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Supporting information for article:

The influence of chalcogen atom on conformation and phase transition in chalcogenazinoquinolinium monoiodides

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Table S1 Comparison of bond lengths in **OQ** and **TQ** crystals at different temperature

Bond	**OQ** 100K	**TQ** 293K	**TQ** 100K	
			Molecule 1	Molecule 2 with index ”A”
I(1)-C(12)	2.165(1)	2.170(3)	2.169(3)	2.177(3)
N(1)-C(1)	1.339(2)	1.333(3)	1.342(5)	1.355(4)
N(1)-C(9)	1.392(2)	1.402(3)	1.400(4)	1.397(4)
N(1)-C(10)	1.499(1)	1.511(3)	1.513(4)	1.504(4)
C(1)-C(2)	1.413(2)	1.392(5)	1.398(5)	1.403(6)
C(2)-C(3)	1.382(2)	1.370(5)	1.379(6)	1.369(6)
C(3)-C(8)	1.424(2)	1.419(4)	1.418(5)	1.428(5)
C(4)-C(5)	1.387(2)	1.359(5)	1.371(6)	1.369(6)
C(4)-C(8)	1.429(2)	1.422(4)	1.414(5)	1.427(5)
C(5)-C(6)	1.414(2)	1.406(5)	1.410(5)	1.418(5)
C(6)-C(7)	1.384(2)	1.390(4)	1.393(5)	1.384(5)
C(7)-C(9)	1.424(2)	1.422(3)	1.431(5)	1.429(4)
C(8)-C(9)	1.430(2)	1.427(3)	1.444(5)	1.430(5)
C(10)-C(11)	1.529(2)	1.526(3)	1.520(5)	1.519(5)
C(10)-C(12)	1.532(2)	1.530(3)	1.542(5)	1.542(5)

Table S2 Comparison of Angles in **OQ** and **TQ** crystals at different temperature

Angles	**OQ** 100K	**TQ** 293K	**TQ** 100K	
			Molecule 1	Molecule 2 with index ”A”
C(1)-N(1)-C(9)	122.02(10)	121.5(2)	122.0(3)	121.4(3)
C(1)-N(1)-C(10)	119.80(10)	116.6(2)	116.3(3)	116.0(3)
C(9)-N(1)-C(10)	118.17(9)	121.83(19)	121.6(3)	122.6(3)

N(1)-C(1)-C(2)	120.65(11)	122.2(3)	121.6(3)	121.4(3)
C(3)-C(2)-C(1)	119.65(11)	119.1(3)	119.3(3)	119.9(3)
C(2)-C(3)-C(8)	120.31(10)	120.3(3)	120.6(3)	119.8(3)
C(5)-C(4)-C(8)	121.01(11)	120.3(3)	120.8(3)	120.4(3)
C(4)-C(5)-C(6)	120.19(11)	120.6(3)	120.0(3)	120.0(3)
C(7)-C(6)-C(5)	120.93(12)	121.4(3)	121.9(3)	121.5(3)
C(6)-C(7)-C(9)	119.19(11)	118.8(2)	118.9(3)	119.4(3)
C(3)-C(8)-C(4)	124.29(11)	121.4(3)	121.5(3)	120.8(3)
C(3)-C(8)-C(9)	118.16(10)	119.3(3)	119.6(3)	119.6(3)
C(4)-C(8)-C(9)	117.55(10)	119.4(3)	118.9(3)	119.6(3)
N(1)-C(9)-C(7)	120.10(10)	123.1(2)	123.6(3)	123.1(3)
N(1)-C(9)-C(8)	119.02(10)	117.6(2)	117.6(3)	118.0(3)
C(7)-C(9)-C(8)	120.88(10)	119.4(2)	118.8(3)	118.9(3)
N(1)-C(10)-C(11)	106.82(9)	109.06(19)	107.8(3)	109.0(3)
N(1)-C(10)-C(12)	111.55(9)	107.51(19)	108.8(3)	107.1(3)
C(11)-C(10)-C(12	110.52(10)	116.7(2)	116.6(3)	116.2(3)
C(10)-C(12)-I(1)	116.14(8)	112.47(17)	113.2(2)	112.0(3)

