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# CRYSTAL PARAMETERS OF NONLINEAR OPTICAL MATERIALS

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## Abstract

The structure is governed by ch arge-assisted $N^{+}$–H•••Cl cation-anion hydrogen bonds that permit alternation between organic/inorganic layers[1]. The intermolecular interactions were investigated using Hirshfeld surface analysis[2-3]. The thermal behavior of (I) was also discussed using TGA/DTA, which showed the thermal stability of the compound up to 190°C. The DFT calculations have been performed using the B3LYP method at the LANL2DZ level. For the new hybrid compound, we have also measured the value of the electronic part of the third-order nonlinear optical susceptibility using the third harmonic generation (THG) method at 1064 nm[4-5].

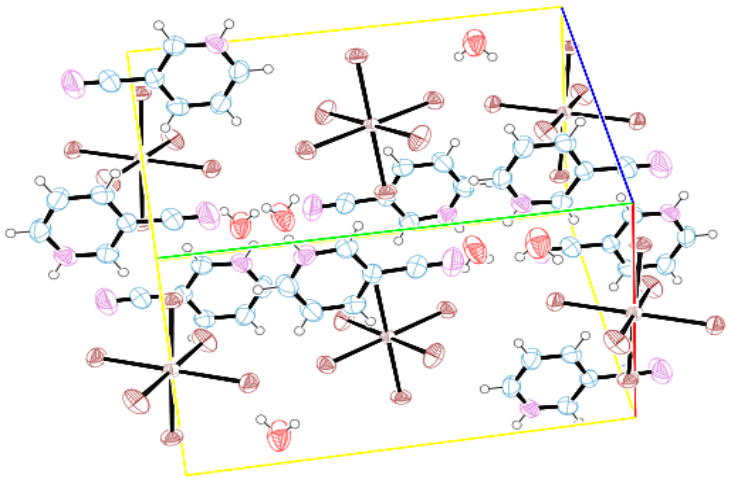

Fig-1. ORTEP-crystal packing drawing of the intermolecular H-bonds and (b) Nonlinear optical (NLO) materials. molecule. Thermal ellipsoids are drawn with the 50% probability level.

**Table -1. Crystal data and structure refinement for $Br_6\,Sn\,(C_6\,H_5N_2)_2\,(H_2O)_2$**

| | |
|---|---|
| Identification code | El-01 |
| Empirical formula | $Br_6\,Sn\,(C_6\,H_5N_2)_2\,(H_2O)_2$ |
| Formula weight ; Temperature/K | 844.22; 107(5) |
| Crystal system | Monoclinic |
| Space group | Pn |
| a/Å ; b/Å ; c/Å | 12.70250(10); 9.45940(10) ;19.25390(10) |
| α/° ; β/° ; γ/° | 90; 92.3510(10) ; 90 |
| Volume/$Å^3$; Z; $\rho_{calc}g/cm^3$ | 2311.56(3) ; 2; 1.487 |
| $\mu/mm^{-1}$ ; F(000) ; Crystal size/$mm^3$ | 11.216; 1060.0; 0.14 × 0.12 × 0.11 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 4.594 to 143.192 |
| Index ranges | $-15 \le h \le 15$, $-11 \le k \le 11$, $-23 \le l \le 23$ |
| Reflections collected | 45306 |
| Independent reflections | 8957 [$R_{int}$ = 0.0551, $R_{sigma}$ = 0.0348] |
| Data/restraints/parameters | 8957/2/520 |
| Goodness-of-fit on $F^2$ | 1.040 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0299, $wR_2$ = 0.0788 |
| Final R indexes [all data] | $R_1$ = 0.0299, $wR_2$ = 0.0788 |
| Largest diff. peak/hole / e $Å^{-3}$ | 1.36/-1.55 |

**Table-3. Bond Distances $Br_6 Sn (C_6 H_5N_2)_2 (H_2O)_2$ ($A^0$). R = 0.03**

| Bond | Distances | Bond | Distances |
|---|---|---|---|
| O(007) –C(00Q) | 1.416(7) | O(00N)–H(G) | 0.87(8) |
| O(007) –C(01G) | 1.440(7) | O(00N)–H(00) | 0.77(8) |
| O(00E)–C(014) | 1.428(7) | N(00D)–C(016) | 1.499(6) |
| O(00E)–C(015) | 1.412(8) | N(00M) –C(01E) | 1.340(7) |
| O(00G) –C(00Y) | 1.429(7) | N(00M)–C(00J) | 1.331(8) |
| O(005)–C(01D) | 1.435(7) | C(00Q) –C(00S) | 1.489(8) |
| O(005)–C(010) | 1.438(7) | C(00Y)–C(018) | 1.507(8) |
| O(006)–C(00W) | 1.424(7) | C(012)–C(015) | 1.501(8) |
| O(006)–C(00O) | 1.403(7) | C(014)–C(01J) | 1.489(9) |
| C(01J) –H(01R) | 0.9900 | C(01K)–H(3) | 0.9500 |
| C(010)–C(01C) | 1.497(9) | C(00P)–C(00T) | 1.503(7) |

**Table-4. Bond Angles. ($A^0$). R = 0.03**

| Bond | Bond Angles | Bond | Bond Angles |
|---|---|---|---|
| C(00P) –N(00F)–H(00L) | 109.00 | H(00A) –C(00Q) –H(00B) | 108.00 |
| C(00P)–N(00F)–H(00M) | 109.00 | H(00C) –C(00S) –H(00D) | 108.00 |
| C(00Y)–C(018)–H(01G) | 110.00 | O(00A) –C(00X) –C(013) | 108.9(5) |
| H(01I)–C(01A)–H(01J) | 108.00 | O(005) –C(010) –C(01C) | 109.3(5) |
| O(00C)–C(013)–H(01X) | 110.00 | O(009) –C(01K) –H(3) | 126.00 |
| H(01W)–C(013)–H(01X) | 108.00 | N(00B) –C(00H) –C(00T) | 123.5(4) |
| O(00I)–C(017)–H(B) | 110.00 | C(00T) –C(00L) –C(00V) | 118.5(5) |
| N(00F)–C(00P)–C(00T) | 112.9(4) | C(016)–C(00R) –C(01B) | 121.3(5) |
| C(00H)–C(00T)–C(00P) | 120.6(4) | C(016) –C(00R) –C(01E) | 120.3(4) |
| C(00L)–C(00T)–C(00P) | 121.1(4) | C(01B) –C(00R) –C(01E) | 118.4(5) |
| C(00H) –C(00T) –C(00L) | 118.2(4) | C(00J) –C(00Z) –C(01B) | 118.2(5) |
| N(00B)–C(00U)–C(00V) | 123.5(5) | N(00D) –C(016) –C(00R) | 112.5(4) |
| C(00L)–C(00V)–C(00U) | 119.3(5) | C(00R) –C(01B) –C(00Z) | 118.9(5) |
| N(00B) –C(00H) –H(00N) | 118.00 | N(00M) –C(01E)–C(00R) | 122.9(5) |
| C(00T) –C(00H) –H(00N) | 118.00 | C(00Z) –C(00J) –H(00X) | 118.00 |

The percent elemental composition of compound 1,4,7,10,13,16-hexaoxacyclooctadecane, pyridin-3-ylmethanaminium salt was determined using a Thermo Scientific FlashSmart (CHNS/O) elemental analyzer. This analysis was performed by gas chromatographic separation of combustion gases based on the modified Dumas method.In order to assess the accuracy of the measurements, the

results obtained from the analysis were compared in practical and theoretical terms. Table-5.

**References**

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