S U P P L E M E N T A R Y M A T E R I A L S

2-(5,6-Diphenyl-1,2,4-triazin-3-yl)pyridinium dichloroiodate (I)

M. Carla Aragoni[1], Vito Lippolis[1], Annalisa Mancini[1], Anna Pintus[1], Enrico Podda[1,2*], James B. Orton[3], Simon J. Coles[3], and Massimiliano Arca[1*]

[1] Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, S.S. 554 bivio Sestu, Monserrato, 09042 Cagliari, Italy
[2] Centro Servizi di Ateneo per la Ricerca (CeSAR), Università degli Studi di Cagliari, S.S. 554 bivio Sestu, Monserrato, 09042 Cagliari, Italy
[3] UK National Crystallography Service, School of Chemistry, Faculty of Engineering and Physical Sciences, University of Southampton, Southampton SO17 1BJ, UK

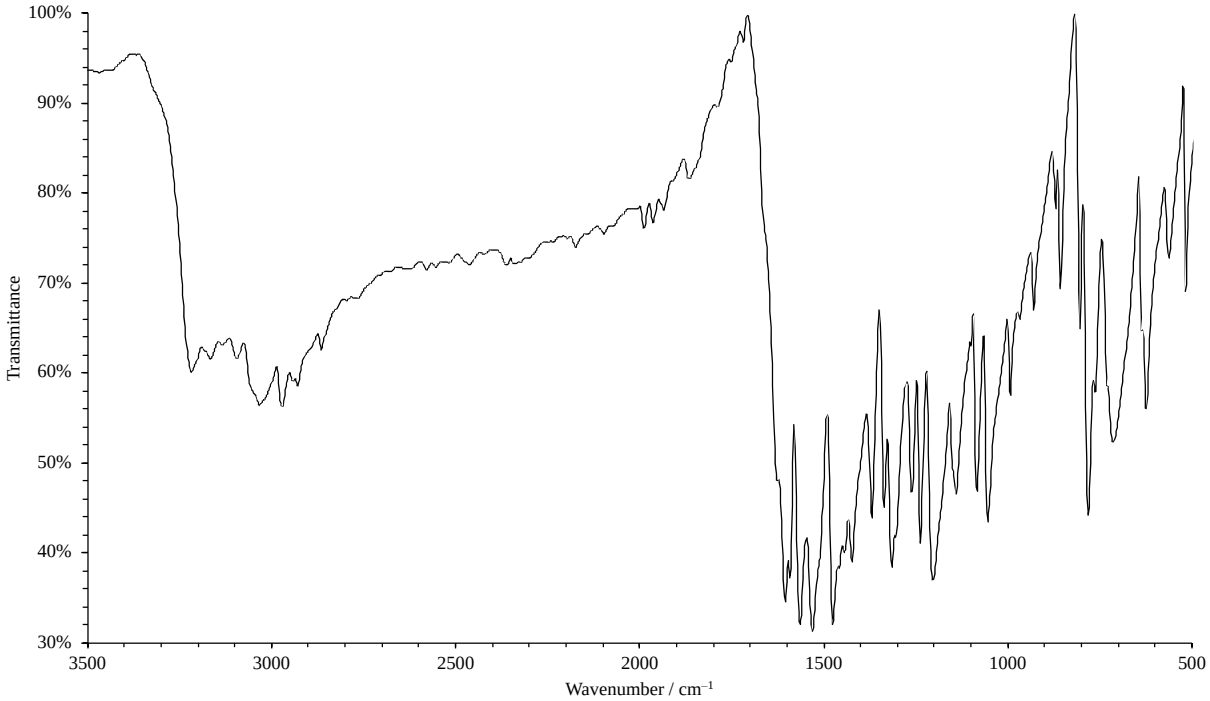

Figure S1. Solid state FT-MIR spectrum recorded for compound **1** (KBr pellet; 500–3500 cm^{-1}).

