Supplementary Material for

New organic–inorganic bromide $(P(C_4H_9)_4)_2[ZnBr_4]$: Crystal Structure, Vibrational Properties, and Electrical Conduction Behavior from Impedance Studies

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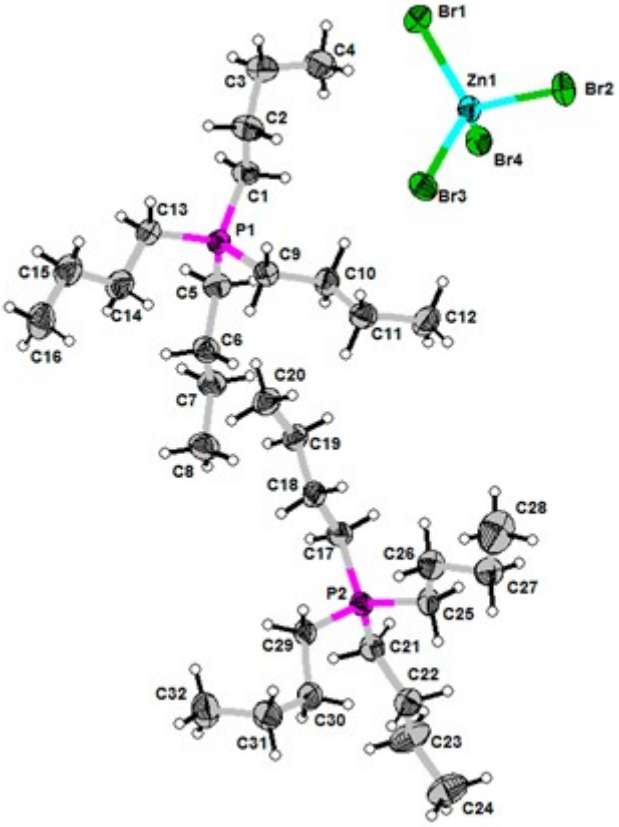

Figure.S1: The asymmetric unit of $(P(C_4H_9)_4)_2[ZnBr_4]$. Displacement ellipsoids are drawn at the 50 % probability level.

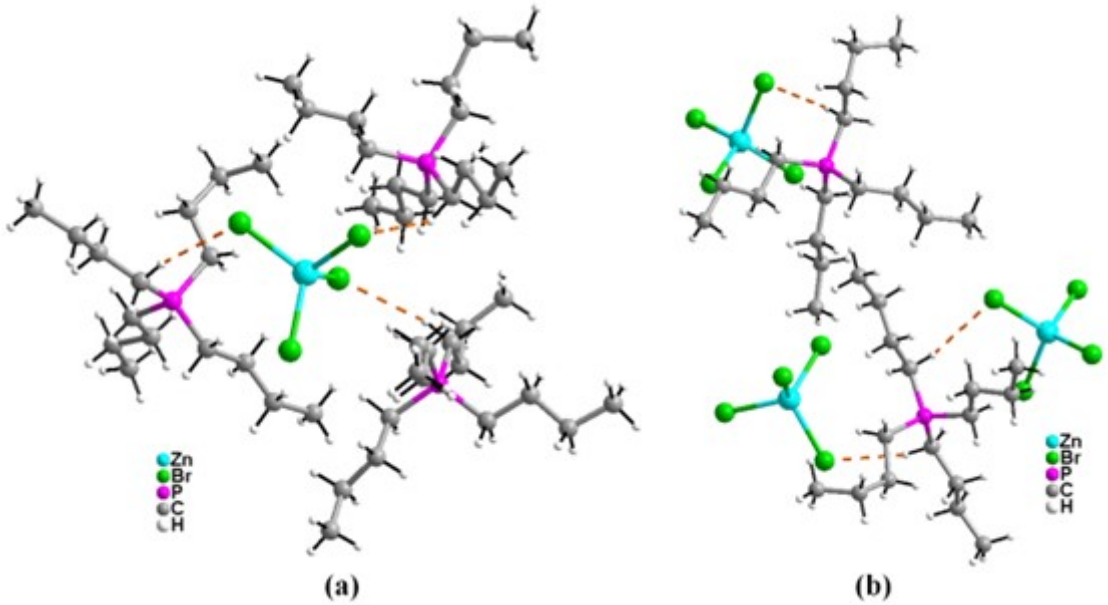

Figure.S2: Hydrogen bonds established by **(a)** the $[ZnBr_4]^{2-}$ tetrahedron and **(b)** the $(P(C_4H_9)_4)^+$ organic cations in $(P(C_4H_9)_4)_2[ZnBr_4]$.

