4.548311</td>
<td>4.227273</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>1</td>
<td>0</td>
<td>4.278362</td>
<td>5.281935</td>
<td>3.710236</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>1</td>
<td>0</td>
<td>3.297264</td>
<td>5.022800</td>
<td>5.139795</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>1</td>
<td>0</td>
<td>4.298076</td>
<td>3.708604</td>
<td>4.518393</td>
<td></td>
</tr>
<tr>
<td>31</td>
<td>6</td>
<td>0</td>
<td>-1.731018</td>
<td>7.419537</td>
<td>6.527122</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>1</td>
<td>0</td>
<td>-1.674108</td>
<td>7.006615</td>
<td>5.525101</td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>6</td>
<td>0</td>
<td>4.760049</td>
<td>7.856705</td>
<td>4.237379</td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>1</td>
<td>0</td>
<td>4.075450</td>
<td>7.882259</td>
<td>5.080173</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>6</td>
<td>0</td>
<td>3.789977</td>
<td>8.74290</td>
<td>7.982726</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>1</td>
<td>0</td>
<td>3.896262</td>
<td>9.795450</td>
<td>8.112689</td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>6</td>
<td>0</td>
<td>-0.010679</td>
<td>4.080066</td>
<td>1.035209</td>
<td></td>
</tr>
<tr>
<td>38</td>
<td>1</td>
<td>0</td>
<td>0.723756</td>
<td>4.389081</td>
<td>0.285412</td>
<td></td>
</tr>
<tr>
<td>39</td>
<td>1</td>
<td>0</td>
<td>0.276408</td>
<td>3.099993</td>
<td>1.421737</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>1</td>
<td>0</td>
<td>-0.974607</td>
<td>3.963648</td>
<td>0.527587</td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>6</td>
<td>0</td>
<td>1.809637</td>
<td>7.616621</td>
<td>-1.279062</td>
<td></td>
</tr>
<tr>
<td>42</td>
<td>1</td>
<td>0</td>
<td>2.204340</td>
<td>6.858938</td>
<td>-1.947516</td>
<td></td>
</tr>
<tr>
<td>43</td>
<td>6</td>
<td>0</td>
<td>-0.035330</td>
<td>1.858085</td>
<td>8.897451</td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>1</td>
<td>0</td>
<td>-0.232719</td>
<td>0.885951</td>
<td>9.335761</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>6</td>
<td>0</td>
<td>3.179016</td>
<td>3.425031</td>
<td>2.074029</td>
<td></td>
</tr>
<tr>
<td>46</td>
<td>1</td>
<td>0</td>
<td>3.765399</td>
<td>4.172059</td>
<td>1.531601</td>
<td></td>
</tr>
<tr>
<td>47</td>
<td>1</td>
<td>0</td>
<td>3.858291</td>
<td>2.620675</td>
<td>2.378790</td>
<td></td>
</tr>
<tr>
<td>48</td>
<td>1</td>
<td>0</td>
<td>2.450907</td>
<td>2.995877</td>
<td>1.383812</td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>6</td>
<td>0</td>
<td>-0.742457</td>
<td>6.401929</td>
<td>1.528608</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>1</td>
<td>0</td>
<td>-0.151667</td>
<td>6.746042</td>
<td>0.677872</td>
<td></td>
</tr>
<tr>
<td>51</td>
<td>1</td>
<td>0</td>
<td>-1.758260</td>
<td>6.191449</td>
<td>1.174922</td>
<td></td>
</tr>
<tr>
<td>52</td>
<td>1</td>
<td>0</td>
<td>-0.804141</td>
<td>7.218946</td>
<td>2.251983</td>
<td></td>
</tr>
<tr>
<td>53</td>
<td>6</td>
<td>0</td>
<td>-0.798620</td>
<td>7.739967</td>
<td>8.716893</td>
<td></td>
</tr>
<tr>
<td>54</td>
<td>1</td>
<td>0</td>
<td>-0.012854</td>
<td>7.569972</td>
<td>9.448148</td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>6</td>
<td>0</td>
<td>1.737637</td>
<td>2.948835</td>
<td>4.069791</td>
<td></td>
</tr>
<tr>
<td>56</td>
<td>1</td>
<td>0</td>
<td>1.252050</td>
<td>3.342570</td>
<td>4.961761</td>
<td></td>
</tr>
<tr>
<td>57</td>
<td>1</td>
<td>0</td>
<td>0.980504</td>
<td>2.483240</td>
<td>3.434825</td>
<td></td>
</tr>
</tbody>
</table>
Table 7. Cartesian coordinates of optimised structure of (E)-2 (ωB97X-D/6-311+G**, THF; Method B).

