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ELECTRONIC SUPPLEMENTARY INFORMATION

Mixed valence trimers in cation radical salts of TMTTF with the planar bis(6-sulfo-8-quinolato) platinum complex $[Pt(qS)_2]^{2-}$

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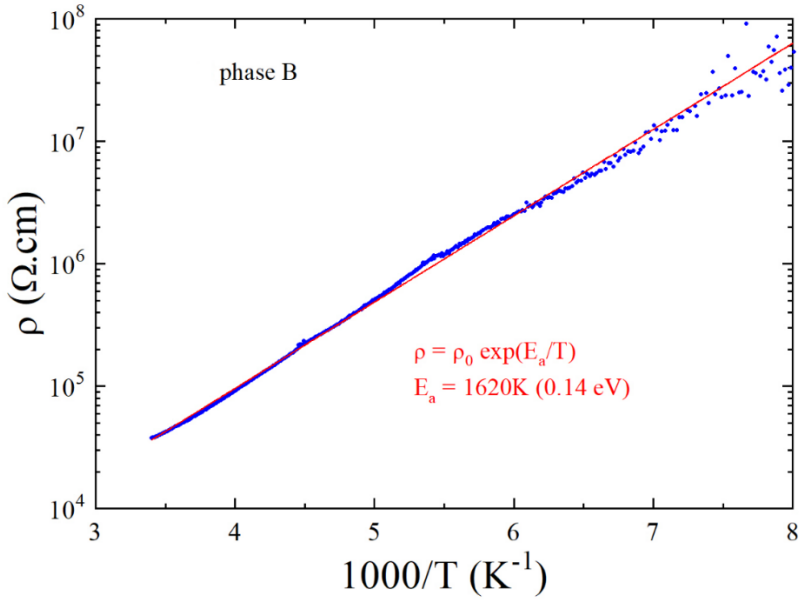

Figure S1. Electrical resistivity ρ plotted as log ρ *versus* the inverse temperature for the B phase $(TMTTF)_3[Pt(qS)_2]$. The red line is the fit to the data with the law $\rho = \rho_0 \exp(E_a/T)$ giving the activation energy E_a = 1620 K.

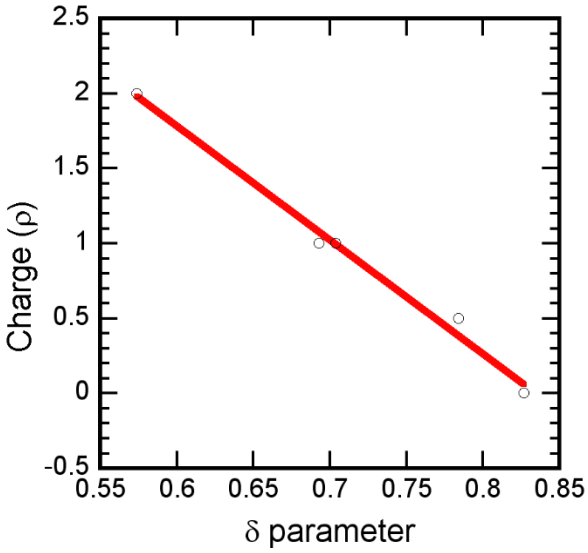

Figure S2. Linear relationship between the structural parameter δ (see text) and the charge ρ of the TMTTF molecule, established from reported structures (Cf Table 2) without ambiguity on the charge.

Infrared and Raman spectra of $[Pt(qS)_2]^{2-}$ anion

Room temperature Raman and IR spectra of $[Pt(qS)_2]K_2$ and $[Pt(qS)_2]Na_2$ powders are displayed in Figure S3 and Figure S4, respectively. As could be expected, there is nearly no difference between vibrational bands of both compounds. The most important vibrational features of $[Pt(qS)_2]^{2-}$ anion, together with the results of numerical calculations of normal modes and proposed assignment, are collected in Table S1.

