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Theoretical, photophysical and biological investigations of an organic charge transfer compound 2-aminobenzimidazolium-2-oxyisoindolate-1,3-dione-2-hydroxyisoindoline-1,3-dione

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Table S1. Crystal data and structure refinement for ABOH

Parameters	ABOH
Empirical formula	$C_{23}H_{17}N_5O_6$
Formula weight	459.42
Temperature (K)	573(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 8.5032(5) Å α = 90° b = 12.9483(7) Å β = 98.797(3)° c = 18.8575(11) Å γ = 90°
Volume (Å^3)	2051.8(2)
Z, Calculated density (Mg/m^{-3})	4, 1.487
F(000)	952
Crystal size (mm)	0.20 × 0.15 × 0.10
Theta range for data collection	1.92 to 27.42°
Limiting indices	$-10 \le h \le 11$, $-16 \le k \le 16$, $-24 \le l \le 24$
Reflections collected/unique	31613/4522 [R(int) = 0.0381]
Completeness to theta	97.00%
Max. and min. transmission	0.9890 and 0.9782
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4522/0/309
Goodness-of-fit on F^2	1.051
Final R indices [I > 2σ(I)]	R1 = 0.0396, wR2 = 0.1016
R indices (all data)	R1 = 0.0575, wR2 = 0.1113
Largest diff. peak and hole	0.223 and –0.170 e.A^{-3}

Table S2. Selected bond lengths (Å) and bond angles (°) for ABOH

Bond	Bond length (Å)	Bond	Bond angle (°)
C(1)-O(1)	1.2049(2)	O(1)-C(1)-N(1)	125.61(1)
C(1)-N(1)	1.3831(2)	O(1)-C(1)-C(2)	130.06(1)
C(8)-O(3)	1.2017(1)	N(1)-C(1)-C(2)	104.32(2)
C(8)-N(1)	1.3895(1)	O(3)-C(8)-N(1)	125.59(1)
C(9)-O(4)	1.2133(1)	O(3)-C(8)-C(7)	130.10(1)
C(9)-N(2)	1.3795(1)	N(1)-C(8)-C(7)	104.31(1)
C(16)-O(6)	1.2126(1)	O(4)-C(9)-N(2)	125.37(1)
C(16)-N(2)	1.3834(1)	O(4)-C(9)-C(10)	128.99(1)
C(17)-N(5)	1.3214(2)	N(2)-C(9)-C(10)	105.64(1)
C(17)-N(4)	1.3321(2)	O(6)-C(16)-N(2)	124.14(1)
C(17)-N(3)	1.3349(2)	O(6)-C(16)-C(15)	130.31(1)
C(18)-N(3)	1.3905(1)	N(2)-C(16)-C(15)	105.55(1)
C(23)-N(4)	1.3975(2)	N(5)-C(17)-N(4)	124.54(1)
N(1)-O(2)	1.3716(2)	N(5)-C(17)-N(3)	126.22(1)
N(2)-O(5)	1.3623(1)	N(4)-C(17)-N(3)	109.23(1)
–	–	C(19)-C(18)-N(3)	131.75(1)
–	–	C(23)-C(18)-N(3)	106.72(1)
–	–	C(22)-C(23)-N(4)	132.32(1)
–	–	C(18)-C(23)-N(4)	105.96(1)
–	–	O(2)-N(1)-C(1)	123.06(1)
–	–	O(2)-N(1)-C(8)	122.43(1)
–	–	C(1)-N(1)-C(8)	114.11(1)
–	–	O(5)-N(2)-C(9)	124.18(1)
–	–	O(5)-N(2)-C(16)	122.98(1)
–	–	C(9)-N(2)-C(16)	112.82(1)
–	–	C(17)-N(3)-C(18)	108.93(1)
–	–	C(17)-N(4)-C(23)	109.15(1)

Table S3. Calculated FT IR spectral band assignments of ABOH crystal

Infrared frequencies (cm^{-1})	Assignments
3449.46	N−H asymmetric stretching vibration(−NH_2)
3225.30	N−H symmetric stretching vibration(−NH_2)
3188.58	N−H stretching vibration
3042.16	C−H stretching vibration
1636.21	C=O Stretching vibration
1532.37	N−H bending vibration
1188.89	C−H in-plane bending vibration
1053.09	C−H out of plane bending vibration
1013.15	C−N stretching vibration
893.33	N−H wagging vibration