Table.S1. Crystallographic data and structure refinements of $(P(C_4H_9)_4)_2[ZnBr_4]$.

Formula	**$(P(C_4H_9)_4)_2[ZnBr_4]$**
Color/Shape	Colorless/plate
Formula weight ($gmol^{-1}$)	903.84
Crystal system	Monoclinic
Space group	$P2_1/c$
Density	1.436
Crystal size (mm)	0.147x0.097x0.081
Diffractometer	Bruker D8 VENTURE PHOTON III-14
a (Å)	15.3260(11)
b (Å)	17.6692(13)
c(Å)	16.9898(11)
β(°)	114.715(2)
V ($Å^3$)	4179.4(5)
Z	4
Radiation type	Mo-Kα radiation
Absorption Correction	Multi-scan
θ range for data collection(°)	2.30-26.37
Measured reflections	208756
Independent reflections	8537
Observed data [I > 2σ (I)]	7679
Index ranges	h = −19→19 k = −22→22 l = −21→21
F(000)	1856
Number of parameters	361
R_1	0.0271
wR_2	0.0678
Goof	1.038

Table.S2. Fractional atomic coordinates and equivalent isotropic temperature factors (Å2).

	x	*y*	*z*	U_{eq}
Zn1	0.65420(2)	0.15810(2)	0.37603(2)	0.02149(7)
Br1	0.78652(2)	0.09569(2)	0.49072(2)	0.03014(7)
Br2	0.61901(2)	0.08458(2)	0.24643(2)	0.02798(7)
Br3	0.51168(2)	0.17458(2)	0.40180(2)	0.02755(7)
Br4	0.70834(2)	0.28467(2)	0.35883(2)	0.02589(7)
P1	0.40297(4)	0.16711(4)	0.66137(4)	0.01925(13)
C1	0.50930(18)	0.12964(14)	0.65638(17)	0.0227(5)
C2	0.52069(19)	0.04391(15)	0.66919(19)	0.0279(6)
C3	0.61885(19)	0.01754(16)	0.67799(19)	0.0292(6)
C4	0.6344(2)	0.02937(18)	0.5974(2)	0.0358(7)
C5	0.40778(18)	0.26817(14)	0.65052(17)	0.0231(5)
C6	0.31632(19)	0.31142(14)	0.63607(17)	0.0245(5)
C7	0.3250(2)	0.39445(15)	0.61801(18)	0.0266(5)
C8	0.2326(2)	0.43819(16)	0.59941(19)	0.0317(6)
C9	0.29741(17)	0.12948(14)	0.57376(15)	0.0214(5)
C10	0.29277(18)	0.14800(16)	0.48376(16)	0.0247(5)
C11	0.19686(19)	0.12372(16)	0.41237(17)	0.0269(5)
C12	0.1923(2)	0.13596(17)	0.32165(17)	0.0341(6)
C13	0.40190(19)	0.14032(16)	0.76324(16)	0.0253(5)
C14	0.3132(2)	0.16019(17)	0.77735(18)	0.0299(6)
C15	0.3090(2)	0.1207(2)	0.85428(19)	0.0370(7)
C16	0.2194(2)	0.1357(2)	0.86711(19)	0.0368(7)
P2	0.17350(5)	0.73170(4)	0.32028(4)	0.01961(13)
C17	0.29628(18)	0.70601(14)	0.38587(16)	0.0229(5)
C18	0.31002(18)	0.63184(14)	0.43629(16)	0.0229(5)
C19	0.41551(18)	0.61586(14)	0.49224(16)	0.0239(5)
C20	0.4270(2)	0.54459(15)	0.54598(17)	0.0275(6)
C21	0.17462(19)	0.82967(14)	0.29143(16)	0.0228(5)
C22	0.08710(19)	0.85981(15)	0.21422(17)	0.0258(5)
C23	0.0951(2)	0.94384(17)	0.2022(2)	0.0393(7)
C24	0.0124(2)	0.97585(19)	0.1238(2)	0.0424(8)
C25	0.12101(19)	0.67718(14)	0.22123(16)	0.0228(5)
C26	0.1159(2)	0.59156(15)	0.22873(17)	0.0275(6)
C27	0.0631(2)	0.55536(15)	0.14013(18)	0.0280(6)
C28	0.0631(3)	0.46992(19)	0.1424(2)	0.0542(10)
C29	0.10507(18)	0.71861(14)	0.38435(16)	0.0226(5)
C30	0.00627(19)	0.75490(16)	0.34704(17)	0.0267(5)
C31	-0.0544(2)	0.72982(17)	0.39473(18)	0.0307(6)
C32	-0.0149(2)	0.7555(2)	0.48794(19)	0.0386(7)

Table.S3. Selected bond distances (Å) and angles (°).

