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Structure and properties of radical anion and dianion salts of organic dye trans-perinone and its mixed salt with gallium(III) phthalocyanine

Maxim A. Faraonov, Nikita R. Romanenko, Maxim V. Mikhailenko, Alexey V. Kuzmin, Salavat S. Khasanov, Dmitri V. Konarev

Supporting information

Crystal structure

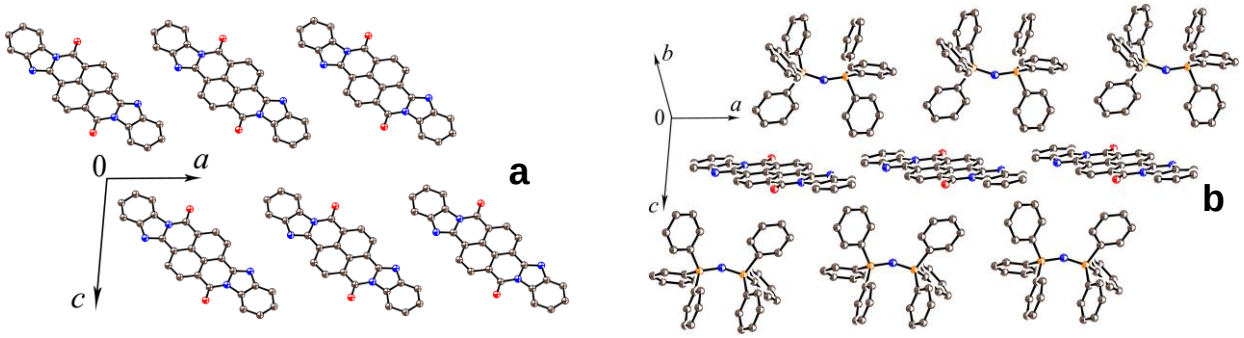

Figure S1. Crystal structure of $\{PPN^{+}\}_2[perinone^{2-}] \cdot 2C_6H_4Cl_2$ (**1**). Views on (a) and along (b) the layers from dianions $perinone^{2-}$.

Optical properties

Table S1. IR spectra of starting compounds and salts **1** and **2**

Components	Cryptand	PPNCl	Perinone	**1**	**2**
Perinone			436w	443w	441w
			462w	462w	462w
			512w	513s	523m
			-	-	537s
			570w	574w	-
			591w	594w	-
			621m	623m	630w
			734m	731w*	744m*
			748m	-	748m
			759s	753s	757m*
			773m	773w	-
			794w	794w	792w
			839w	827m	-
			875w	872m	-
			902m	902m	903w
			991m	985m*	997w
			1010m	1008m	1005w
			1100w	1100s*	1084w
			1133w	-	1116s
			1153w	1155w	-
			1233m	1235s	-
			1285m	1284s	1289s
			1313m	1300w*	1316m
			1337w	1330m	
			1351s	1354m	1363m
			1384s	1394m	1382w
			1432w	1434w	1438s
			1445m	1448s*	1445s
			-	-	1466m
			-	-	1473m
			1480w	1477m	1483w*
			1494w	-	
			-	-	1524s
			1551w	1543s	-
			1579w	1585w	-
Cation			1612w	1603s	-
			1697s (C=O)	1632s(C=O)	1614s(C=O)
				Cryptand(K^+)	PPN^+
	476w	500s		-	502m
	528w	531s		524w	527m
	581w	550s		-	548s
	735m	694m		731w*	691s
	922m	724m		921w	723s
	948w	746m		946m	744m*
	982m	754m		985m*	757m*
	1038w	1024w		1022m	1028w*
	1071m	1250s		1077s	1218w
	1100s	1439s		1100s*	1245m
	1127s	1483m		1127s	1483w*
	1213w	1575w		1216s	1569s
	1295m	1587m		1300w*	1581s
	1329m			-	
	1360s			1359m	
	1446m			1448s*	
	1462m			-	
	1490w			1504m	
	2790w			-	
	2877w			-	
	2943w			-	
Solvent					$C_6H_4Cl_2$
	653m				-
	757m				757m*
	1035w				1028w*
	1456s				-