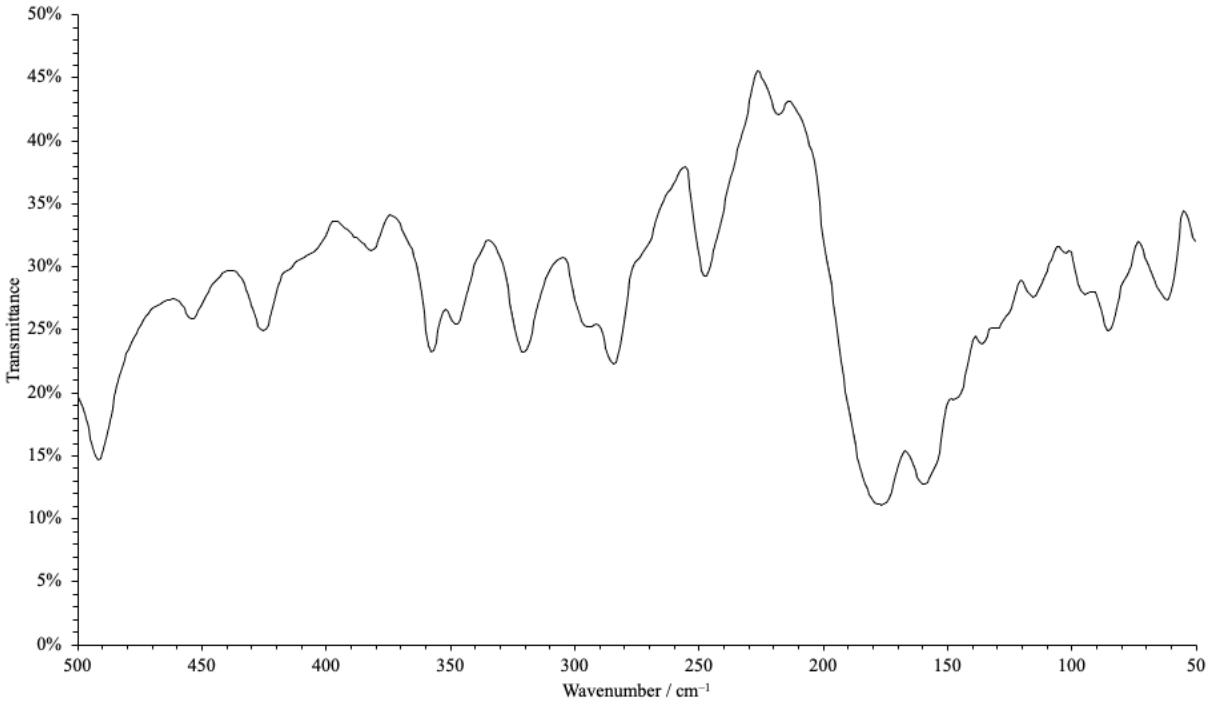

Figure S2. Solid state FT-FIR spectrum recorded for compound **1** (polythene pellet; 50–500 cm^{-1}).

Table S1 Crystal data and structure refinement parameters for compound **1.**

Empirical formula	$C_{20}H_{15}Cl_2IN_4$
Formula weight (g mol^{-1})	509.16
Temperature/K	120(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.7427(13)
b/Å	7.4326(5)
c/Å	15.5351(12)
α/°	90
β/°	100.659(7)
γ/°	90
Volume/Å^3	2013.3(3)
Z	4
ρ_{calc}g/cm^3	1.680
μ/mm^{-1}	1.868
F(000)	1000.0
Crystal size/mm^3	0.4 × 0.16 × 0.03
Radiation	Mo$K\alpha$ (λ = 0.71073)
2Θ range for data collection/°	5.958 to 55.072
Index ranges	-22 ≤ h ≤ 21, -9 ≤ k ≤ 9, -18 ≤ l ≤ 20
Reflections collected	19110
Independent reflections	4624 [R_{int} = 0.0302, R_{sigma} = 0.0297]
Data/restraints/parameters	4624/0/247
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1 = 0.0270, wR_2 = 0.0604
Final R indexes [all data]	R_1 = 0.0335, wR_2 = 0.0634
Largest diff. peak/hole / e Å^{-3}	0.64/-0.74

Table S2 Bond lengths (Å) for compound **1**.

C1−C2	1.423(3)	C10−N4	1.341(3)
C1−C4	1.475(3)	C11−C12	1.385(3)
C1−N1	1.325(3)	C12−C13	1.384(4)
C2−C15	1.479(3)	C13−C14	1.374(3)
C2−N3	1.331(3)	C14−N4	1.333(3)
C3−C10	1.473(3)	C15−C16	1.392(3)
C3−N1	1.333(3)	C15−C20	1.392(3)
C3−N2	1.329(3)	C16−C17	1.381(3)
C4−C5	1.398(3)	C17−C18	1.384(4)
C4−C9	1.391(3)	C18−C19	1.384(4)
C5−C6	1.383(3)	C19−C20	1.380(3)
C6−C7	1.381(3)	N2−N3	1.337(3)
C7−C8	1.383(3)	Cl1−I1	2.4860(7)
C8−C9	1.385(3)	Cl2−I1	2.6003(6)
C10−C11	1.379(3)		

Table S3 Bond angles (°) for compound **1**.

C2–C1–C4	125.47(19)	N4–C10–C11	119.0(2)
N1–C1–C2	118.93(19)	C10–C11–C12	119.1(2)
N1–C1–C4	115.60(18)	C13–C12–C11	120.1(2)
C1–C2–C15	123.71(19)	C14–C13–C12	118.8(2)
N3–C2–C1	120.6(2)	N4–C14–C13	119.8(2)
N3–C2–C15	115.72(18)	C16–C15–C2	120.5(2)
N1–C3–C10	116.85(19)	C16–C15–C20	119.2(2)
N2–C3–C10	116.57(19)	C20–C15–C2	120.31(19)
N2–C3–N1	126.6(2)	C17–C16–C15	120.2(2)
C5–C4–C1	122.19(19)	C16–C17–C18	120.2(2)
C9–C4–C1	118.2(2)	C19–C18–C17	120.1(2)
C9–C4–C5	119.6(2)	C20–C19–C18	119.9(2)
C6–C5–C4	119.4(2)	C19–C20–C15	120.5(2)
C7–C6–C5	120.7(2)	C1–N1–C3	116.46(19)
C6–C7–C8	120.2(2)	C3–N2–N3	117.45(18)
C7–C8–C9	119.7(2)	C2–N3–N2	119.67(18)
C8–C9–C4	120.4(2)	C14–N4–C10	123.2(2)
C11–C10–C3	123.4(2)	Cl1–I1–Cl2	178.27(2)
N4–C10–C3	117.55(19)		

