Supplementary Material for

A zero-dimensional $(C_6H_9N_2)_3[BiCl_6]$ hybrid material: Synthesis, structural, optical, and electrical conductivity

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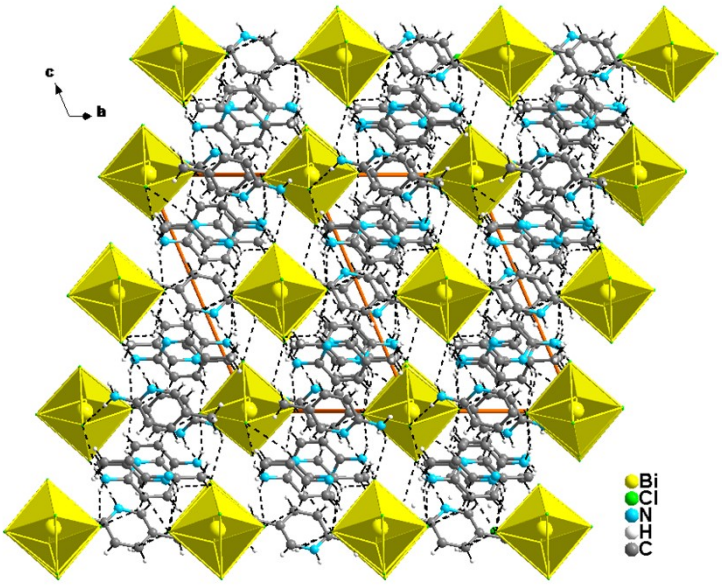


Figure S1: Projection of the structure of $(C_6H_9N_2)_3[BiCl_6]$ along the [1 -1 0] direction.

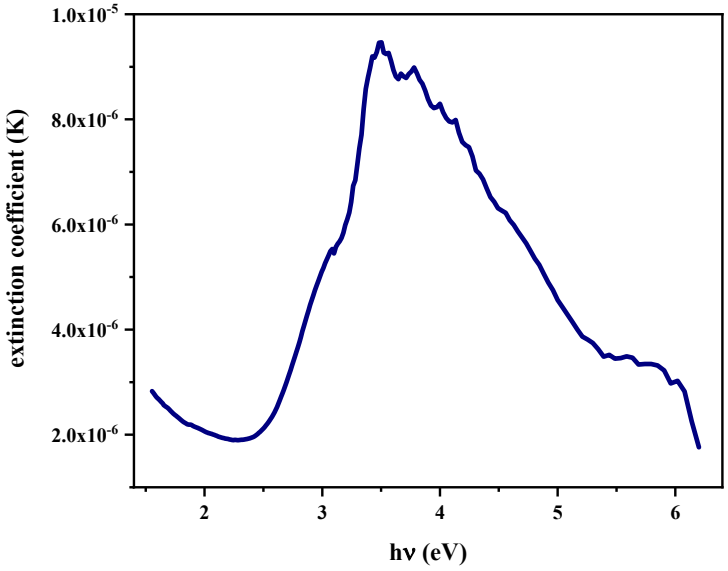
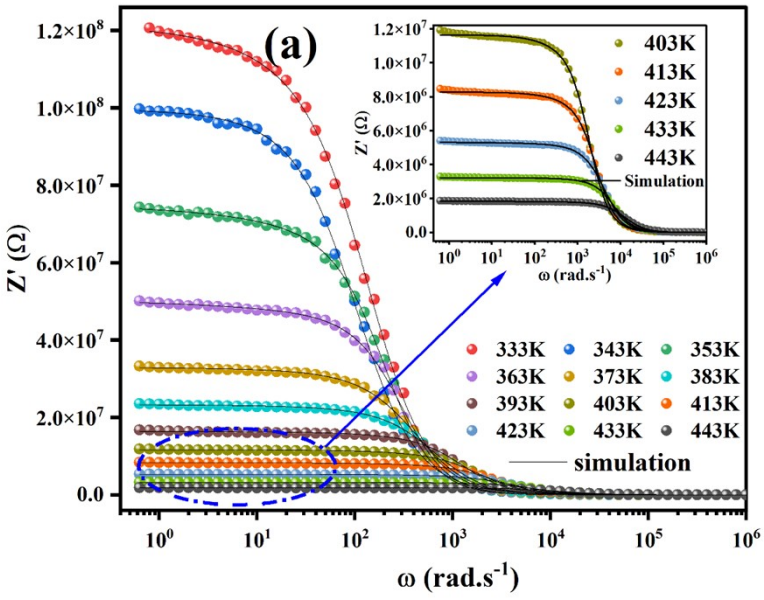


Figure S2: Extinction Coefficient against photon energy.