* - bands are coincided

w – weak, m –middle and s – strong intensity

Table S2. IR spectra of starting compounds and salt **3**

Components	Cryptand	Perinone	GaClPc	**3**
perinone		436w		441w
		462w		460w
		512w		518w
		570w		572w*
		591w		585m*
		621m		624m
		734m		732s*
		748m		-
		759s		755s*
		773m		772w
		794w		794w
		839w		830m
		875w		-
		902m		902w
		991m		985w*
		1010m		1009w
		1100w		1101s*
		1133w		-
		1153w		1154w
		1233m		1221m
		1285m		1285s*
		1313m		-
		1337w		-
		1351s		1354m
		1384s		-
		1432w		1434w
		1445m		1444m*
		1480w		1474w
		1494w		-
		1551w		-
		1579w		1571w
		1612w		-
		1697s(C=O)		1626s(C=O)
GaClPc			507w	507w
			572w	572w*
			733s	732s*
			755m	755s*
			780m	-
			897m	894w
			1062s	-
			1121s	1120s*
			1169m	1168m
			1288m	-
			1332s	-
			1423m	1423m
			3050w	-
Cryptand	476w			-
	528w			-
	581w			585m*
	735m			732s*
	922m			-
	948w			948m
	982m			985w*
	1038w			1031w*
	1071m			1080s
	1100s			1101s*
	1127s			1120s*
	1213w			-
	1295m			1285s*
	1329m			1329m
	1360s			1359m
	1446m			1444m*
	1462m			1458m*
	1490w			1502w
	2790w			-
	2877w			-
	2943w			-
Solvent				$C_6H_4Cl_2$
	653m			654s
	757m			755s*
	1035w			1031w*
	1456s			1458m*

* - bands are coincided

w – weak, m –middle and s – strong intensity

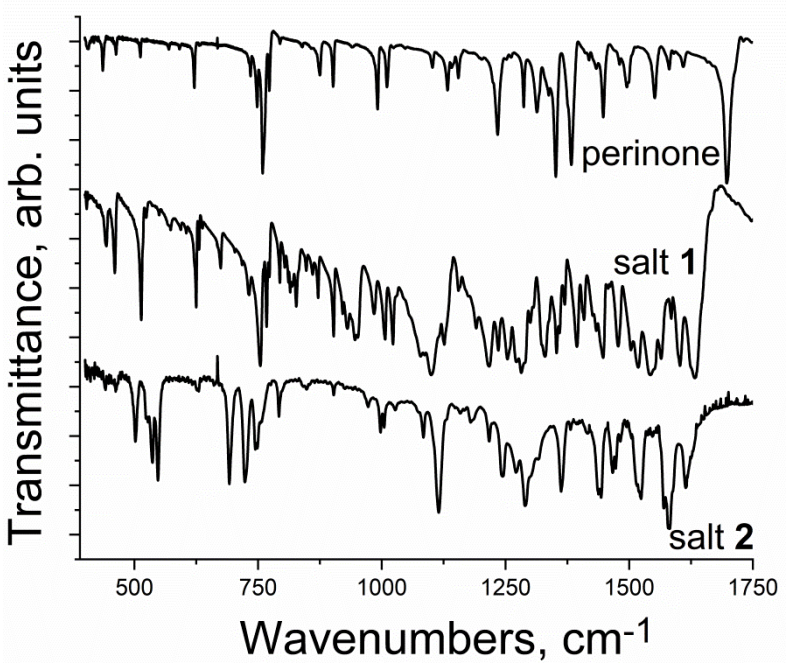

Figure S2. IR spectra of starting perinone and salts {cryptand(K^+)}[perinone$^{\bullet-}$] (**1**) and {PPN^+}$_2$[perinone^{2-}]·2$C_6H_4Cl_2$ (**2**) in KBr pellets prepared in anaerobic condition.