Table S4. Experimental and calculated bond lengths (Å) and bond angles (°) of ABOH

Bond length (Å)			Bond angle (°)		
	Experimental	DFT		Experimental	DFT
C(1)-O(1)	1.2049(2)	1.2108	O(1)-C(1)-N(1)	125.61(1)	126.96
C(1)-N(1)	1.3831(2)	1.3923	O(1)-C(1)-C(2)	130.06(1)	130.15
C(8)-O(3)	1.2017(1)	1.2203	N(1)-C(1)-C(2)	104.32(2)	104.72
C(8)-N(1)	1.3895(1)	1.3869	O(3)-C(8)-N(1)	125.59(1)	126.01
C(9)-O(4)	1.2133(1)	1.2259	O(3)-C(8)-C(7)	130.10(1)	129.95
C(9)-N(2)	1.3795(1)	1.3743	N(1)-C(8)-C(7)	104.31(1)	104.03
C(16)-O(6)	1.2126(1)	1.2086	O(4)-C(9)-N(2)	125.37(1)	126.06
C(16)-N(2)	1.3834(1)	1.4008	O(4)-C(9)-C(10)	128.99(1)	129.95
C(17)-N(5)	1.3214(2)	1.3233	N(2)-C(9)-C(10)	105.64(1)	105.17
C(17)-N(4)	1.3321(2)	1.3628	O(6)-C(16)-N(2)	124.14(1)	122.32
C(17)-N(3)	1.3349(2)	1.3423	O(6)-C(16)-C(15)	130.31(1)	132.94
C(18)-N(3)	1.3905(1)	1.3938	N(2)-C(16)-C(15)	105.55(1)	104.77
C(23)-N(4)	1.3975(2)	1.3971	N(5)-C(17)-N(4)	124.54(1)	122.70
N(1)-O(2)	1.3716(2)	1.3793	N(5)-C(17)-N(3)	126.22(1)	125.17
N(2)-O(5)	1.3623(1)	1.3643	N(4)-C(17)-N(3)	109.23(1)	112.07
–	–	–	C(19)-C(18)-N(3)	131.75(1)	130.25
–	–	–	C(23)-C(18)-N(3)	106.72(1)	106.02
–	–	–	C(22)-C(23)-N(4)	132.32(1)	132.61
–	–	–	C(18)-C(23)-N(4)	105.96(1)	104.72
–	–	–	O(2)-N(1)-C(1)	123.06(1)	122.88
–	–	–	O(2)-N(1)-C(8)	122.43(1)	122.84
–	–	–	C(1)-N(1)-C(8)	114.11(1)	115.14
–	–	–	O(5)-N(2)-C(9)	124.18(1)	124.12
–	–	–	O(5)-N(2)-C(16)	122.98(1)	120.72
–	–	–	C(9)-N(2)-C(16)	112.82(1)	113.78
–	–	–	C(17)-N(3)-C(18)	108.93(1)	107.46
–	–	–	C(17)-N(4)-C(23)	109.15(1)	106.00

Table S5. The energy of experimental absorption bands and the electronic transitions calculated with the TD-DFT method for ABOH

E (eV)	*F*	Wavelength λ (nm)		Major contribution
		(Cal)	(Exp)	
2.36	0.0027	355	−	HOMO→LUMO (100%)
2.89	0.0002	342	345	HOMO→LUMO+1 (100%) HOMO−1→LUMO (99%)
2.92	0.0007	275	271	HOMO−6→LUMO (61%) HOMO−3→LUMO (30%)