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Ångstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>1</td>
<td>32</td>
<td>5.864258</td>
<td>5.384577</td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>6.677482</td>
<td>9.807642</td>
</tr>
<tr>
<td>3</td>
<td>14</td>
<td>4.970644</td>
<td>9.788171</td>
</tr>
<tr>
<td>4</td>
<td>15</td>
<td>6.743866</td>
<td>6.731972</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>5.359645</td>
<td>8.448936</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>6.208529</td>
<td>8.271898</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>8.542584</td>
<td>9.816931</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>5.575393</td>
<td>9.805229</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>4.242055</td>
<td>9.342298</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>9.165068</td>
<td>8.643003</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>8.868460</td>
<td>11.17956</td>
</tr>
<tr>
<td>12</td>
<td>6</td>
<td>9.187433</td>
<td>9.883358</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>6.200033</td>
<td>8.896818</td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>5.552503</td>
<td>11.247466</td>
</tr>
<tr>
<td>15</td>
<td>1</td>
<td>3.823316</td>
<td>9.931469</td>
</tr>
<tr>
<td>16</td>
<td>1</td>
<td>4.229949</td>
<td>8.288883</td>
</tr>
<tr>
<td>17</td>
<td>1</td>
<td>3.585196</td>
<td>9.461494</td>
</tr>
<tr>
<td>18</td>
<td>1</td>
<td>10.241010</td>
<td>8.831553</td>
</tr>
<tr>
<td>19</td>
<td>1</td>
<td>9.042069</td>
<td>7.701248</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>8.755883</td>
<td>8.522380</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>21</td>
<td>1</td>
<td>0</td>
<td>8.399566</td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>0</td>
<td>9.952474</td>
</tr>
<tr>
<td>23</td>
<td>1</td>
<td>0</td>
<td>8.555810</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
<td>0</td>
<td>8.827418</td>
</tr>
<tr>
<td>25</td>
<td>1</td>
<td>0</td>
<td>10.273669</td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>0</td>
<td>8.984110</td>
</tr>
<tr>
<td>27</td>
<td>1</td>
<td>0</td>
<td>6.387453</td>
</tr>
<tr>
<td>28</td>
<td>1</td>
<td>0</td>
<td>5.463283</td>
</tr>
<tr>
<td>29</td>
<td>1</td>
<td>0</td>
<td>7.123049</td>
</tr>
<tr>
<td>30</td>
<td>1</td>
<td>0</td>
<td>5.105796</td>
</tr>
<tr>
<td>31</td>
<td>1</td>
<td>0</td>
<td>4.911013</td>
</tr>
<tr>
<td>32</td>
<td>1</td>
<td>0</td>
<td>6.520756</td>
</tr>
<tr>
<td>33</td>
<td>6</td>
<td>0</td>
<td>5.843870</td>
</tr>
<tr>
<td>34</td>
<td>6</td>
<td>0</td>
<td>8.014711</td>
</tr>
<tr>
<td>35</td>
<td>6</td>
<td>0</td>
<td>6.443280</td>
</tr>
<tr>
<td>36</td>
<td>6</td>
<td>0</td>
<td>4.761377</td>
</tr>
<tr>
<td>37</td>
<td>6</td>
<td>0</td>
<td>8.615884</td>
</tr>
<tr>
<td>38</td>
<td>6</td>
<td>0</td>
<td>8.643714</td>
</tr>
<tr>
<td>39</td>
<td>6</td>
<td>0</td>
<td>7.827698</td>
</tr>
<tr>
<td>40</td>
<td>6</td>
<td>0</td>
<td>5.821983</td>
</tr>
<tr>
<td>41</td>
