

Identification Code	A	B(1)	B(2)
CCDC	1504948	1446763	1510071
Empirical formula	C <sub>10</sub> H <sub>6</sub> Br N O <sub>2</sub>	C <sub>10</sub> H <sub>7</sub> NO <sub>2</sub>	C <sub>10</sub> H <sub>7</sub> N O <sub>2</sub>
Formula weight	252.07	173.17	173.17
Temperature	273(2) K	296(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	1.54178 Å
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>C</i>	<i>P</i> 2 <sub>1</sub> / <i>C</i>	<i>P</i> 2 <sub>1</sub> / <i>C</i>
Unit cell dimensions	a = 15.2305(14) Å b = 3.9184(4) Å, β = 110.700(3)° c = 15.9439(14) Å	a = 14.6144(9) Å b = 3.9568(2) Å β = 108.336(5)° c = 14.726(3) Å	a = 14.5758(6) Å b = 3.8648(2) Å β = 108.5550(10)° c = 14.6609(6) Å
Volume	890.09(15) Å <sup>3</sup>	808.30(17) Å <sup>3</sup>	782.96(6) Å <sup>3</sup>
Z	4	4	4
Density (calculated)	1.881 Mg/m <sup>3</sup>	1.423 Mg/m <sup>3</sup>	1.469 Mg/m <sup>3</sup>
Absorption coefficient	4.585 mm <sup>-1</sup>	0.101 mm <sup>-1</sup>	0.861 mm <sup>-1</sup>
F(000)	496	360	360
Crystal size	0.24 × 0.18 × 0.14 mm <sup>3</sup>	0.319 × 0.287 × 0.241 mm <sup>3</sup>	0.421 × 0.285 × 0.071 mm <sup>3</sup>
Theta range for data collection	2.86 to 24.98°	2.821 to 28.439°	6.150 to 68.276°
Index ranges	-18 ≤ h ≤ 18, -4 ≤ k ≤ 4, -18 ≤ l ≤ 14	-19 ≤ h ≤ 19, -5 ≤ k ≤ 5, -19 ≤ l ≤ 19	-17 ≤ h ≤ 17, -4 ≤ k ≤ 4, -17 ≤ l ≤ 17
Reflections collected	5752	14289	4266
Independent reflections	1532 [R(int) = 0.0861]	2020 [R(int) = 0.1340]	1341 [R(int) = 0.0254]
Completeness to theta = 24.98°	97.1 %	99.9%	93.4 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.5661 and 0.4058	-	0.941 and 0.745
Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	1532 / 0 / 127	2020 / 0 / 119	1341 / 0 / 118
Goodness-of-fit on F <sup>2</sup>	1.122	1.003	1.042
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0617, wR <sub>2</sub> = 0.1515	R <sub>1</sub> = 0.0726, wR <sub>2</sub> = 0.1125	R <sub>1</sub> = 0.0381, wR <sub>2</sub> = 0.1017

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### **Table of Contents Crystal Structure Data Of Inor Volume Pt B**

1. Understanding the eBook Crystal Structure Data Of Inor Volume Pt B
  - The Rise of Digital Reading Crystal Structure Data Of Inor Volume Pt B
  - Advantages of eBooks Over Traditional Books
2. Identifying Crystal Structure Data Of Inor Volume Pt B
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Crystal Structure Data Of Inor Volume Pt B
  - User-Friendly Interface
4. Exploring eBook Recommendations from Crystal Structure Data Of Inor Volume Pt B
  - Personalized Recommendations

- Crystal Structure Data Of Inor Volume Pt B User Reviews and Ratings
- Crystal Structure Data Of Inor Volume Pt B and Bestseller Lists
- 5. Accessing Crystal Structure Data Of Inor Volume Pt B Free and Paid eBooks
  - Crystal Structure Data Of Inor Volume Pt B Public Domain eBooks
  - Crystal Structure Data Of Inor Volume Pt B eBook Subscription Services
  - Crystal Structure Data Of Inor Volume Pt B Budget-Friendly Options
- 6. Navigating Crystal Structure Data Of Inor Volume Pt B eBook Formats
  - ePub, PDF, MOBI, and More
  - Crystal Structure Data Of Inor Volume Pt B Compatibility with Devices
  - Crystal Structure Data Of Inor Volume Pt B Enhanced eBook Features
- 7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Crystal Structure Data Of Inor Volume Pt B
  - Highlighting and Note-Taking Crystal Structure Data Of Inor Volume Pt B
  - Interactive Elements Crystal Structure Data Of Inor Volume Pt B
- 8. Staying Engaged with Crystal Structure Data Of Inor Volume Pt B
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Crystal Structure Data Of Inor Volume Pt B
- 9. Balancing eBooks and Physical Books Crystal Structure Data Of Inor Volume Pt B
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Crystal Structure Data Of Inor Volume Pt B
- 10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
- 11. Cultivating a Reading Routine Crystal Structure Data Of Inor Volume Pt B
  - Setting Reading Goals Crystal Structure Data Of Inor Volume Pt B
  - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Crystal Structure Data Of Inor Volume Pt B
  - Fact-Checking eBook Content of Crystal Structure Data Of Inor Volume Pt B

- Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
  - Utilizing eBooks for Skill Development
  - Exploring Educational eBooks
- 14. Embracing eBook Trends
  - Integration of Multimedia Elements
  - Interactive and Gamified eBooks

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