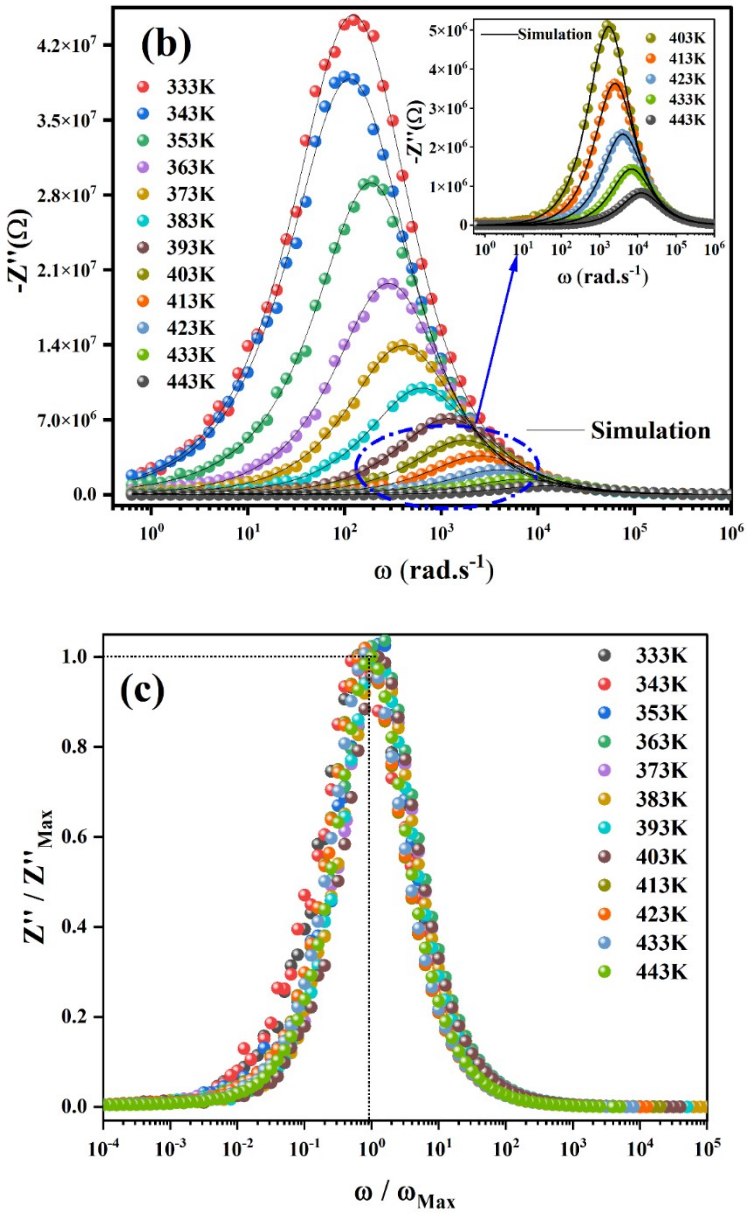


Figure S3: Variation of (a) the real part (Z') and (b) the imaginary part (Z") of the impedance as a function of angular frequency, and **(c)** Variation of Z''/Z''_{max} with ω/ω_{max} at several temperatures.