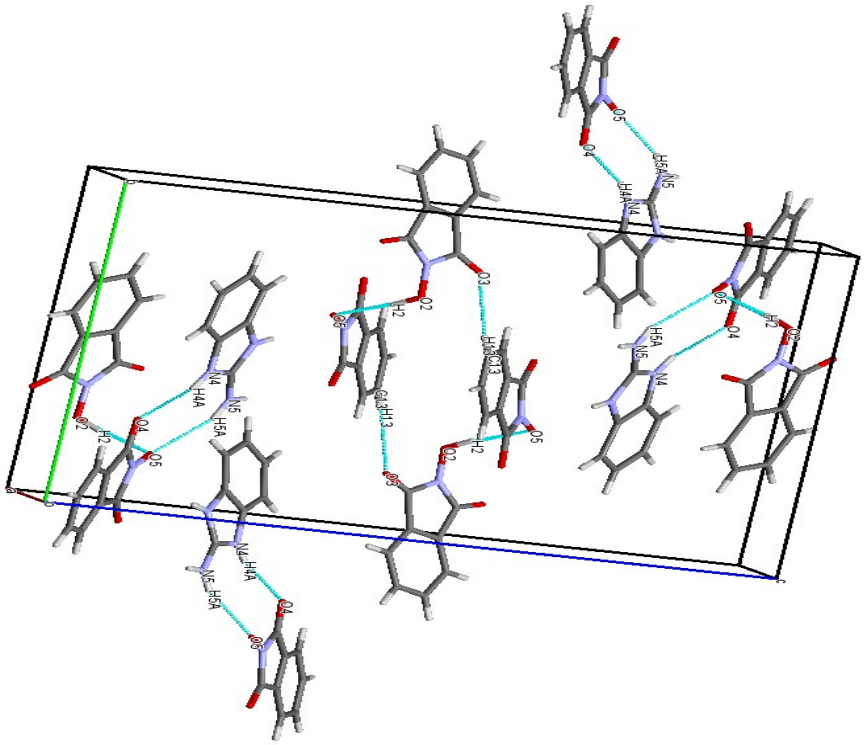

Fig. S1 Packing diagram of ABOH view down ‘b’ axis.

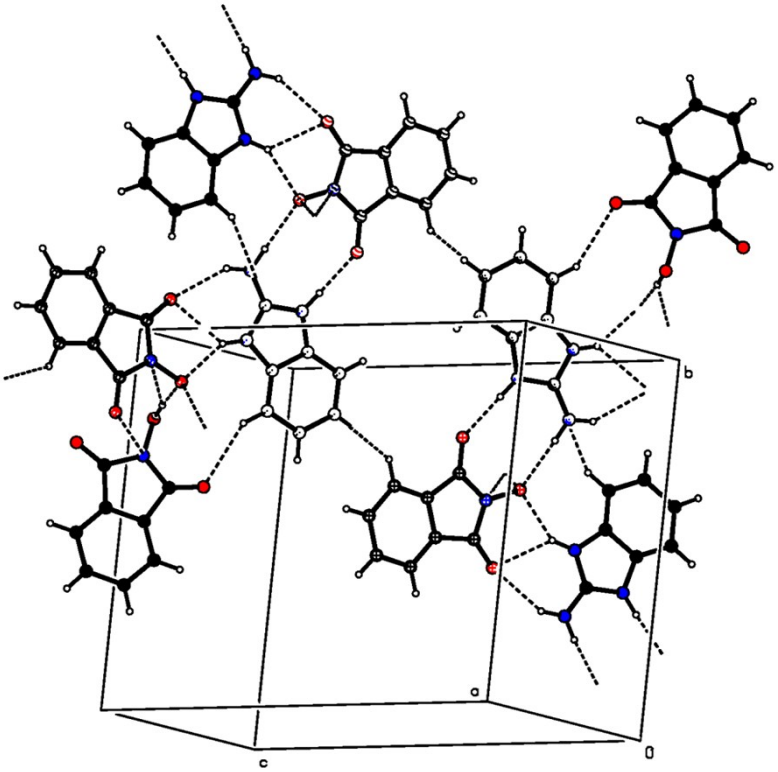

Fig. S2 Packing diagram of the compund ABOH running along ‘bc’ plane.