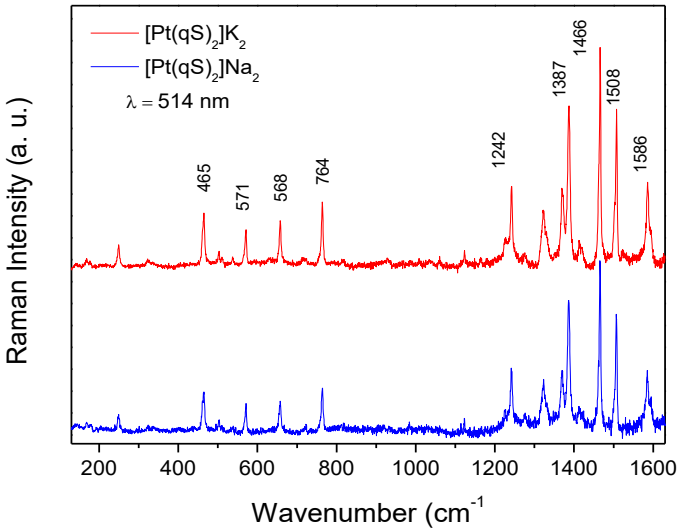

Figure S3. Raman spectra of the salts $[Pt(qS)_2]K_2$ and $[Pt(qS)_2]Na_2$ (excit. λ = 514.5 nm).

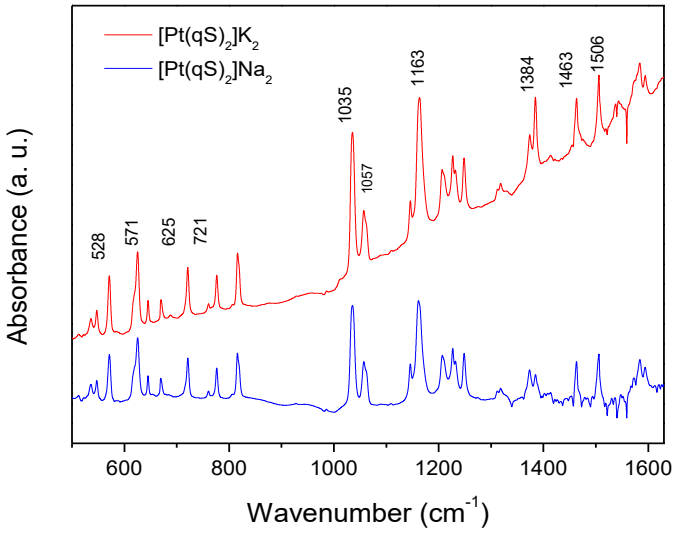

Figure S4. Infrared spectra of the salts $[Pt(qS)_2]K_2$ and $[Pt(qS)_2]Na_2$.

Table S1. Vibrational spectra of $[Pt(qS)_2]^{2-}$ anion.

Experiment $[Pt(qS)_2]X_2$ (X=Na, K)		Theory $[Pt(qS)_2]^{2-}$	Assignment*
Raman (cm^{-1})	IR (cm^{-1})	(cm^{-1})	
1586	-	1623	CCs+CNs+COs+CCHb
1508	1506	1534	CCs+CCHb+CNs+COs « s »
-	-	1533	CCs+CCHb+CNs+COs « as »
1466	-	1485	CCHb+CCs+CNs+COs « s »
-	1463	1482	CCHb+CCs+CNs+COs « as »
1387	-	1445	CCs+CCHb
-	1384	1410 ?	HCNb+CCs
-	1374	-	
1370	-	1426	CCHb+CNs+CCs
1323	-	1350	CNs+CCs+CCHb « s »
-	1318	1350	CNs+CCs+CCHb « as »
-	1248	1297	COs+CCHb+CCCb
1242	-	1270	CCHb+CNs « s »
-	1227	1265	CCHb+CNs « as »
-	1163	1154 ?	CCHb
-	1146	-	
-	1057	?	
-	1035	?	
-	816	886	SOs+CHb oop+CCCb oop
-	777	828	CCCb (in-plane rings def)
764	-	763	CCCb+PtOs+PtNs+CNCb
-	721	734	SOs+CCCb
658	-	671	PtNs+CCCb+CNCb+PtOs
-	670	685	NptNb oop+rings def oop
-	645	671	PtOs+PtNs+in-plane rings def
-	625	652	PtOs+CCOb
571	-	558	breathing mode« s »