Distances (Å)		**Angles (°)**	
Zn1-Br1	2.4127(4)	Br1-Zn1-Br2	106.402(15)

Zn1-Br2	2.4152(4)	Br1-Zn1-Br3	115.254(15)
Zn1-Br3	2.4181(4)	Br2-Zn1-Br3	110.828(15)
Zn1-Br4	2.4450(4)	Br1-Zn1-Br4	107.574(15)
P1-C1	1.793(3)	Br2-Zn1-Br4	109.913(14)
P1-C5	1.800(3)	Br3-Zn1-Br4	106.787(14)
P1-C13	1.801(3)	C1-P1-C5	106.52(12)
P1-C9	1.806(2)	C1-P1-C13	108.78(12)
C1-C2	1.530(4)	C5-P1-C13	112.12(13)
C2-C3	1.521(4)	C1-P1-C9	110.10(12)
C3-C4	1.500(4)	C5-P1-C9	109.99(12)
C5-C6	1.524(3)	C13-P1-C9	109.29(12)
C6-C7	1.516(4)	C2-C1-P1	114.25(18)
C7-C8	1.526(4)	C3-C2-C1	111.5(2)
C9-C10	1.536(3)	C4-C3-C2	113.3(2)
C10-C11	1.525(3)	C6-C5-P1	116.09(18)
C11-C12	1.529(4)	C7-C6-C5	111.4(2)
C13-C14	1.517(4)	C6-C7-C8	112.3(2)
C14-C15	1.507(4)	C10-C9-P1	113.25(17)
C15-C16	1.502(4)	C11-C10-C9	111.1(2)
P2-C17	1.799(3)	C10-C11-C12	112.6(2)
P2-C21	1.801(3)	C14-C13-P1	117.37(18)
P2-C25	1.810(2)	C15-C14-C13	113.3(2)
P2-C29	1.815(3)	C16-C15-C14	114.7(2)
C17-C18	1.531(3)	C17-P2-C21	106.53(12)
C18-C19	1.521(3)	C17-P2-C25	112.64(12)
C19-C20	1.522(3)	C21-P2-C25	108.04(12)
C21-C22	1.527(4)	C17-P2-C29	108.27(12)
C22-C23	1.511(4)	C21-P2-C29	111.06(12)
C23-C24	1.513(4)	C25-P2-C29	110.26(12)
C25-C26	1.523(4)	C18-C17-P2	115.22(18)
C26-C27	1.520(4)	C19-C18-C17	111.7(2)
C27-C28	1.510(4)	C18-C19-C20	110.8(2)
C29-C30	1.518(4)	C22-C21-P2	117.65(18)
C30-C31	1.531(4)	C23-C22-C21	111.5(2)
C31-C32	1.510(4)	C22-C23-C24	113.6(3)
		C26-C25-P2	117.99(18)
		C27-C26-C25	111.1(2)
		C28-C27-C26	113.6(2)
		C30-C29-P2	114.93(17)
		C29-C30-C31	112.1(2)
		C32-C31-C30	113.7(2)

Table.S4. C-H…Br interaction geometry (Å, °).

D—H···A	**D—H**	**H···A**	**D···A**	**D—H···A**
C1-H1B…Br4[i]	0.99	2.86	3.828(3)	165.9

C17-H17A…Br2[ii]	0.99	2.92	3.712(3)	138.1
C21-H21A…Br1[iii]	0.99	2.78	3.735(3)	162.3

Symmetry codes : [i] x, -y+1/2, z+1/2; [ii] –x+1, y+1/2, -z+1/2; [iii] –x+1, -y+1, -z+1

Table.S5. Jonscher Law parameters for $(P(C_4H_9)_4)_2[ZnBr_4]$ at different temperatures.

T (K)	s	σ_{dc} (x10$^{-8}\Omega^{-1}$.cm^{-1})	A(x10^{-13})	R^2
303	0.9056	3.190	7.513	0.99201
308	0.9035	4.285	8.878	0.99151
313	0.8967	5.445	9.164	0.99288
318	0.8960	7.180	9.90	0.99360
323	0.8904	10.190	11.60	0.99650
328	0.8740	17.079	15.98	0.99837