<td>6</td>
<td>0</td>
<td>9.679431</td>
</tr>
<tr>
<td>42</td>
<td>6</td>
<td>0</td>
<td>8.293128</td>
</tr>
<tr>
<td>43</td>
<td>6</td>
<td>0</td>
<td>4.761377</td>
</tr>
<tr>
<td>44</td>
<td>6</td>
<td>0</td>
<td>8.615884</td>
</tr>
<tr>
<td>45</td>
<td>6</td>
<td>0</td>
<td>7.314298</td>
</tr>
<tr>
<td>46</td>
<td>6</td>
<td>0</td>
<td>7.215224</td>
</tr>
<tr>
<td>47</td>
<td>6</td>
<td>0</td>
<td>6.359785</td>
</tr>
<tr>
<td>48</td>
<td>6</td>
<td>0</td>
<td>7.980820</td>
</tr>
<tr>
<td>49</td>
<td>6</td>
<td>0</td>
<td>7.511126</td>
</tr>
<tr>
<td>50</td>
<td>6</td>
<td>0</td>
<td>3.901143</td>
</tr>
<tr>
<td>51</td>
<td>6</td>
<td>0</td>
<td>3.218559</td>
</tr>
<tr>
<td>52</td>
<td>6</td>
<td>0</td>
<td>3.158683</td>
</tr>
<tr>
<td>53</td>
<td>6</td>
<td>0</td>
<td>1.828961</td>
</tr>
<tr>
<td>54</td>
<td>6</td>
<td>0</td>
<td>3.770322</td>
</tr>
<tr>
<td>55</td>
<td>6</td>
<td>0</td>
<td>1.768880</td>
</tr>
<tr>
<td>56</td>
<td>6</td>
<td>0</td>
<td>3.668851</td>
</tr>
<tr>
<td>57</td>
<td>6</td>
<td>0</td>
<td>1.101388</td>
</tr>
<tr>
<td>58</td>
<td>6</td>
<td>0</td>
<td>1.313628</td>
</tr>
<tr>
<td>59</td>
<td>6</td>
<td>0</td>
<td>1.207814</td>
</tr>
<tr>
<td>60</td>
<td>6</td>
<td>0</td>
<td>0.017727</td>
</tr>
<tr>
<td>61</td>
<td>6</td>
<td>0</td>
<td>6.558706</td>
</tr>
<tr>
<td>62</td>
<td>6</td>
<td>0</td>
<td>6.826555</td>
</tr>
<tr>
<td>63</td>
<td>6</td>
<td>0</td>
<td>7.506223</td>
</tr>
<tr>
<td>64</td>
<td>6</td>
<td>0</td>
<td>8.015658</td>
</tr>
<tr>
<td>65</td>
<td>6</td>
<td>0</td>
<td>6.103824</td>
</tr>
<tr>
<td>66</td>
<td>6</td>
<td>0</td>
<td>8.691282</td>
</tr>
<tr>
<td>67</td>
<td>6</td>
<td>0</td>
<td>7.320909</td>
</tr>
<tr>
<td>68</td>
<td>6</td>
<td>0</td>
<td>8.951753</td>
</tr>
<tr>
<td>69</td>
<td>6</td>
<td>0</td>
<td>8.209584</td>
</tr>
<tr>
<td>70</td>
<td>6</td>
<td>0</td>
<td>9.409702</td>
</tr>
<tr>
<td>71</td>
<td>6</td>
<td>0</td>
<td>9.878766</td>
</tr>
<tr>
<td>72</td>
<td>6</td>
<td>0</td>
<td>3.889278</td>
</tr>
<tr>
<td>73</td>
<td>6</td>
<td>0</td>
<td>4.087242</td>
</tr>
<tr>
<td>74</td>
<td>6</td>
<td>0</td>
<td>2.495572</td>
</tr>
<tr>
<td>75</td>
<td>6</td>
<td>0</td>
<td>3.574626</td>
</tr>
<tr>
<td>76</td>
<td>6</td>
<td>0</td>
<td>5.481537</td>
</tr>
<tr>
<td>77</td>
<td>6</td>
<td>0</td>
<td>1.655969</td>
</tr>
<tr>
<td>78</td>
<td>6</td>
<td>0</td>
<td>2.048480</td>
</tr>
<tr>
<td>79</td>
<td>6</td>
<td>0</td>
<td>2.194500</td>
</tr>
<tr>
<td>80</td>
<td>6</td>
<td>0</td>
<td>4.003002</td>
</tr>
<tr>
<td>81</td>
<td>6</td>
<td>0</td>
<td>0.581397</td>
</tr>
<tr>
<td>82</td>
<td>6</td>
<td>0</td>
<td>1.527988</td>
</tr>
<tr>
<td>83</td>
<td>6</td>
<td>0</td>
<td>3.981007</td>
</tr>
<tr>
<td>84</td>
<td>6</td>
<td>0</td>
<td>4.258665</td>
</tr>
<tr>
<td>85</td>
<td>6</td>
<td>0</td>
<td>2.940382</td>
</tr>
<tr>
<td>86</td>
<td>6</td>
<td>0</td>
<td>3.531912</td>
</tr>
</tbody>
</table>
Table 8. Cartesian coordinates of optimised structure of (Z)-2 (ωB97X-D/6-311+G**, THF; Method B).

