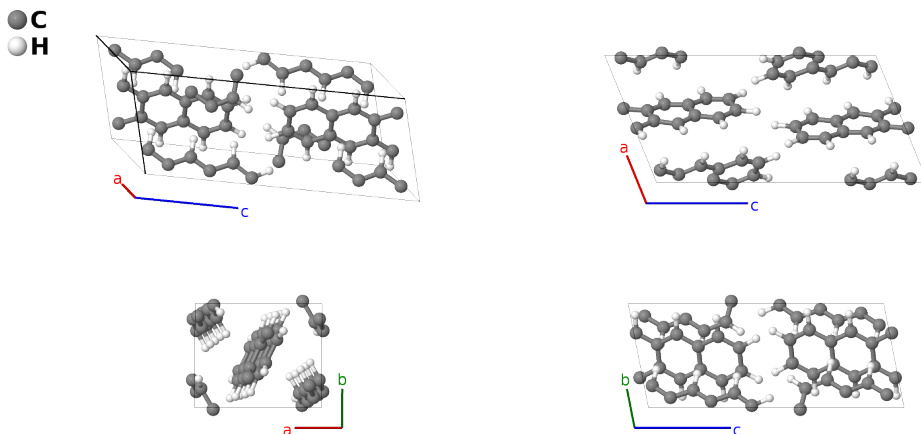


# Pentacene (C<sub>11</sub>H<sub>7</sub>) Structure: A11B7\_aP72\_2\_22i\_14i-001

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<https://aflow.org/p/C9KZ>

[https://aflow.org/p/A11B7\\_aP72\\_2\\_22i\\_14i-001](https://aflow.org/p/A11B7_aP72_2_22i_14i-001)

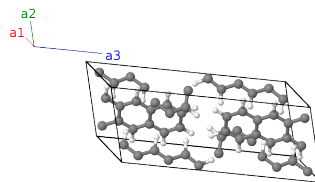


Prototype	C <sub>11</sub> H <sub>7</sub>
AFLOW prototype label	A11B7_aP72_2_22i_14i-001
Mineral name	pentacene
CCDC	1818858
Pearson symbol	aP72
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<pre>aflow --proto=A11B7_aP72_2_22i_14i-001       --params=a,b/a,c/a,α,β,γ,x<sub>1</sub>,y<sub>1</sub>,z<sub>1</sub>,x<sub>2</sub>,y<sub>2</sub>,z<sub>2</sub>,x<sub>3</sub>,y<sub>3</sub>,z<sub>3</sub>,x<sub>4</sub>,y<sub>4</sub>,z<sub>4</sub>,x<sub>5</sub>,y<sub>5</sub>,z<sub>5</sub>,x<sub>6</sub>,y<sub>6</sub>,       z<sub>6</sub>,x<sub>7</sub>,y<sub>7</sub>,z<sub>7</sub>,x<sub>8</sub>,y<sub>8</sub>,z<sub>8</sub>,x<sub>9</sub>,y<sub>9</sub>,z<sub>9</sub>,x<sub>10</sub>,y<sub>10</sub>,z<sub>10</sub>,x<sub>11</sub>,y<sub>11</sub>,z<sub>11</sub>,x<sub>12</sub>,y<sub>12</sub>,z<sub>12</sub>,x<sub>13</sub>,y<sub>13</sub>,z<sub>13</sub>,x<sub>14</sub>,y<sub>14</sub>,z<sub>14</sub>,       x<sub>15</sub>,y<sub>15</sub>,z<sub>15</sub>,x<sub>16</sub>,y<sub>16</sub>,z<sub>16</sub>,x<sub>17</sub>,y<sub>17</sub>,z<sub>17</sub>,x<sub>18</sub>,y<sub>18</sub>,z<sub>18</sub>,x<sub>19</sub>,y<sub>19</sub>,z<sub>19</sub>,x<sub>20</sub>,y<sub>20</sub>,z<sub>20</sub>,x<sub>21</sub>,y<sub>21</sub>,z<sub>21</sub>,x<sub>22</sub>,       y<sub>22</sub>,z<sub>22</sub>,x<sub>23</sub>,y<sub>23</sub>,z<sub>23</sub>,x<sub>24</sub>,y<sub>24</sub>,z<sub>24</sub>,x<sub>25</sub>,y<sub>25</sub>,z<sub>25</sub>,x<sub>26</sub>,y<sub>26</sub>,z<sub>26</sub>,x<sub>27</sub>,y<sub>27</sub>,z<sub>27</sub>,x<sub>28</sub>,y<sub>28</sub>,z<sub>28</sub>,x<sub>29</sub>,y<sub>29</sub>,       z<sub>29</sub>,x<sub>30</sub>,y<sub>30</sub>,z<sub>30</sub>,x<sub>31</sub>,y<sub>31</sub>,z<sub>31</sub>,x<sub>32</sub>,y<sub>32</sub>,z<sub>32</sub>,x<sub>33</sub>,y<sub>33</sub>,z<sub>33</sub>,x<sub>34</sub>,y<sub>34</sub>,z<sub>34</sub>,x<sub>35</sub>,y<sub>35</sub>,z<sub>35</sub>,x<sub>36</sub>,y<sub>36</sub>,z<sub>36</sub></pre>