Table S3 Comparison of some torsion angles in **OQ** and **TQ** crystals at different temperature (for **OQ**, the chalcogen atom Ch = O, for TQ, Ch = S)

Torsion angles	**OQ** 100K	**TQ** 293K	**TQ** 100K	
			Molecule 1	Molecule 2 with index ”A”
C(10)-N(1)-C(9)-C(7)	-2.19(15)	-5.7(3)	-4.9(6)	-4.9(5)
C(11)-O(1)-C(7)-C(6)	158.50(11)	160.9(2)	160.2(3)	160.3(3)
Ch(1)-C(7)-C(9)-N(1)	-6.35(17)	-2.8(3)	-3.3(5)	-3.5(5)
C(7)-Ch(1)-C(11)-C(10)	55.83(13)	52.8(2)	53.8(3)	52.9(3)
C(12)-C(10)-C(11)-Ch(1)	60.28(12)	55.7(3)	54.9(3)	54.9(4)
N(1)-C(10)-C(11)-Ch(1)	-61.24(12)	-66.3(2)	-67.2(3)	-66.3(3)

N(1)-C(10)-C(12)-I(1)	-67.25(11)	179.68(15)	177.2(2)	-178.4(2)

Table S4 Comparative geometric and QTAIM (Bader, 1990) characteristics at the bond critical points: electron density, Laplacian of electron density, the kinetic energy density for OQ and TQ molecules in **OQ** and **TQ** crystals.

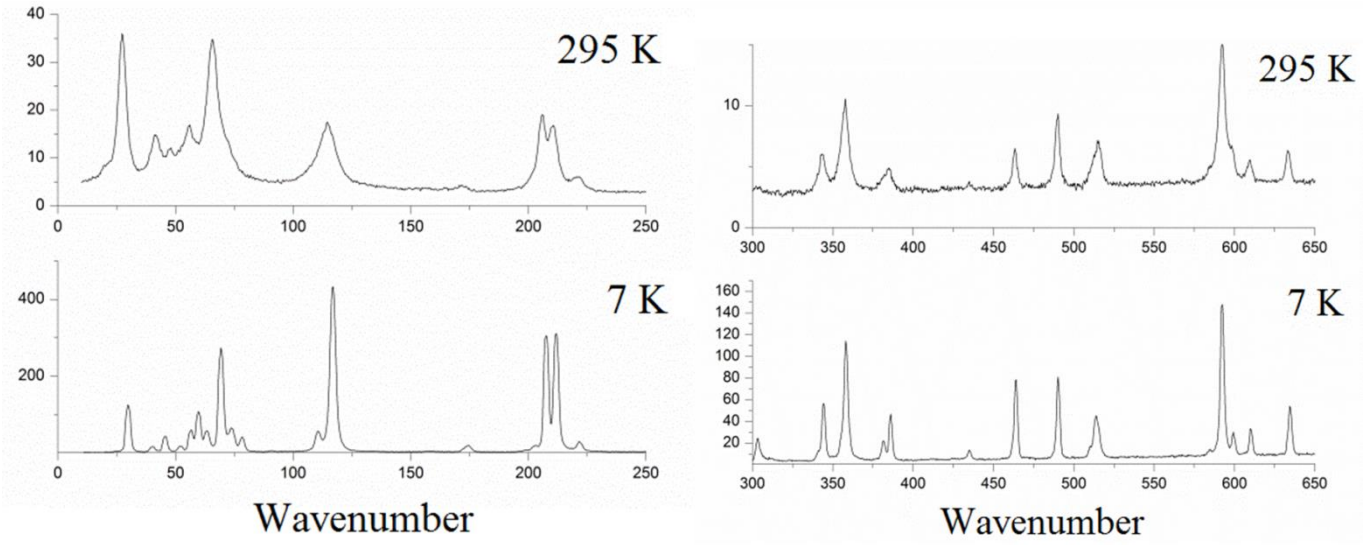
Bond	Crystal	Bond length (Å)	$\rho(r_{bcp})$, a.u.	$\nabla^2\rho(r_{bcp})$, a.u.	$G(r_{bcp})$, a.u.	$ELF(r_{bcp})$
C12-I1	**OQ**	2,1932	0.104	-0.0039	0.043	0.707
	TQ	2,2026	0.103	-0.0025	0.043	0.696
C4-Cl1	**OQ**	1,7834	0.173	-0.185	0.060	0.869
O1-C7	**OQ**	1,3675	0.288	-0.695	0.243	0.688
S1-C7	**TQ**	1,7666	0.197	-0.369	0.060	0.912
O1-C11	**OQ**	1,4458	0.237	-0.484	0.164	0.715
S1-C11	**TQ**	1,8152	0.181	-0.293	0.050	0.918
N1-C1	**OQ**	1,3329	0.332	-0.904	0.298	0.702
	TQ	1,3409	0.326	-0.549	0.399	0.552
N1-C9	**OQ**	1,3815	0.301	-0.854	0.194	0.802
	TQ	1,3900	0.298	-0.746	0.274	0.661
N1-C10	**OQ**	1,4895	0.239	-0.522	0.115	0.840
	TQ	1,4977	0.239	-0.592	0.133	0.798
C1-C2	**OQ**	1,3881	0.321	-0.979	0.101	0.948
	TQ	1,3943	0.315	-0.897	0.100	0.946
C2-C3	**OQ**	1,3658	0.332	-1,00	0.112	0.944
	TQ	1,3761	0.325	-0.928	0.107	0.944
C3-C8	**OQ**	1,4094	0.307	-0.895	0.089	0.953
	TQ	1,4130	0.305	-0.832	0.089	0.952
C4-C5	**OQ**	1,3619	0.334	-1,01	0.118	0.939
	TQ	1,3758	0.324	-0.918	0.108	0.943
C4-C8	**OQ**	1,4080	0.307	-0.888	0.092	0.951
	TQ	1,4137	0.303	-0.818	0.090	0.950
C6-C7	**OQ**	1,3681	0.333	-1,02	0.114	0.942