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>32</td>
<td>0</td>
<td>2.505768   8.925122   2.695827</td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>0</td>
<td>1.604306   5.549092   2.762130</td>
</tr>
<tr>
<td>3</td>
<td>15</td>
<td>0</td>
<td>1.122153   8.164501   4.420425</td>
</tr>
<tr>
<td>4</td>
<td>14</td>
<td>0</td>
<td>0.748485   6.071650   7.020162</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>0</td>
<td>0.747899   5.712604   5.351746</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>2.629413   10.848148  3.106888</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0</td>
<td>2.507373   3.987210   3.348857</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>0</td>
<td>0.470246   4.385748   7.773591</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>0</td>
<td>1.853328   8.740745   0.864133</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>0</td>
<td>-0.682124  7.203827   7.189931</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>0</td>
<td>-0.699344  2.241884  7.721528</td>
</tr>
<tr>
<td>12</td>
<td>1</td>
<td>0</td>
<td>-1.337822  1.549987   7.221182</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>0</td>
<td>1.159486   6.461145   4.309137</td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>0</td>
<td>2.402235   6.798670   7.501742</td>
</tr>
<tr>
<td>15</td>
<td>6</td>
<td>0</td>
<td>4.323548   8.237784   2.947311</td>
</tr>
<tr>
<td>16</td>
<td>6</td>
<td>0</td>
<td>2.583844   8.197824   7.652306</td>
</tr>
<tr>
<td>17</td>
<td>1</td>
<td>0</td>
<td>1.735884   8.490553   7.554730</td>
</tr>
<tr>
<td>18</td>
<td>6</td>
<td>0</td>
<td>-0.142395  5.103259   2.139811</td>
</tr>
<tr>
<td>19</td>
<td>6</td>
<td>0</td>
<td>-0.395750  3.478110   7.149845</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>0</td>
<td>-0.856926  3.737676   6.201688</td>
</tr>
<tr>
<td>21</td>
<td>6</td>
<td>0</td>
<td>0.769232   9.517340   0.446419</td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>0</td>
<td>0.327129   10.243383  1.122598</td>
</tr>
<tr>
<td>23</td>
<td>6</td>
<td>0</td>
<td>3.524048   5.969201   7.62974</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
<td>0</td>
<td>3.419137   4.893589   7.523405</td>
</tr>
<tr>
<td>25</td>
<td>6</td>
<td>0</td>
<td>2.388164   7.809730  -0.029023</td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>0</td>
<td>3.207492   7.170570   0.280191</td>
</tr>
<tr>
<td>27</td>
<td>6</td>
<td>0</td>
<td>3.637454   4.491122   4.259261</td>
</tr>
<tr>
<td>28</td>
<td>1</td>
<td>0</td>
<td>4.271950   5.217386   3.746350</td>
</tr>
<tr>
<td>29</td>
<td>1</td>
<td>0</td>
<td>3.256506   4.959490   5.167253</td>
</tr>
<tr>
<td>30</td>
<td>1</td>
<td>0</td>
<td>4.266111   3.644354   4.556942</td>
</tr>
<tr>
<td>31</td>
<td>6</td>
<td>0</td>
<td>-1.753148  7.357333  6.532332</td>
</tr>
<tr>
<td>32</td>
<td>1</td>
<td>0</td>
<td>-1.728117  6.867550  5.564126</td>
</tr>
<tr>
<td>33</td>
<td>6</td>
<td>0</td>
<td>4.752575   7.801140   4.203881</td>
</tr>
<tr>
<td>34</td>
<td>1</td>
<td>0</td>
<td>4.054296   7.745050   5.033906</td>
</tr>
<tr>
<td>35</td>
<td>6</td>
<td>0</td>
<td>3.841484   8.713570   7.906734</td>
</tr>
<tr>
<td>36</td>
<td>1</td>
<td>0</td>
<td>3.962715   9.785983   8.011109</td>
</tr>
<tr>
<td>37</td>
<td>6</td>
<td>0</td>
<td>0.001114   4.040159   1.034807</td>
</tr>
<tr>
<td>38</td>
<td>1</td>
<td>0</td>
<td>0.749612   4.325961   0.289637</td>
</tr>
<tr>
<td>39</td>