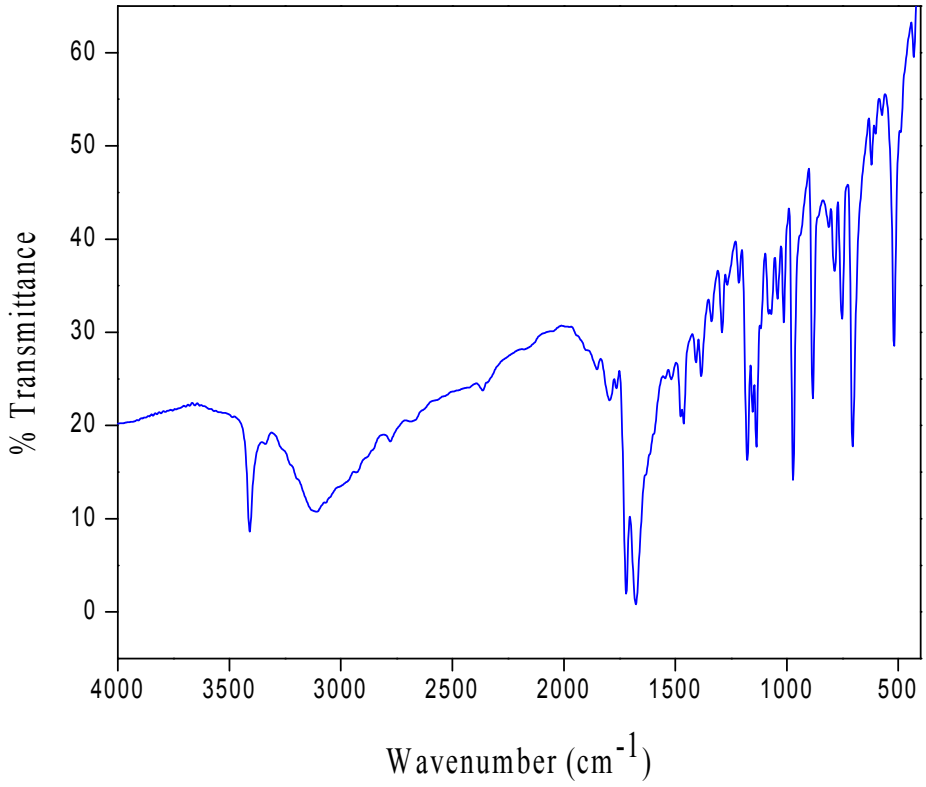

Fig. S3 FT IR spectrum of ABOH crystal.

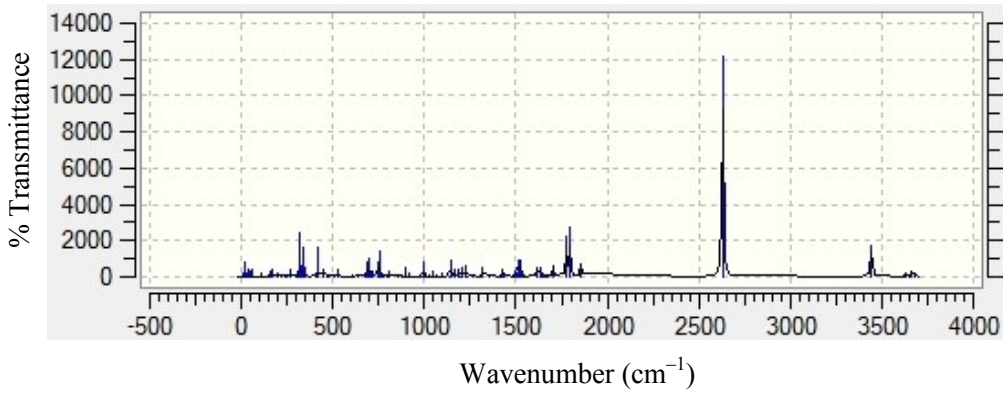

Fig. S4 Calculated FT IR spectrum of ABOH crystal.