	TQ	1,3898	0.315	-0.861	0.105	0.940
C7-C9	**OQ**	1,4087	0.312	-0.925	0.091	0.954
	TQ	1,4234	0.296	-0.771	0.090	0.947
C8-C9	**OQ**	1,4159	0.304	-0.873	0.091	0.950
	TQ	1,4311	0.295	-0.774	0.087	0.949
C10-C12	**OQ**	1,5151	0.254	-0.651	0.058	0.962
	TQ	1,5164	0.255	-0.605	0.060	0.961
C10-C11	**OQ**	1,5193	0.258	-0.680	0.056	0.966
	TQ	1,5248	0.250	-0.584	0.058	0.960

Table S5 Temperature dependency of the unit cell parameters in **TQ** crystal

T, K	**a**	**b**	**c**	α	β	γ	V, Å^3
100	8.1178(2)	12.0928(3)	14.4689(3)	88.188(1)	89.472(1)	73.923(1)	1364.14(9)
113	8.1228(2)	12.1002(3)	14.4723(3)	88.367(1)	89.524(1)	73.942(1)	1366.39(9)
133	8.1294(3)	12.1079(3)	14.4767(4)	88.704(1)	89.621(1)	73.969(1)	1369.17(10)
153	8.1370(3)	12.1168(4)	14.4794(4)	89.160(1)	89.757(1)	74.000(1)	1372.14(11)
173	8.1468(2)	12.1275(3)	14.4892(3)	89.901(1)	89.958(1)	74.055(1)	1376.46(8)
223	8.1675(3)	12.1433(3)	14.5062(3)	89.987(1)	89.977(1)	74.216(1)	1384.49(9)
230	8.1701(4)	12.1472(4)	14.5137(4)	89.986(1)	89.968(2)	74.254(1)	1386.34(12)
273	8.1899(3)	12.1591(3)	14.5241(4)	90.001(1)	90.02(1)	74.395(1)	1393.02(10)
293	8.2078(2)	12.1709(4)	14.5397(5)	90	90	74.515(1)	1399.74(8)

Figure S1 The yellowish crystal of **TQ** wrapped into indium foil and prepared for low-temperature Raman measurements



a b

Figure S2 Comparison of experimental Raman spectra of **TQ** at 295 K and 7K in the low-frequency region 15–250 cm^{-1} (a) and medium frequency region 300-650 cm^{-1} (b)