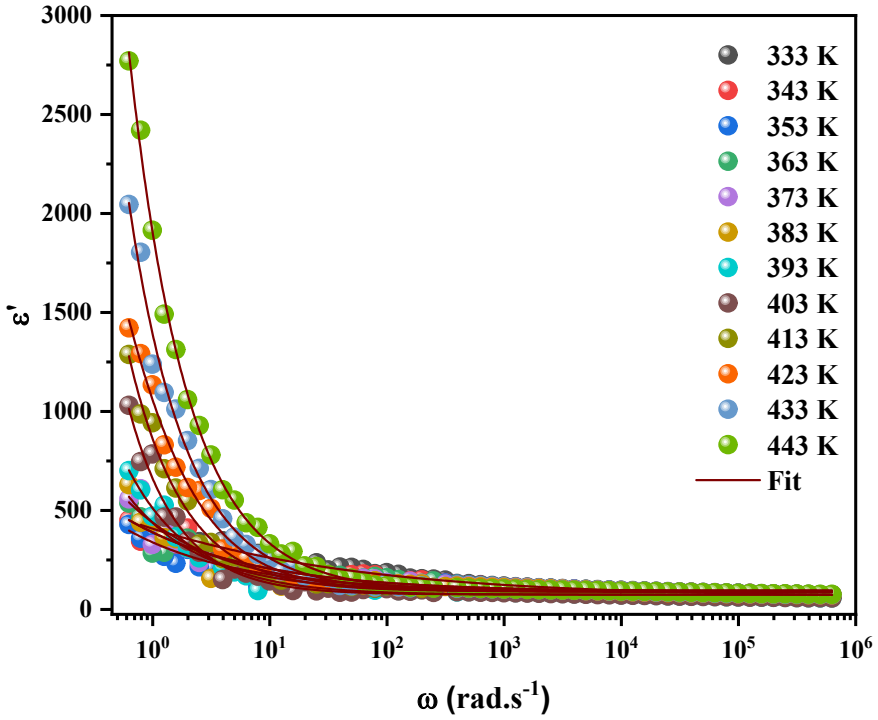


Figure S4: Frequency-dependent real part of dielectric constants (ε′) of $(C_6H_9N_2)_3[BiCl_6]$ at different temperatures.

Table S1: Fractional atomic coordinates and equivalent isotropic temperature factors (Å^2).

	x	*y*	*z*	U_{eq}
Bi1	0.24339(2)	0.2547(2)	0.50310(2)	0.03005(7)
Bi2	0.25517(2)	0.74146(2)	0.99767(2)	0.02953(7)
Cl9	0.17836(11)	0.72252(11)	0.79118(11)	0.0465(4)
Cl6	0.22842(11)	0.18227(11)	0.31303(10)	0.0429(4)
Cl10	0.32791(11)	0.75939(11)	1.18713(10)	0.0479(4)
Cl2	0.10984(12)	0.09066(11)	0.48891(11)	0.0485(4)
Cl11	0.41692(11)	0.88064(12)	1.00967(11)	0.0493(4)
Cl8	0.09269(11)	0.60689(12)	0.98503(12)	0.0514(4)
Cl7	0.35228(13)	0.59866(13)	0.93907(12)	0.0571(4)
Cl4	0.09386(12)	0.34445(12)	0.43645(12)	0.0541(4)
Cl5	0.37850(12)	0.41789(11)	0.51281(12)	0.0540(5)
Cl12	0.16295(13)	0.87982(13)	1.05120(13)	0.0610(5)
Cl3	0.26282(12)	0.33325(13)	0.70813(11)	0.0569(5)
Cl1	0.38357(13)	0.16694(14)	0.55743(13)	0.0624(5)
N7	0.2476(4)	0.4067(4)	0.2752(4)	0.0498(14)
N6	0.2469(4)	0.0711(4)	0.7079(4)	0.0488(14)
C17	0.3237(4)	0.0388(4)	0.8544(4)	0.0379(14)
N11	0.4254(4)	0.7603(4)	0.7830(4)	0.0473(13)
N8	0.0765(4)	0.3476(4)	0.2021(4)	0.0614(16)
N4	0.2485(4)	0.2828(4)	0.9063(4)	0.0555(15)
N5	0.4181(4)	0.1365(4)	0.7810(4)	0.0666(17)
N2	0.0489(4)	0.7543(4)	1.2121(4)	0.0517(14)
C35	0.4595(4)	0.6834(4)	0.6366(4)	0.0387(14)
C16	0.3317(4)	0.0840(4)	0.7800(5)	0.0428(15)
C22	0.1644(5)	0.3974(4)	0.2026(5)	0.0418(14)
C34	0.4140(4)	0.6755(4)	0.7104(4)	0.0389(14)
N12	0.3620(4)	0.5899(4)	0.7117(4)	0.0581(15)
N9	0.2113(4)	0.7433(4)	0.5865(4)	0.0516(14)
C4	0.0523(4)	0.8293(5)	1.3604(5)	0.0478(16)
N1	0.1429(4)	0.9257(4)	1.2812(4)	0.0671(18)
C23	0.1744(4)	0.4435(4)	0.1285(4)	0.0434(15)
C2	-0.0032(4)	0.6514(4)	1.2825(5)	0.0450(15)
C8	0.1905(5)	0.1937(5)	1.0074(5)	0.0521(17)
C32	0.5233(4)	0.8609(4)	0.7167(5)	0.0440(15)
N3	0.4118(4)	0.3644(5)	0.9378(5)	0.0736(19)
C25	0.1860(5)	0.6479(4)	0.5282(5)	0.0432(15)
N10	0.1324(4)	0.5790(4)	0.5538(4)	0.0682(18)
C18	0.2339(4)	-0.0133(4)	0.8518(4)	0.0409(14)
C11	0.3435(5)	0.3100(5)	0.9643(5)	0.0517(17)
C36	0.5122(4)	0.7732(4)	0.6399(4)	0.0402(14)
C24	0.2657(5)	0.4938(4)	0.1349(5)	0.0448(15)
C5	0.0950(5)	0.8392(5)	1.2845(5)	0.0462(15)
C3	0.0044(4)	0.7375(4)	1.3580(4)	0.0448(15)
C9	0.2897(5)	0.2215(5)	1.0700(5)	0.0581(18)