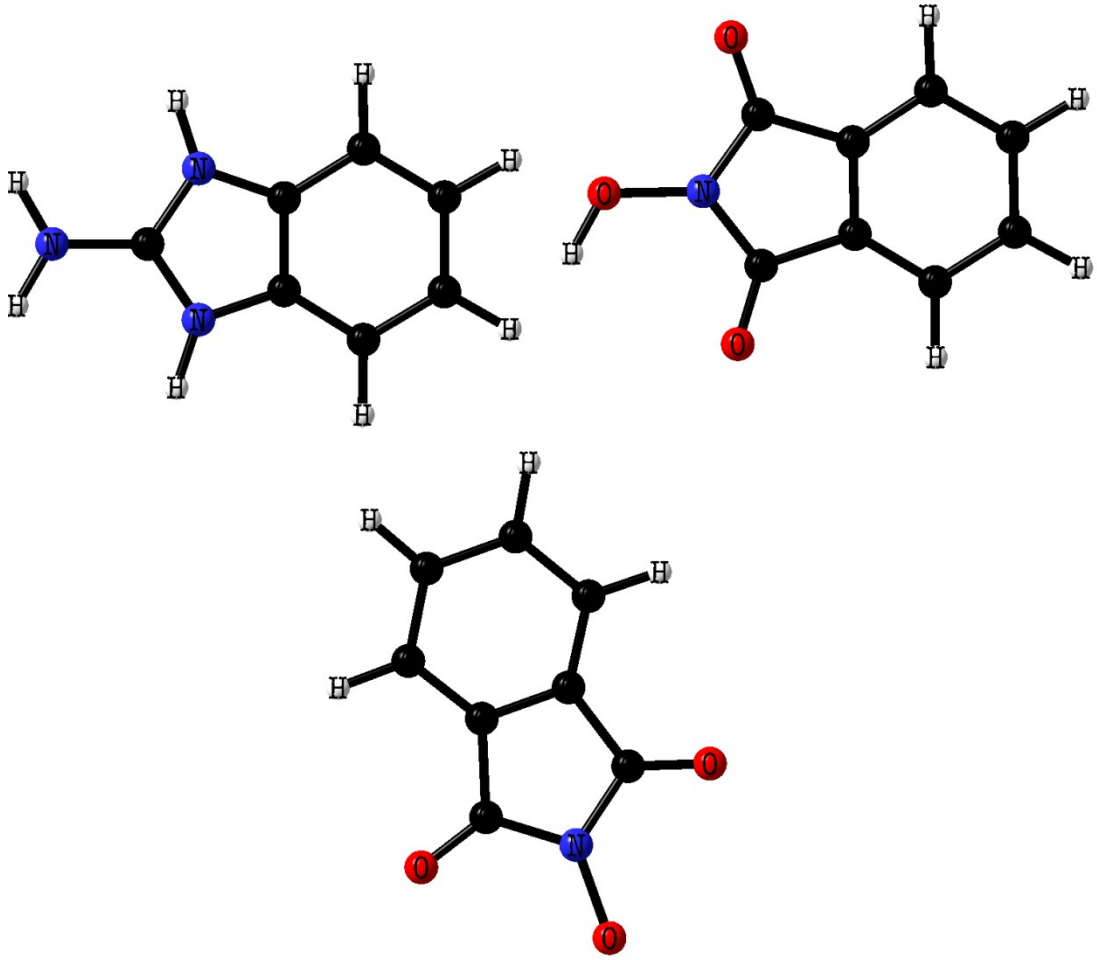

Fig. S5 Optimized geometry of ABOH crystal.