-	571	558	breathing mode« as »
-	547	?	
-	536	?	
503	-	513	CCCb
465	-	460	OSOb+NPtOb
-	471	468	SO_3 umbrella mode+CCCb
249	-	256	SO_3w/r+in-plane rings def

* s – stretching, b – bending, w – wagging, r – rocking, oop – out-of-plane, def – deformation, « s » - symmetric, « as » - antisymmetric

Polarized IR reflectance of $(TMTTF)_3[Pt(qS)_2]$

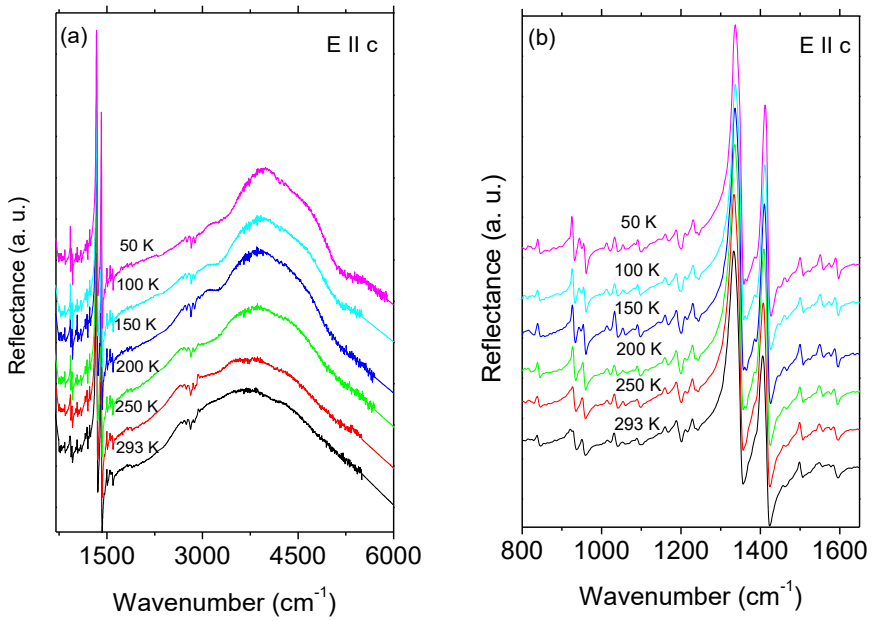

Figure S5. (a) Temperature dependence of the reflectance spectra of $(TMTTF)_3[Pt(qS)_2]$; (b) within the region of strong vibrational features (polarization $E \parallel c$).

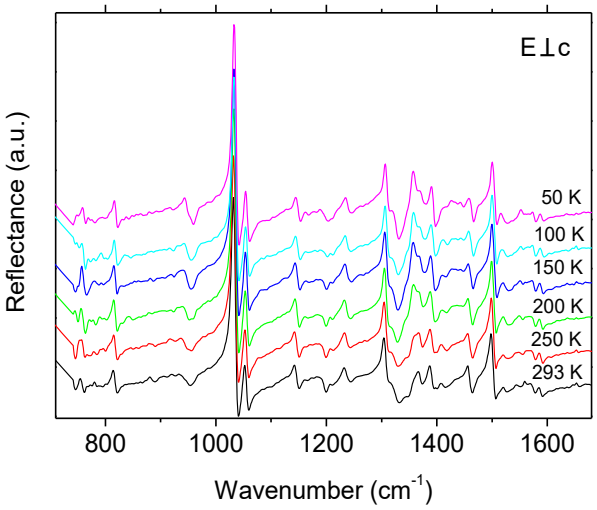

Figure S6. Temperature dependence of reflectance spectra of $(TMTTF)_3[Pt(qS)_2]$ within the region of strong vibrational features (polarization $E \perp c$).