

## 基于 Lewis 酸-碱作用合成“看得见”的 B←N 键配位化合物在实验教学中的设计与探索

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## Designing and Exploring “Visible” B←N Bond Coordination Compounds Based on Lewis Acid-Base Interaction in Laboratory Teaching

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表S1 配合物1–5的晶体学数据与精修参数

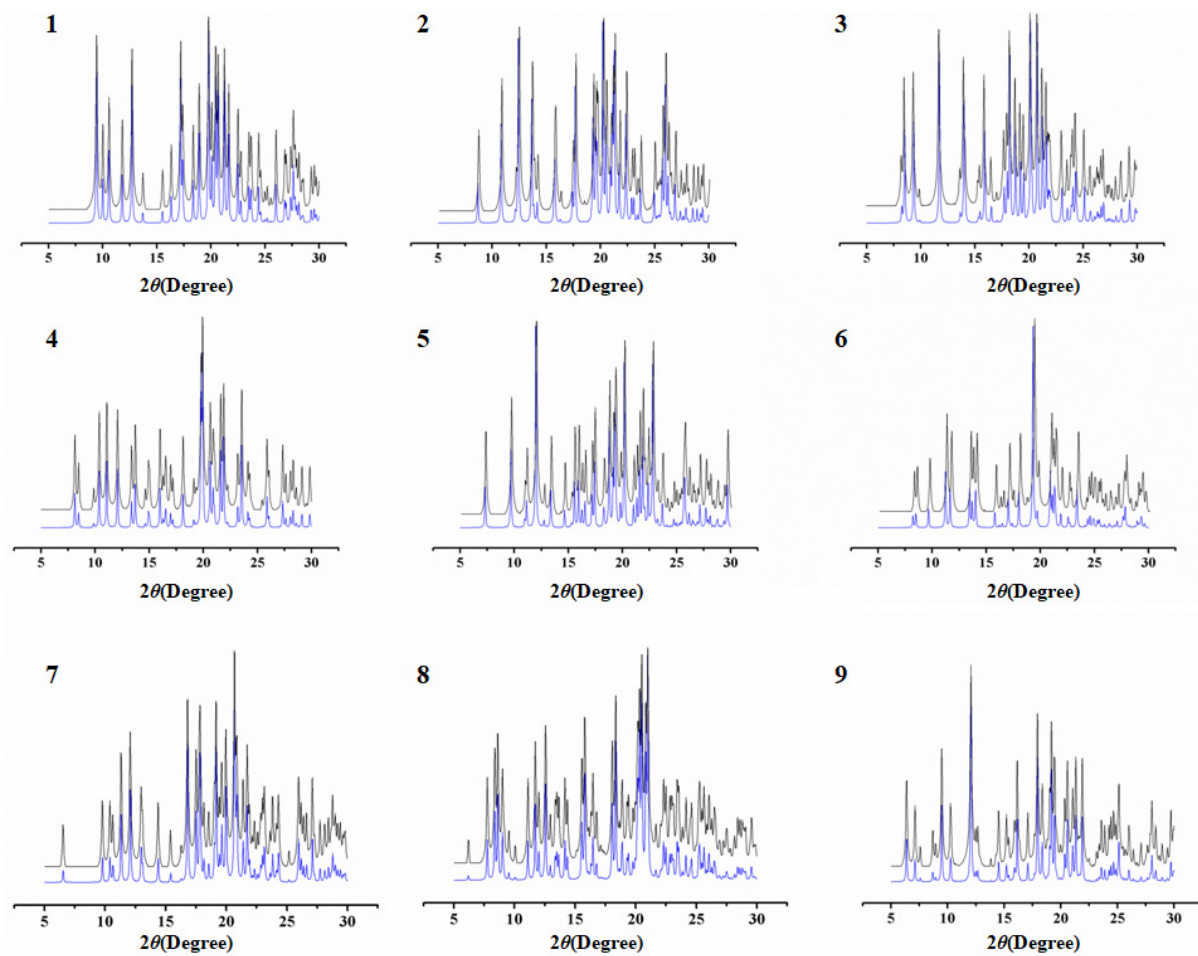
| 晶体参数                                               | 1                                  | 2                                                             | 3                                                                            | 4                                                                            | 5                                                             |
|----------------------------------------------------|------------------------------------|---------------------------------------------------------------|------------------------------------------------------------------------------|------------------------------------------------------------------------------|---------------------------------------------------------------|
| 分子式                                                | C <sub>11</sub> H <sub>10</sub> BN | C <sub>48</sub> H <sub>42</sub> B <sub>2</sub> N <sub>2</sub> | C <sub>56</sub> H <sub>50</sub> B <sub>2</sub> N <sub>2</sub> O <sub>2</sub> | C <sub>54</sub> H <sub>46</sub> B <sub>2</sub> N <sub>2</sub> O <sub>2</sub> | C <sub>58</sub> H <sub>46</sub> B <sub>2</sub> N <sub>2</sub> |
| 分子量                                                | 153.00                             | 668.45                                                        | 804.60                                                                       | 776.55                                                                       | 792.59                                                        |
| 测试温度/K                                             | 293(2)                             | 293(2)                                                        | 293(2)                                                                       | 293(2)                                                                       | 293(2)                                                        |
| 晶系                                                 | Triclinic                          | Monoclinic                                                    | Triclinic                                                                    | Triclinic                                                                    | Monoclinic                                                    |
| 空间群                                                | <i>P</i> -1                        | <i>P</i> 2 <sub>1</sub> / <i>n</i>                            | <i>P</i> -1                                                                  | <i>P</i> -1                                                                  | <i>P</i> 2 <sub>1</sub> / <i>n</i>                            |
| <i>a</i> /Å                                        | 9.739(2)                           | 8.9310(2)                                                     | 9.1189(6)                                                                    | 9.0011(5)                                                                    | 7.52367(17)                                                   |
| <i>b</i> /Å                                        | 10.0341(18)                        | 14.5678(3)                                                    | 11.2873(5)                                                                   | 10.9920(6)                                                                   | 18.2449(6)                                                    |
| <i>c</i> /Å                                        | 10.3005(19)                        | 14.4739(4)                                                    | 11.6683(6)                                                                   | 11.7998(6)                                                                   | 16.1724(4)                                                    |
| <i>α</i> (°)                                       | 65.934(18)                         | 90                                                            | 110.972(5)                                                                   | 104.599(3)                                                                   | 90                                                            |
| <i>β</i> (°)                                       | 86.710(16)                         | 100.585(2)                                                    | 97.189(5)                                                                    | 105.261(3)                                                                   | 94.304(3)                                                     |
| <i>γ</i> (°)                                       | 74.702(17)                         | 90                                                            | 96.445(4)                                                                    | 96.532(3)                                                                    | 90                                                            |
| <i>V</i> /Å <sup>3</sup>                           | 885.1(3)                           | 1851.07(7)                                                    | 1096.52(11)                                                                  | 1069.47(10)                                                                  | 2213.69(11)                                                   |
| <i>Z</i>                                           | 4                                  | 2                                                             | 1                                                                            | 1                                                                            | 2                                                             |
| $\rho_{\text{calc}}/(\text{g}\cdot\text{cm}^{-3})$ | 1.148                              | 1.199                                                         | 1.218                                                                        | 1.206                                                                        | 1.189                                                         |