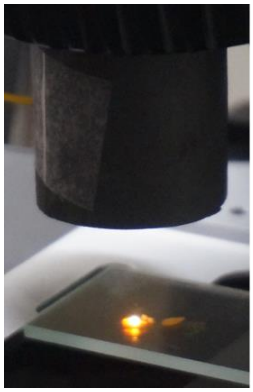
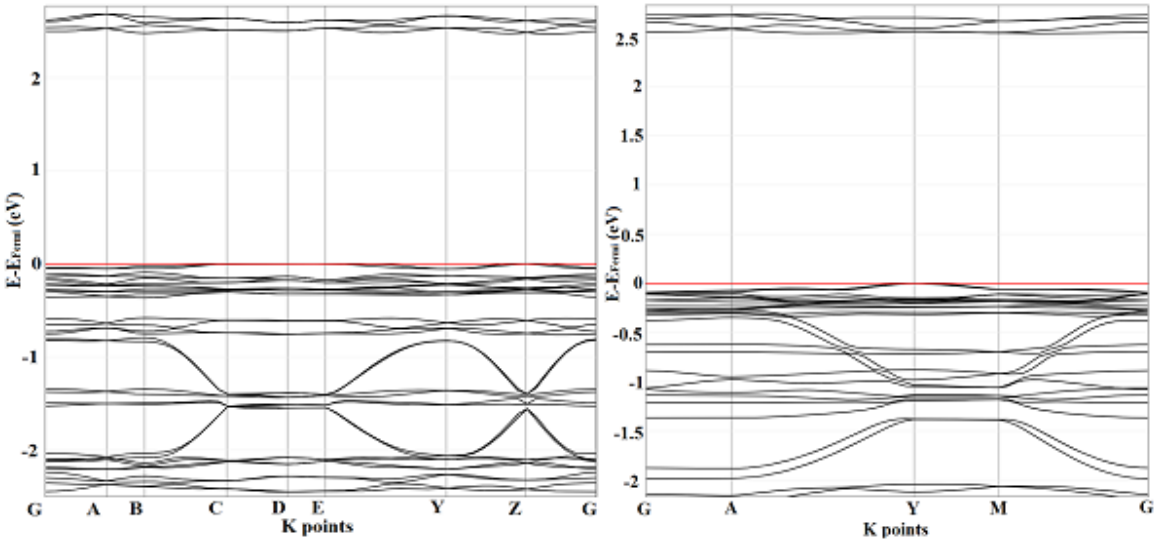


Figure S3 Reddish luminescence of **OQ** under irradiation of microscope light.



a b

Figure S4 Calculated band structure of **TQ** (a) and **OQ** (b) crystals

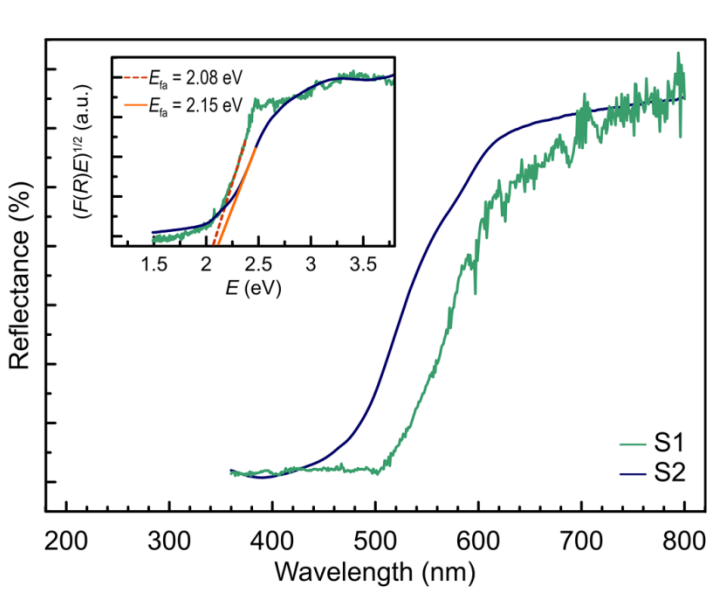


Figure S5 Kubelka-Munk graph for experimental band gap estimation for **OQ** (blue line) and **TQ** (green line) samples