<td>1</td>
<td>0</td>
<td>0.267433   3.061301   1.438086</td>
</tr>
<tr>
<td>40</td>
<td>1</td>
<td>0</td>
<td>-0.958614  3.932071  0.517750</td>
</tr>
<tr>
<td>41</td>
<td>6</td>
<td>0</td>
<td>1.859063   7.662148  -1.306605</td>
</tr>
<tr>
<td>42</td>
<td>1</td>
<td>0</td>
<td>2.285564   6.932500  -1.966439</td>
</tr>
<tr>
<td>43</td>
<td>6</td>
<td>0</td>
<td>-0.08456   1.892924   8.935525</td>
</tr>
<tr>
<td>44</td>
<td>1</td>
<td>0</td>
<td>-0.295813  0.977765   9.382626</td>
</tr>
<tr>
<td>45</td>
<td>6</td>
<td>0</td>
<td>3.167489   3.362520   2.105793</td>
</tr>
<tr>
<td>46</td>
<td>1</td>
<td>0</td>
<td>3.767423   4.097580   1.561548</td>
</tr>
<tr>
<td>47</td>
<td>1</td>
<td>0</td>
<td>3.834221   2.553296   2.424692</td>
</tr>
<tr>
<td>48</td>
<td>1</td>
<td>0</td>
<td>2.440698   2.935903   1.412960</td>
</tr>
<tr>
<td>49</td>
<td>6</td>
<td>0</td>
<td>-0.704736  6.377965   1.485890</td>
</tr>
<tr>
<td>50</td>
<td>1</td>
<td>0</td>
<td>-0.092997  6.704479  0.642719</td>
</tr>
<tr>
<td>51</td>
<td>1</td>
<td>0</td>
<td>-1.716152  6.173155  1.116986</td>
</tr>
<tr>
<td>52</td>
<td>1</td>
<td>0</td>
<td>-0.769645  7.204521  2.198131</td>
</tr>
<tr>
<td>53</td>
<td>6</td>
<td>0</td>
<td>-0.745623  7.856553   8.655564</td>
</tr>
<tr>
<td>54</td>
<td>1</td>
<td>0</td>
<td>0.068338   7.754390   9.367940</td>
</tr>
</tbody>
</table>
Table 9. Cartesian coordinates of optimised structure of (E)-2 (M06-2x/6-311+G**, THF, GD3; Method C).

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>1</td>
<td>32</td>
<td>0</td>
<td>5.825412</td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>0</td>
<td>6.688527</td>
</tr>
<tr>
<td>3</td>
<td>14</td>
<td>0</td>
<td>4.939987</td>
</tr>
<tr>
<td>4</td>
<td>15</td>
<td>0</td>
<td>6.738742</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>0</td>
<td>5.345299</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>6.203440</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0</td>
<td>8.559976</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>0</td>
<td>5.717105</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>0</td>
<td>4.295558</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>0</td>
<td>9.198891</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>0</td>
<td>8.902753</td>
</tr>
<tr>
<td>12</td>
<td>6</td>
<td>0</td>
<td>9.182637</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>0</td>
<td>6.295545</td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>0</td>
<td>5.618104</td>
</tr>
<tr>
<td>15</td>
<td>6</td>
<td>0</td>
<td>3.856687</td>
</tr>
<tr>
<td>Center Number</td>
<td>Atomic Number</td>
<td>Atomic Type</td>
<td>Coordinates (Angstroms)</td>
</tr>
<tr>
<td>---------------</td>
<td>---------------</td>
<td>-------------</td>
<td>------------------------</td>
</tr>
<tr>
<td>1</td>
<td>32</td>
<td>0</td>
<td>2.498290 8.917254 2.704566</td>
</tr>
<tr>
<td>2</td>
<td>15</td>
<td>0</td>
<td>1.599112 5.580376 2.741196</td>
</tr>
<tr>
<td>3</td>
<td>15</td>
<td>0</td>
<td>1.106787 8.172297 4.445717</td>
</tr>
<tr>
<td>4</td>
<td>14</td>
<td>0</td>
<td>0.762817 6.053167 7.005287</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>0</td>
<td>0.733036 5.695998 5.338713</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>2.596681 10.853112 3.098209</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0</td>
<td>2.480660 4.005671 3.324633</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>0</td>