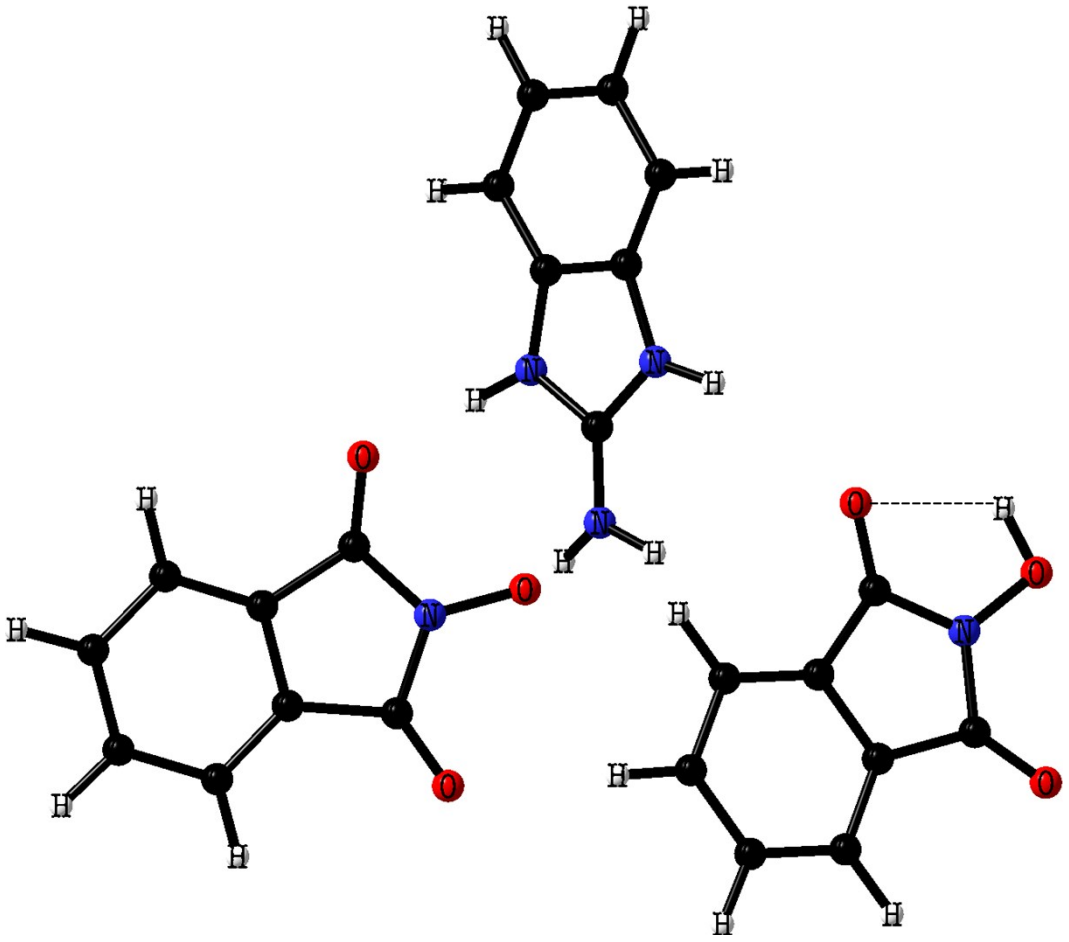

Fig. S6 Intramolecular interaction of ABOH crystal.

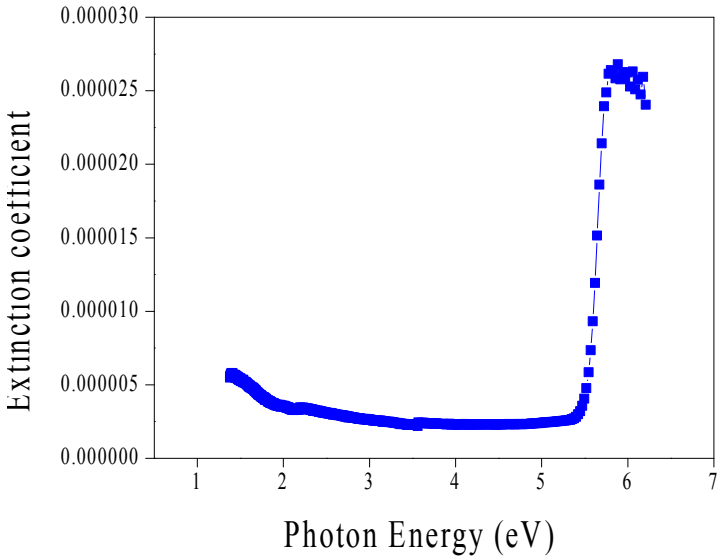

Fig. S7 Plot of photon energy *vs*. extinction coefficient of ABOH crystal.