C27	0.2972(5)	0.8031(5)	0.4840(5)	0.0506(17)
C20	0.3522(4)	0.5024(4)	0.2111(5)	0.0435(15)
C12	0.1731(5)	0.2265(5)	0.9268(5)	0.0576(19)
C14	0.1461(4)	-0.0248(4)	0.7756(4)	0.0421(15)
C15	0.1562(4)	0.0182(4)	0.7047(5)	0.0483(16)
C6	0.0373(5)	0.6630(5)	1.2104(5)	0.0525(17)
C21	0.3391(5)	0.4584(5)	0.2809(5)	0.0508(17)
C28	0.2649(5)	0.8180(5)	0.5652(5)	0.0550(18)
C29	0.2174(5)	0.6283(5)	0.4428(4)	0.0552(18)
C33	0.4793(5)	0.8507(5)	0.7861(5)	0.0499(17)
C30	0.2720(5)	0.7047(5)	0.4229(5)	0.0552(18)
C10	0.3636(5)	0.2774(5)	1.0488(5)	0.0579(19)
C1	-0.0541(6)	0.5511(5)	1.2838(5)	0.068(2)
C19	0.4537(5)	0.5587(5)	0.2166(6)	0.068(2)
C13	0.0459(5)	-0.0822(5)	0.7739(6)	0.067(2)
C31	0.5834(5)	0.9599(5)	0.7206(6)	0.071(2)
C7	0.1093(6)	0.1305(6)	1.0295(6)	0.077(2)
C26	0.3576(6)	0.8851(6)	0.4607(6)	0.077(2)

Table S2: Selected bond distances (Å) and angles (°) in the $BiCl_6$ octahedra.

Distances (Å)		Angles (°)	
Bi1-Cl6	2.6140(14)	Cl6-Bi1-Cl1	91.25(5)
Bi1-Cl1	2.6364(17)	Cl6-Bi1-Cl2	89.96(5)
Bi1-Cl2	2.6918(14)	Cl1-Bi1-Cl2	87.45(6)
Bi1-Cl5	2.7005(14)	Cl6-Bi1-Cl5	88.56(5)
Bi1-Cl4	2.7889(17)	Cl1-Bi1-Cl5	91.97(6)
Bi1-Cl3	2.8061(15)	Cl2-Bi1-Cl5	178.40(4)
Bi2-Cl10	2.5961(14)	Cl6-Bi1-Cl4	86.15(5)
Bi2-Cl12	2.6506(16)	Cl1-Bi1-Cl4	177.38(5)
Bi2-Cl8	2.6806(14)	Cl2-Bi1-Cl4	92.22(5)
Bi2-Cl11	2.7130(14)	Cl5-Bi1-Cl4	88.29(5)
Bi2-Cl7	2.7667(16)	Cl6-Bi1-Cl3	178.96(5)
Bi2-Cl9	2.8274(14)	Cl1-Bi1-Cl3	87.75(5)
		Cl2-Bi1-Cl3	90.30(5)
		Cl5-Bi1-Cl3	91.17(5)
		Cl4-Bi1-Cl3	94.85(5)
		Cl10-Bi2-Cl12	88.33(5)
		Cl10-Bi2-Cl8	89.82(5)
		Cl12-Bi2-Cl8	87.41(6)
		Cl10-Bi2-Cl11	90.72(5)
		Cl12-Bi2-Cl11	91.36(6)
		Cl8-Bi2-Cl11	178.65(5)
		Cl10-Bi2-Cl7	92.50(5)
		Cl12-Bi2-Cl7	178.90(5)
		Cl8-Bi2-Cl7	93.31(5)
		Cl11-Bi2-Cl7	87.91(5)
		Cl10-Bi2-Cl9	179.29(4)
		Cl12-Bi2-Cl9	92.04(5)
		Cl8-Bi2-Cl9	90.80(5)