<td>0.501956 4.371278 7.771671</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>0</td>
<td>1.872635 8.712308 0.857114</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>0</td>
<td>-0.656422 7.190843 7.427005</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>0</td>
<td>-0.649443 2.231685 7.741322</td>
</tr>
<tr>
<td>12</td>
<td>1</td>
<td>0</td>
<td>-1.330008 1.542208 7.255397</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>0</td>
<td>1.144528 6.468656 4.305384</td>
</tr>
<tr>
<td>14</td>
<td>6</td>
<td>0</td>
<td>2.414685 6.791730 7.480315</td>
</tr>
<tr>
<td>15</td>
<td>6</td>
<td>0</td>
<td>4.315674 8.216630 2.967434</td>
</tr>
<tr>
<td>16</td>
<td>6</td>
<td>0</td>
<td>2.578186 8.175284 7.642998</td>
</tr>
<tr>
<td>17</td>
<td>1</td>
<td>0</td>
<td>1.720504 8.832794 7.543039</td>
</tr>
<tr>
<td>18</td>
<td>6</td>
<td>0</td>
<td>-0.149216 5.148882 2.111994</td>
</tr>
<tr>
<td>19</td>
<td>6</td>
<td>0</td>
<td>-0.380042 3.467149 7.162809</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>0</td>
<td>-0.856594 3.731988 6.222911</td>
</tr>
<tr>
<td>21</td>
<td>6</td>
<td>0</td>
<td>0.806470 9.499301 4.092747</td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>0</td>
<td>0.363892 10.243076 1.068006</td>
</tr>
<tr>
<td>23</td>
<td>6</td>
<td>0</td>
<td>3.544264 5.971731 7.611282</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
<td>0</td>
<td>3.449302 4.895255 7.502245</td>
</tr>
<tr>
<td>25</td>
<td>6</td>
<td>0</td>
<td>2.408873 7.757847 -0.013267</td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>0</td>
<td>3.211978 7.110403 0.322512</td>
</tr>
<tr>
<td>27</td>
<td>6</td>
<td>0</td>
<td>3.610563 4.504879 4.236773</td>
</tr>
<tr>
<td>28</td>
<td>1</td>
<td>0</td>
<td>4.266443 5.201751 3.709559</td>
</tr>
<tr>
<td>29</td>
<td>1</td>
<td>0</td>
<td>3.226545 5.008930 5.125427</td>
</tr>
<tr>
<td>30</td>
<td>1</td>
<td>0</td>
<td>4.212843 3.650188 4.563463</td>
</tr>
<tr>
<td>31</td>
<td>6</td>
<td>0</td>
<td>-1.709186 7.407091 6.530703</td>
</tr>
<tr>
<td>32</td>
<td>1</td>
<td>0</td>
<td>-1.672755 6.964411 5.540103</td>
</tr>
<tr>
<td>33</td>
<td>6</td>
<td>0</td>
<td>4.737496 7.791818 4.252424</td>
</tr>
<tr>
<td>34</td>
<td>1</td>
<td>0</td>
<td>4.036126 7.752769 5.083068</td>
</tr>
<tr>
<td>35</td>
<td>6</td>
<td>0</td>
<td>3.829007 8.722036 7.912682</td>
</tr>
<tr>
<td>36</td>
<td>1</td>
<td>0</td>
<td>3.937909 9.794274 8.027817</td>
</tr>
<tr>
<td>37</td>
<td>6</td>
<td>0</td>
<td>-0.012732 4.074460 1.024821</td>
</tr>
<tr>
<td>38</td>
<td>1</td>
<td>0</td>
<td>0.744263 4.346933 0.283144</td>
</tr>
<tr>
<td>39</td>
<td>1</td>
<td>0</td>
<td>0.238404 3.096987 1.439096</td>
</tr>
<tr>
<td>40</td>
<td>1</td>
<td>0</td>
<td>-0.971198 3.977567 0.504243</td>
</tr>
<tr>
<td>41</td>
<td>6</td>
<td>0</td>
<td>1.898223 7.597960 -1.298382</td>
</tr>
<tr>
<td>42</td>
<td>1</td>
<td>0</td>
<td>2.324993 6.853168 -1.960564</td>
</tr>
<tr>
<td>43</td>
<td>6</td>
<td>0</td>
<td>-0.043354 1.882206 8.946251</td>
</tr>
<tr>
<td>44</td>
<td>1</td>
<td>0</td>
<td>-0.250758 0.919163 9.398157</td>
</tr>
<tr>
<td>45</td>
<td>6</td>
<td>0</td>
<td>3.142041 3.377517 2.084921</td>
</tr>
<tr>
<td>46</td>
<td>1</td>
<td>0</td>
<td>3.739626 4.113572 1.539926</td>
</tr>
<tr>
<td>47</td>
<td>1</td>
<td>0</td>
<td>3.810591 2.573554 2.411040</td>
</tr>
</tbody>
</table>

Table 10. Cartesian coordinates of optimised structure of (Z)-2 (M06-2x/6-311+G**, THF, GD3; Method C).
