

Figure S7. The X-ray structure of 13c (CCDC: 2446154, 50% probability thermal ellipsoids)

|  |  |
| --- | --- |
| **Table S1 Crystal data and structure refinement for 20250422LYJ-31837-1\_auto.** | |
| Identification code | 20250422LYJ-31837-1\_auto |
| Empirical formula | C10H9Br4NO2 |
| Formula weight | 494.82 |
| Temperature/K | 100.00(10) |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 13.62980(10) |
| b/Å | 25.7396(2) |
| c/Å | 8.33400(10) |
| α/° | 90 |
| β/° | 95.7650(10) |
| γ/° | 90 |
| Volume/Å3 | 2908.99(5) |
| Z | 8 |
| ρcalcg/cm3 | 2.260 |
| μ/mm‑1 | 13.444 |
| F(000) | 1856.0 |
| Crystal size/mm3 | 0.14 × 0.12 × 0.1 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 6.518 to 151.686 |
| Index ranges | -17 ≤ h ≤ 16, -31 ≤ k ≤ 31, -6 ≤ l ≤ 10 |
| Reflections collected | 21226 |
| Independent reflections | 5742 [Rint = 0.0292, Rsigma = 0.0199] |
| Data/restraints/parameters | 5742/0/315 |
| Goodness-of-fit on F2 | 1.049 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0313, wR2 = 0.0850 |
| Final R indexes [all data] | R1 = 0.0330, wR2 = 0.0862 |
| Largest diff. peak/hole / e Å-3 | 1.59/-1.07 |

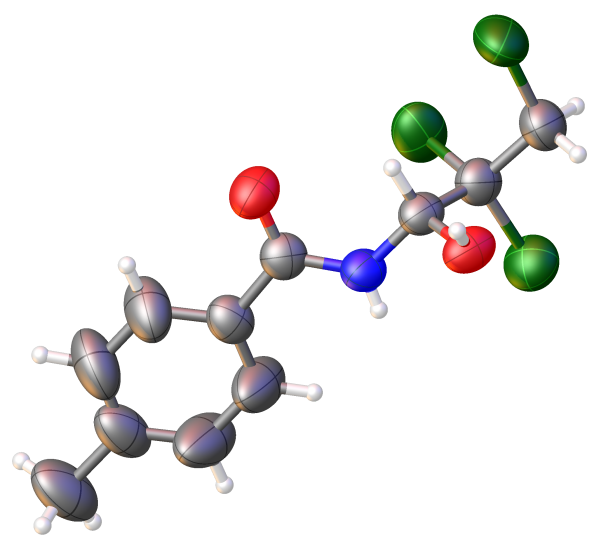


Figure S7. The X-ray structure of 13c (CCDC: 2442144, 50% probability thermal ellipsoids)

|  |  |
| --- | --- |
| **Table S1 Crystal data and structure refinement for t.** | |
| Identification code | t |
| Empirical formula | C11H12Cl3O2N |
| Formula weight | 296.57 |
| Temperature/K | 298(2) |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 6.8567(3) |
| b/Å | 10.4133(4) |
| c/Å | 11.2353(4) |
| α/° | 116.575(4) |
| β/° | 98.166(3) |
| γ/° | 99.590(3) |
| Volume/Å3 | 685.76(5) |
| Z | 2 |
| ρcalcg/cm3 | 1.436 |
| μ/mm‑1 | 5.978 |
| F(000) | 304.0 |
| Crystal size/mm3 | 0.15 × 0.14 × 0.12 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 9.078 to 155.008 |
| Index ranges | -8 ≤ h ≤ 7, -12 ≤ k ≤ 13, -13 ≤ l ≤ 14 |
| Reflections collected | 8303 |
| Independent reflections | 2756 [Rint = 0.0217, Rsigma = 0.0168] |
| Data/restraints/parameters | 2756/0/160 |
| Goodness-of-fit on F2 | 1.083 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0516, wR2 = 0.1511 |
| Final R indexes [all data] | R1 = 0.0551, wR2 = 0.1543 |
| Largest diff. peak/hole / e Å-3 | 0.35/-0.34 |