表S2 配合物6–9的晶体学数据与精修参数

| 晶体参数                                               | 6                                                             | 7                                                             | 8                                                             | 9                                                             |
|----------------------------------------------------|---------------------------------------------------------------|---------------------------------------------------------------|---------------------------------------------------------------|---------------------------------------------------------------|
| 分子式                                                | C <sub>60</sub> H <sub>46</sub> B <sub>2</sub> N <sub>2</sub> | C <sub>64</sub> H <sub>50</sub> B <sub>2</sub> N <sub>2</sub> | C <sub>75</sub> H <sub>60</sub> B <sub>3</sub> N <sub>3</sub> | C <sub>98</sub> H <sub>78</sub> B <sub>4</sub> N <sub>4</sub> |
| 分子量                                                | 816.61                                                        | 868.6                                                         | 1035.69                                                       | 1354.88                                                       |
| 测试温度/K                                             | 293(2)                                                        | 293(2)                                                        | 293(2)                                                        | 293(2)                                                        |
| 晶系                                                 | Triclinic                                                     | Triclinic                                                     | Monoclinic                                                    | Monoclinic                                                    |
| 空间群                                                | <i>P</i> -1                                                   | <i>P</i> -1                                                   | <i>P</i> 2 <sub>1</sub> / <i>n</i>                            | <i>P</i> 2 <sub>1</sub> / <i>n</i>                            |
| <i>a</i> /Å                                        | 9.4405(4)                                                     | 9.5810(4)                                                     | 21.1712(4)                                                    | 17.8358(11)                                                   |
| <i>b</i> /Å                                        | 11.1257(5)                                                    | 10.2357(5)                                                    | 19.3308(3)                                                    | 23.2967(14)                                                   |
| <i>c</i> /Å                                        | 11.5880(4)                                                    | 13.9200(7)                                                    | 14.1400(2)                                                    | 19.2818(12)                                                   |
| <i>α</i> (°)                                       | 108.102(4)                                                    | 101.144(3)                                                    | 90                                                            | 90                                                            |
| <i>β</i> (°)                                       | 99.904(3)                                                     | 93.004(2)                                                     | 93.788(2)                                                     | 104.791(2)                                                    |
| <i>γ</i> (°)                                       | 96.679(4)                                                     | 114.700(2)                                                    | 90                                                            | 90                                                            |
| <i>V</i> /Å <sup>3</sup>                           | 1120.75(8)                                                    | 1203.17(10)                                                   | 5774.24(16)                                                   | 9367.5(2)                                                     |
| <i>Z</i>                                           | 1                                                             | 1                                                             | 4                                                             | 4                                                             |
| $\rho_{\text{calc}}/(\text{g}\cdot\text{cm}^{-3})$ | 1.210                                                         | 1.199                                                         | 1.191                                                         | 1.162                                                         |

表S3 化合物1–9的B←N键长(Å)

|   |       |            |   |       |            |
|---|-------|------------|---|-------|------------|
| 1 | N1—B1 | 1.661(5)   | 7 | N1—B1 | 1.6555(17) |
| 2 | N1—B1 | 1.6524(19) | 8 | N1—B3 | 1.649(2)   |
| 3 | N1—B1 | 1.662(2)   |   | N3—B1 | 1.657(3)   |
| 4 | N1—B1 | 1.660(4)   |   | N2—B2 | 1.650(3)   |
| 5 | N1—B1 | 1.651(2)   | 9 | N1—B1 | 1.659(4)   |
| 6 | N1—B1 | 1.6662(15) |   | N2—B3 | 1.661(4)   |



图S1 化合物1-9的XRPD图

蓝色：模拟曲线；黑色：测试曲线