<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>1</td>
<td>0</td>
<td>2.416424</td>
<td>2.945663</td>
<td>1.394896</td>
</tr>
<tr>
<td>49</td>
<td>6</td>
<td>0</td>
<td>-0.697176</td>
<td>6.421640</td>
<td>1.450110</td>
</tr>
<tr>
<td>50</td>
<td>1</td>
<td>0</td>
<td>-0.087552</td>
<td>6.723549</td>
<td>0.595663</td>
</tr>
<tr>
<td>51</td>
<td>1</td>
<td>0</td>
<td>-1.714962</td>
<td>6.223970</td>
<td>1.096412</td>
</tr>
<tr>
<td>52</td>
<td>1</td>
<td>0</td>
<td>-0.740844</td>
<td>7.258912</td>
<td>2.151717</td>
</tr>
<tr>
<td>53</td>
<td>6</td>
<td>0</td>
<td>-0.725809</td>
<td>7.785551</td>
<td>8.693473</td>
</tr>
<tr>
<td>54</td>
<td>1</td>
<td>0</td>
<td>0.076363</td>
<td>7.632013</td>
<td>9.410636</td>
</tr>
<tr>
<td>55</td>
<td>6</td>
<td>0</td>
<td>1.665665</td>
<td>2.941374</td>
<td>4.062141</td>
</tr>
<tr>
<td>56</td>
<td>1</td>
<td>0</td>
<td>1.187756</td>
<td>3.348574</td>
<td>4.952534</td>
</tr>
<tr>
<td>57</td>
<td>1</td>
<td>0</td>
<td>0.901655</td>
<td>7.632013</td>
<td>9.410636</td>
</tr>
<tr>
<td>58</td>
<td>6</td>
<td>0</td>
<td>-0.725809</td>
<td>7.785551</td>
<td>8.693473</td>
</tr>
<tr>
<td>59</td>
<td>1</td>
<td>0</td>
<td>0.283577</td>
<td>9.334925</td>
<td>-0.871332</td>
</tr>
<tr>
<td>60</td>
<td>1</td>
<td>0</td>
<td>-0.549919</td>
<td>9.946008</td>
<td>-1.198096</td>
</tr>
<tr>
<td>61</td>
<td>6</td>
<td>0</td>
<td>2.880343</td>
<td>13.581025</td>
<td>3.714402</td>
</tr>
<tr>
<td>62</td>
<td>1</td>
<td>0</td>
<td>2.986921</td>
<td>14.633239</td>
<td>3.951582</td>
</tr>
<tr>
<td>63</td>
<td>6</td>
<td>0</td>
<td>2.664414</td>
<td>11.287964</td>
<td>4.428048</td>
</tr>
<tr>
<td>64</td>
<td>1</td>
<td>0</td>
<td>2.611177</td>
<td>10.567100</td>
<td>5.240263</td>
</tr>
<tr>
<td>65</td>
<td>6</td>
<td>0</td>
<td>5.252307</td>
<td>8.241014</td>
<td>1.946438</td>
</tr>
<tr>
<td>66</td>
<td>1</td>
<td>0</td>
<td>4.962493</td>
<td>8.589904</td>
<td>0.959767</td>
</tr>
<tr>
<td>67</td>
<td>6</td>
<td>0</td>
<td>-2.847927</td>
<td>8.787155</td>
<td>8.144954</td>
</tr>
<tr>
<td>68</td>
<td>1</td>
<td>0</td>
<td>-3.693211</td>
<td>9.406914</td>
<td>8.420717</td>
</tr>
<tr>
<td>69</td>
<td>6</td>
<td>0</td>
<td>0.831030</td>
<td>8.383828</td>
<td>-1.727803</td>
</tr>
<tr>
<td>70</td>
<td>1</td>
<td>0</td>
<td>0.426455</td>
<td>8.253153</td>
<td>-2.724833</td>
</tr>
<tr>
<td>71</td>
<td>6</td>
<td>0</td>
<td>4.941398</td>
<td>7.891429</td>
<td>8.024585</td>
</tr>
<tr>
<td>72</td>
<td>1</td>
<td>0</td>
<td>5.917732</td>
<td>8.317158</td>
<td>8.226417</td>
</tr>
<tr>
<td>73</td>
<td>6</td>
<td>0</td>