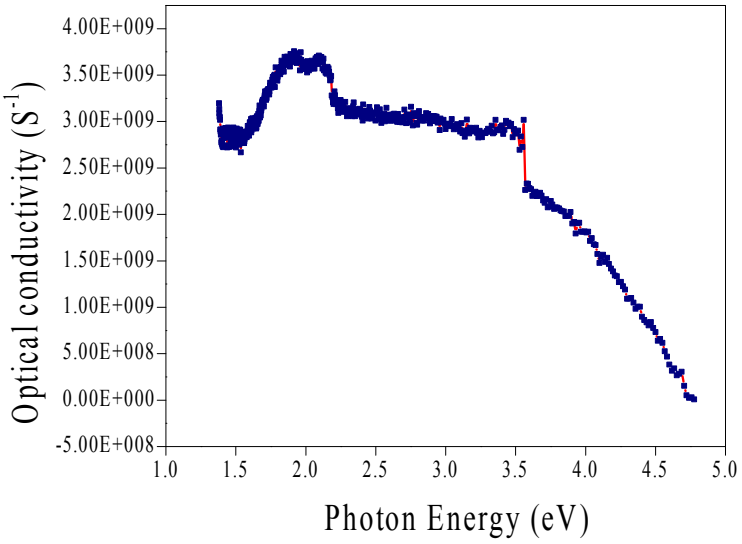

Fig. S8 Plot of photon energy *vs*. optical conductivity of ABOH crystal.

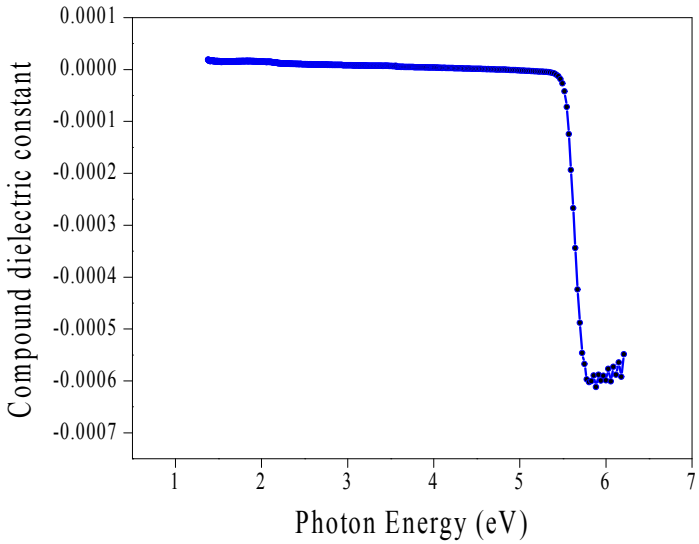

Fig. S9 Plot of photon energy *vs*. compound dielectric constant of ABOH crystal.

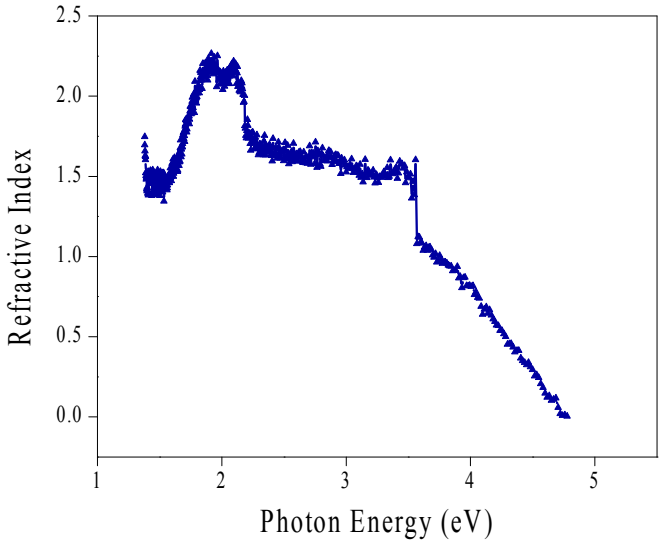

Fig. S10 Plot of photon energy *vs*. refractive index of ABOH crystal.