Table S4. Optimized geometry calculated at DFT level (mPW1PW functional; def2-SVP basis set) for **L** in orthogonal Cartesian coordinate format.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.718583	-0.966005	-0.104529
2	6	1.859275	-0.442680	-0.042828
3	6	-0.263370	0.383559	-0.104321
4	6	-1.113009	1.583976	-0.275955
5	6	-2.282716	1.566541	-1.049229
6	6	-0.686744	2.794565	0.289730
7	6	-3.018316	2.732795	-1.235042
8	1	-2.611602	0.641085	-1.522427
9	6	-1.434247	3.954442	0.115034
10	1	0.244452	2.804424	0.856970
11	6	-2.602721	3.926595	-0.645765
12	1	-3.920875	2.709598	-1.847898
13	1	-1.099021	4.888275	0.569554
14	1	-3.186417	4.838038	-0.787066
15	6	-2.110138	-1.418678	0.108221
16	6	-2.578999	-2.555266	-0.565704
17	6	-2.950776	-0.780662	1.031589
18	6	-3.869862	-3.024182	-0.342206
19	1	-1.912253	-3.064144	-1.261862
20	6	-4.237205	-1.259088	1.260203
21	1	-2.591506	0.088542	1.584180
22	6	-4.703547	-2.377045	0.569165
23	1	-4.226407	-3.903955	-0.880759
24	1	-4.878152	-0.757797	1.987380
25	1	-5.714811	-2.747481	0.746246
26	6	3.316865	-0.233231	0.161829
27	6	4.207540	-1.301618	-0.008099
28	6	5.009050	1.199341	0.703765
29	6	5.563951	-1.069277	0.187752
30	1	3.818579	-2.279614	-0.287593
31	6	5.980555	0.208265	0.551540
32	1	5.300468	2.214194	0.994756
33	1	6.286573	-1.877212	0.059585
34	1	7.034085	0.437323	0.717604
35	7	0.176899	-1.938564	-0.295788
36	7	1.455704	-1.689418	-0.317524
37	7	1.039180	0.598983	0.008366
38	7	3.713680	0.990316	0.513831

Table S5. Optimized geometry calculated at DFT level (mPW1PW functional; def2-SVP basis set) for H**L**$^{+}$ in orthogonal Cartesian coordinate format.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.042665	0.044362	-0.011807
2	6	-0.121419	0.061104	2.595831
3	6	1.186022	0.064952	0.736926
4	6	2.535660	-0.055626	0.159904
5	6	2.790576	-0.944802	-0.895883
6	6	3.597386	0.670231	0.720333
7	6	4.085572	-1.101628	-1.376595
8	1	1.978450	-1.528942	-1.329962
9	6	4.886230	0.527904	0.218313
10	1	3.399945	1.364614	1.537926
11	6	5.132702	-0.360686	-0.828214
12	1	4.279145	-1.806487	-2.186138
13	1	5.703326	1.112181	0.643747
14	1	6.145127	-0.476976	-1.217953
15	6	-0.159536	0.243655	-1.463377
16	6	-1.209323	-0.383317	-2.156164
17	6	0.699252	1.112912	-2.157688
18	6	-1.373580	-0.170088	-3.519336
19	1	-1.887284	-1.039465	-1.610934
20	6	0.515428	1.337730	-3.516460
21	1	1.499143	1.634834	-1.632110
22	6	-0.513101	0.689923	-4.201928
23	1	-2.181140	-0.673455	-4.052495
24	1	1.176400	2.026198	-4.044501
25	1	-0.647656	0.861499	-5.271064
26	6	-0.201527	0.155391	4.059451
27	6	-1.375176	0.100645	4.806030
28	6	1.090005	0.396656	6.034136
29	6	-1.291363	0.198296	6.190612
30	1	-2.319684	-0.018061	4.276214
31	6	-0.047469	0.350019	6.816416
32	1	2.096875	0.507680	6.436340
33	1	-2.200505	0.157276	6.792779
34	1	0.038657	0.429054	7.899482
35	7	-1.198631	-0.144211	0.636081
36	7	-1.247176	-0.177164	1.939629
37	7	1.091738	0.154721	2.058111
38	7	0.973780	0.298327	4.701178
39	1	1.789269	0.318183	4.075001