		Cl11-Bi2-Cl9	88.67(4)
		Cl7-Bi2-Cl9	87.11(5)

Table S3: Selected bond distances (Å) and angles (°) in $(C_6H_9N_2)^+$ cations.

Distances (Å)		Angles (°)	
N7-C22	1.337(7)	C22-N7-C21	123.2(5)
N7-C21	1.358(7)	C16-N6-C15	123.4(5)
N6-C16	1.337(7)	C18-C17-C16	120.5(5)
N6-C15	1.367(7)	C34-N11-C33	122.6(5)
C17-C18	1.355(7)	C11-N4-C12	123.2(6)
C17-C16	1.403(8)	C5-N2-C6	123.6(6)
N11-C34	1.346(7)	C36-C35-C34	120.4(5)
N11-C33	1.371(7)	N5-C16-N6	121.7(6)
N8-C22	1.331(7)	N5-C16-C17	122.1(6)
N4-C11	1.335(8)	N6-C16-C17	116.2(5)
N4-C12	1.369(8)	N8-C22-N7	120.5(6)
N5-C16	1.325(7)	N8-C22-C23	122.3(6)
N2-C5	1.350(7)	N7-C22-C23	117.2(5)
N2-C6	1.357(8)	N12-C34-N11	120.0(6)
C35-C36	1.357(7)	N12-C34-C35	123.3(6)
C35-C34	1.397(7)	N11-C34-C35	116.7(5)
C22-C23	1.414(8)	C25-N9-C28	122.6(5)
C34-N12	1.325(7)	C3-C4-C5	119.8(6)
N9-C25	1.346(7)	C24-C23-C22	118.8(6)
N9-C28	1.352(7)	C6-C2-C3	116.9(6)
C4-C3	1.362(8)	C6-C2-C1	122.4(6)
C4-C5	1.406(8)	C3-C2-C1	120.6(6)
N1-C5	1.327(7)	C12-C8-C9	116.4(7)
C23-C24	1.345(7)	C12-C8-C7	122.2(7)
C2-C6	1.341(8)	C9-C8-C7	121.4(7)
C2-C3	1.396(8)	C33-C32-C36	116.2(6)
C2-C1	1.502(8)	C33-C32-C31	122.3(6)
C8-C12	1.345(9)	C36-C32-C31	121.4(6)
C8-C9	1.404(9)	N10-C25-N9	118.9(6)
C8-C7	1.494(9)	N10-C25-C29	124.1(6)
C32-C33	1.333(8)	N9-C25-C29	116.9(6)
C32-C36	1.408(8)	C17-C18C14	122.0(6)
C32-C31	1.506(8)	N3-C11-N4	118.9(6)
N3-C11	1.332(8)	N3-C11-C10	124.7(6)
C25-N10	1.327(7)	N4-C11-C10	116.4(6)
C25-C29	1.395(8)	C35-C36-C32	121.9(5)

C18-C14	1.402(7)	C23-C24-C20	123.3(6)
C11-C10	1.396(9)	N1-C5-N2	120.1(6)
C24-C20	1.400(8)	N1-C5-C4	123.6(6)
C9-C10	1.356(9)	N2-C5-C4	116.3(6)
C27-C28	1.345(9)	C4-C3-C2	122.3(6)
C27-C30	1.393(9)	C10-C9-C8	121.3(7)
C27-C26	1.493(9)	C28-C27-C30	115.4(6)
C20-C21	1.349(8)	C28-C27-C26	123.0(7)
C20-C19	1.505(8)	C30-C27-C26	121.6(6)
C14-C15	1.344(8)	C21-C20-C24	115.9(6)
C14-C13	1.513(8)	C21-C20-C19	121.6(6)
C29-C30	1.364(8)	C24-C20-C19	122.4(6)
		C8-C12-N4	121.7(6)
		C15-C14-C18	116.2(5)
		C15-C14-C13	122.2(6)
		C18-C14-C13	121.6(6)
		C14-C15-N6	121.7(5)
		C2-C6-N2	121.3(6)
		C20-C21-N7	121.5(6)
		C27-C28-N9	122.8(6)
		C30-C29-C25	119.5(6)
		C32-C33-N11	122.2(6)
		C29-C30-C27	122.7(6)
		C9-C10-C11	121.1(6)

Table S4: Hydrogen bonding geometry (Å, °).