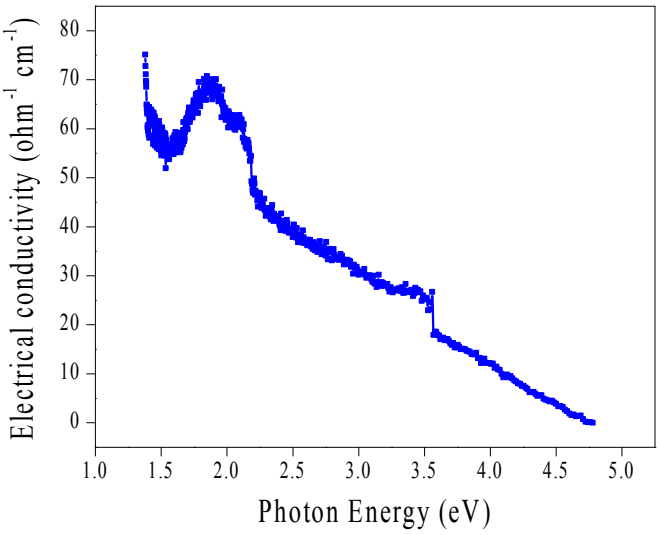

Fig. S11 Plot of photon energy *vs*. electrical conductivity of ABOH crystal.

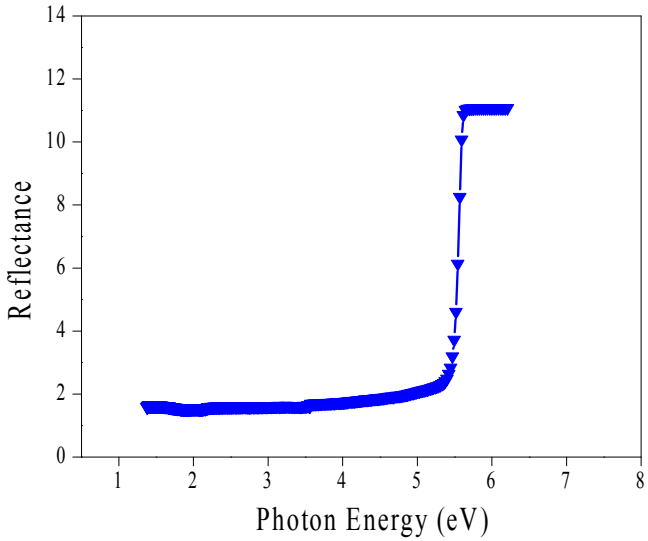

Fig. S12 Plot of photon energy *vs.* reflectance of ABOH crystal.

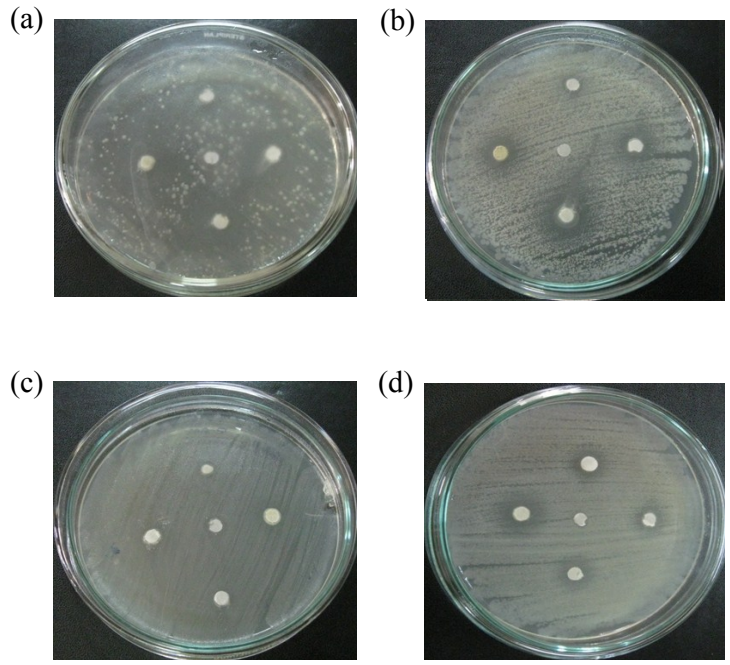

Fig. S13 Antibacterial activity of ABOH against *E. coli* (a), *P. aeruginosa* (b), *K. pneumoniae* (c) and *S. aureus* (d).