- The CCSD entry has a CIF with the lattice constants but no atomic positions.

## Triclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
 c_x &= c \cos \beta \\
 c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
 c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
 \end{aligned}$$



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**Basis vectors**

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(2i)	C I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} - (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} - c_z z_1 \hat{\mathbf{z}}$	(2i)	C I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(2i)	C II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} - (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} - c_z z_2 \hat{\mathbf{z}}$	(2i)	C II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(2i)	C III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$	(2i)	C III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(2i)	C IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$	(2i)	C IV
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(2i)	C V
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$	(2i)	C V
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(2i)	C VI
$\mathbf{B}_{12}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$	(2i)	C VI
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(2i)	C VII
$\mathbf{B}_{14}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}}$	(2i)	C VII
$\mathbf{B}_{15}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(2i)	C VIII
$\mathbf{B}_{16}$	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}}$	(2i)	C VIII
$\mathbf{B}_{17}$	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$	(2i)	C IX
$\mathbf{B}_{18}$	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} - (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} - c_z z_9 \hat{\mathbf{z}}$	(2i)	C IX
$\mathbf{B}_{19}$	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}}$	(2i)	C X
$\mathbf{B}_{20}$	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} - (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} - c_z z_{10} \hat{\mathbf{z}}$	(2i)	C X
$\mathbf{B}_{21}$	$= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} + (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} + c_z z_{11} \hat{\mathbf{z}}$	(2i)	C XI
$\mathbf{B}_{22}$	$= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} - (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} - c_z z_{11} \hat{\mathbf{z}}$	(2i)	C XI





$$\begin{aligned}
\mathbf{B}_{71} &= x_{36} \mathbf{a}_1 + y_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3 &= (ax_{36} + by_{36} \cos \gamma + c_x z_{36}) \hat{\mathbf{x}} + & (2i) & \text{H XIV} \\
&&& (by_{36} \sin \gamma + c_y z_{36}) \hat{\mathbf{y}} + c_z z_{36} \hat{\mathbf{z}} \\
\mathbf{B}_{72} &= -x_{36} \mathbf{a}_1 - y_{36} \mathbf{a}_2 - z_{36} \mathbf{a}_3 &= -(ax_{36} + by_{36} \cos \gamma + c_x z_{36}) \hat{\mathbf{x}} - & (2i) & \text{H XIV} \\
&&& (by_{36} \sin \gamma + c_y z_{36}) \hat{\mathbf{y}} - c_z z_{36} \hat{\mathbf{z}}
\end{aligned}$$

## References

- [1] R. B. Campbell, J. M. Robertson, and J. Trotter, *The Crystal and Molecular Structure of Pentacene*, *Acta Cryst.* **14**, 705–711 (1961), doi:10.1107/S0365110X61002163.