D—H···A	**D—H**	**H···A**	**D···A**	**D—H···A**
N7—H7···Cl6	0.86	2.77	2.386(5)	129.7
N7—H7···Cl5	0.86	2.81	3.419(5)	129.0
N6—H6···Cl2	0.86	2.74	2.386(5)	133.0
N6—H6···Cl1	0.86	2.90	3.617(5)	142.3
C17—H17···Cl11^{i}	0.93	2.74	3.563(6)	147.4
N11—H11···Cl9	0.86	2.98	3.525(5)	122.8
N11—H11···Cl11	0.86	2.67	3.335(5)	135.1
N8—H8A···Cl4	0.86	2.57	3.336(6)	148.5
N8—H8B···Cl8^{ii}	0.86	2.63	3.438(6)	156.5
N4—H4···Cl3	0.86	2.37	3.164(5)	153.6
N5—H5A···Cl1	0.86	2.49	3.288(6)	155.1
N5—H5B···Cl11^{i}	0.86	2.63	3.436(6)	157.2
N2—H2···Cl8	0.86	2.86	2.465(5)	129.4
N2—H2···Cl12	0.86	2.81	2.544(5)	144.8
C35—H35···Cl5	0.93	2.83	3.616(6)	143.5
N12—H12A···Cl7	0.86	2.51	3.287(6)	150.2
N12—H12B···Cl5	0.86	2.56	3.376(6)	159.3
N9—H9···Cl9	0.86	2.41	3.178(5)	148.9
C4—H4A···Cl2^{iii}	0.93	2.77	3.589(6)	147.6
N1—HN1A···Cl12	0.86	2.52	3.309(6)	153.8

N1—HN1B···Cl2^{iii}	0.86	2.72	3.519(6)	154.4
C23—H23···Cl8^{ii}	0.93	2.84	3.629(6)	143.1
N3—H3A···Cl3	0.86	2.60	3.333(6)	144.4
N3—H3B···Cl7^{i}	0.86	2.44	3.283(6)	168.9
N10—H10A···Cl9	0.86	2.64	3.351(6)	141.0
N10—H10B···Cl4	0.86	2.40	3.250(6)	170.0
C15—H15···Cl2	0.93	2.88	3.473(6)	122.7
C6—H6A···Cl8	0.93	2.83	3.469(6)	126.6
C21—H21···Cl5	0.93	2.86	3.463(7)	123.4
C33—H33···Cl11	0.93	2.95	3.499(7)	118.8
Symmetry codes : ^{i} –x+1, -y+1, -z+2 ; ^{ii} –x, -y+1, -z+1 ; ^{iii} x, y+1, z+1 ;				

Table S5: AC conductivity parameters for the CBH model for the $(C_6H_9N_2)_3[BiCl_6]$ compound at various frequencies.

Frequency (Hz)		10	10^2	10^3
N_T (eV/Cm^3)	Region I	2.36×10^{18}	2.41×10^{18}	1.21×10^{19}
	Region II	3.62×10^{18}	4.06×10^{18}	3.01×10^{19}
U_{eff} (eV)	Region I	0.022	0.020	0.009
	Region II	0.051	0.041	0.022

Table S6: The extracted fitting parameters obtained from the Cole-Davison equation.

T(K)	ε_s	ε_∞	**τ(s)**	α
333	2602	62.550	0.098	0.268
343	416062	87.718	0.053	0.406
353	875564	90.076	0.054	0.458
363	417535	87.718	0.053	0.406
373	3.746×10^6	94.203	0.072	0.557
383	1.679×10^7	95.577	0.005	0.699
393	3.490×10^6	74.122	0.009	0.782
403	1.652×10^7	75.391	0.002	0.801
413	111776	92.074	2.089×10^{-4}	0.939
423	493445	92.888	2.810×10^{-4}	0.986
433	3.713×10^8	88.786	1.401×10^{-4}	0.884
443	2.605×10^8	90.135	1.108×10^{-4}	0.873