<td>0.826011</td>
<td>2.771481</td>
<td>9.570358</td>
</tr>
<tr>
<td>74</td>
<td>1</td>
<td>0</td>
<td>1.296468</td>
<td>2.502808</td>
<td>10.508975</td>
</tr>
<tr>
<td>75</td>
<td>6</td>
<td>0</td>
<td>6.054129</td>
<td>7.391713</td>
<td>4.467516</td>
</tr>
<tr>
<td>76</td>
<td>1</td>
<td>0</td>
<td>6.358987</td>
<td>7.063601</td>
<td>5.454967</td>
</tr>
<tr>
<td>77</td>
<td>6</td>
<td>0</td>
<td>-1.144156</td>
<td>4.687746</td>
<td>3.180945</td>
</tr>
<tr>
<td>78</td>
<td>1</td>
<td>0</td>
<td>-1.356670</td>
<td>5.489734</td>
<td>3.898660</td>
</tr>
<tr>
<td>79</td>
<td>1</td>
<td>0</td>
<td>-2.085707</td>
<td>4.413337</td>
<td>2.691877</td>
</tr>
<tr>
<td>80</td>
<td>1</td>
<td>0</td>
<td>-0.788316</td>
<td>3.825347</td>
<td>3.743493</td>
</tr>
<tr>
<td>81</td>
<td>6</td>
<td>0</td>
<td>1.094602</td>
<td>4.007417</td>
<td>8.865637</td>
</tr>
<tr>
<td>82</td>
<td>1</td>
<td>0</td>
<td>1.776096</td>
<td>4.690493</td>
<td>9.484658</td>
</tr>
<tr>
<td>83</td>
<td>6</td>
<td>0</td>
<td>-2.797544</td>
<td>8.198586</td>
<td>6.884027</td>
</tr>
<tr>
<td>84</td>
<td>1</td>
<td>0</td>
<td>-3.602473</td>
<td>8.359833</td>
<td>6.176470</td>
</tr>
<tr>
<td>85</td>
<td>6</td>
<td>0</td>
<td>6.968703</td>
<td>7.401237</td>
<td>3.418179</td>
</tr>
<tr>
<td>86</td>
<td>1</td>
<td>0</td>
<td>7.991032</td>
<td>7.081375</td>
<td>3.583677</td>
</tr>
<tr>
<td>87</td>
<td>6</td>
<td>0</td>
<td>2.682882</td>
<td>11.813005</td>
<td>2.083983</td>
</tr>
<tr>
<td>88</td>
<td>1</td>
<td>0</td>
<td>2.642862</td>
<td>11.507558</td>
<td>1.042939</td>
</tr>
<tr>
<td>89</td>
<td>6</td>
<td>0</td>
<td>2.804137</td>
<td>12.638556</td>
<td>4.736505</td>
</tr>
<tr>
<td>90</td>
<td>1</td>
<td>0</td>
<td>2.853139</td>
<td>12.954591</td>
<td>5.772343</td>
</tr>
<tr>
<td>91</td>
<td>6</td>
<td>0</td>
<td>-1.810933</td>
<td>8.580280</td>
<td>9.050898</td>
</tr>
<tr>
<td>92</td>
<td>1</td>
<td>0</td>
<td>-1.847431</td>
<td>9.037758</td>
<td>10.032676</td>
</tr>
<tr>
<td>93</td>
<td>6</td>
<td>0</td>
<td>6.566221</td>
<td>7.828070</td>
<td>2.155594</td>
</tr>
<tr>
<td>94</td>
<td>1</td>
<td>0</td>
<td>7.274775</td>
<td>7.845025</td>
<td>1.353324</td>
</tr>
<tr>
<td>95</td>
<td>6</td>
<td>0</td>
<td>2.922410</td>
<td>13.166085</td>
<td>2.387252</td>
</tr>
<tr>
<td>96</td>
<td>1</td>
<td>0</td>
<td>2.886555</td>
<td>13.895035</td>
<td>1.587349</td>
</tr>
<tr>
<td>97</td>
<td>6</td>
<td>0</td>
<td>4.798349</td>
<td>6.514550</td>
<td>7.877885</td>
</tr>
<tr>
<td>98</td>
<td>1</td>
<td>0</td>
<td>5.660658</td>
<td>5.864193</td>
<td>7.970211</td>
</tr>
</tbody>
</table>
REFERENCES