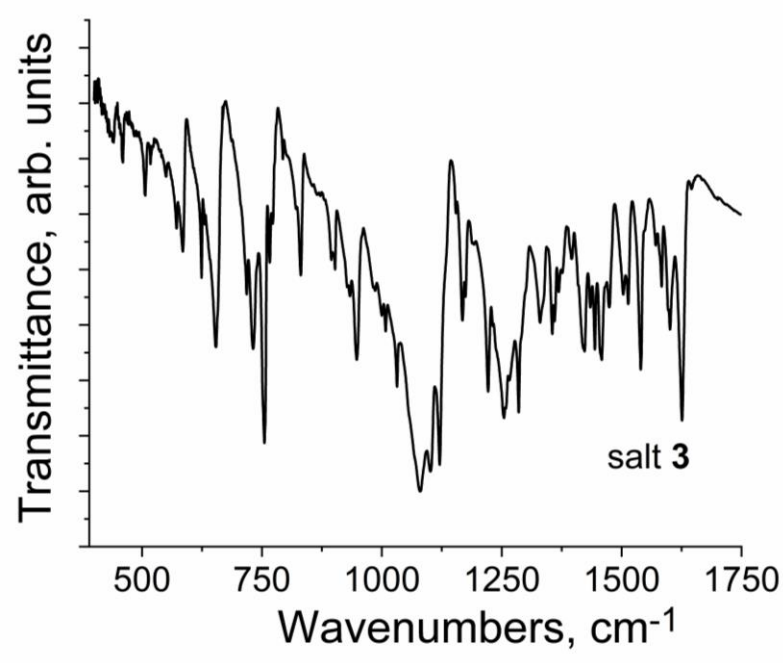

Figure S3. IR spectra of salt {PPN^+}$_2$[(perinone)$_{0.5}$(GaClPc)]$^-$·3$C_6H_4Cl_2$ (**3**) in KBr pellets prepared in anaerobic condition.

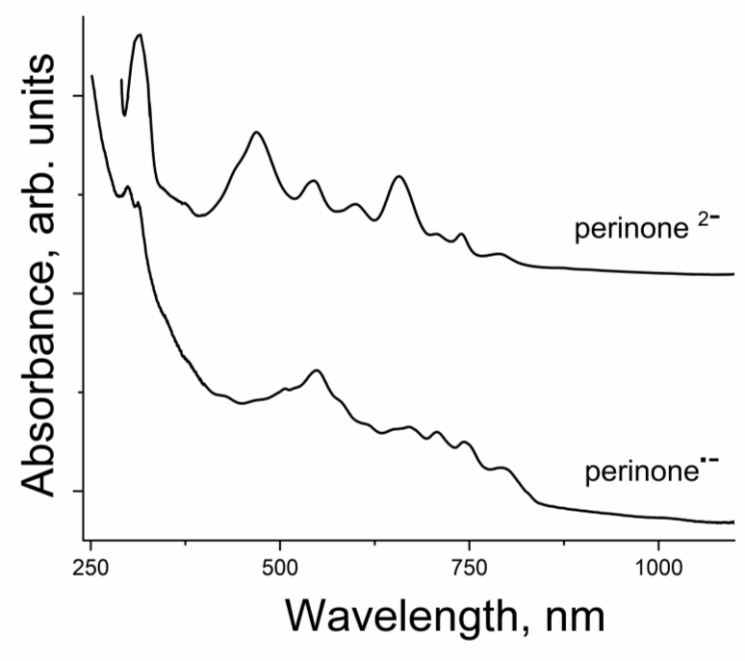

Figure S4 UV-visible-NIR spectra of perinone$^{\bullet-}$ and perinone^{2-} *o*-dichlorobenzene solution prepared in anaerobic conditions.

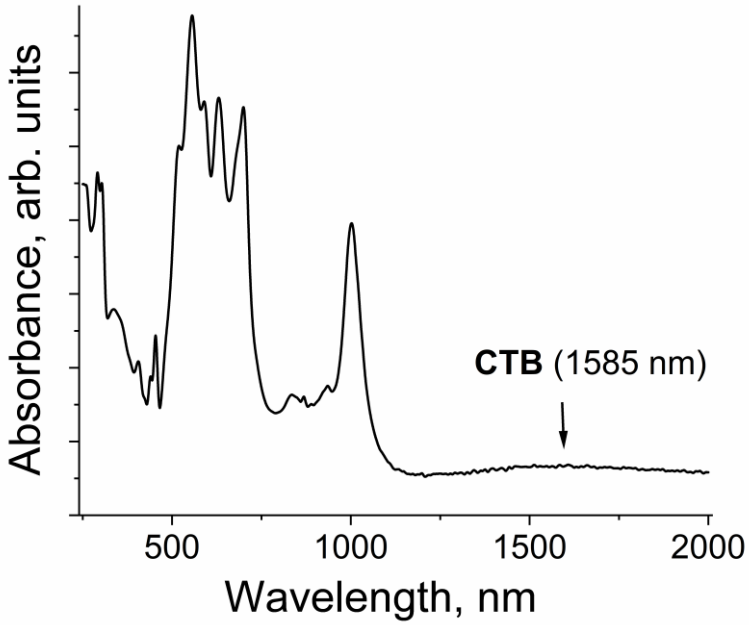

Figure S5. UV-visible-NIR spectra of salts **3** in KBr pellets in anaerobic conditions.

Magnetic measurements

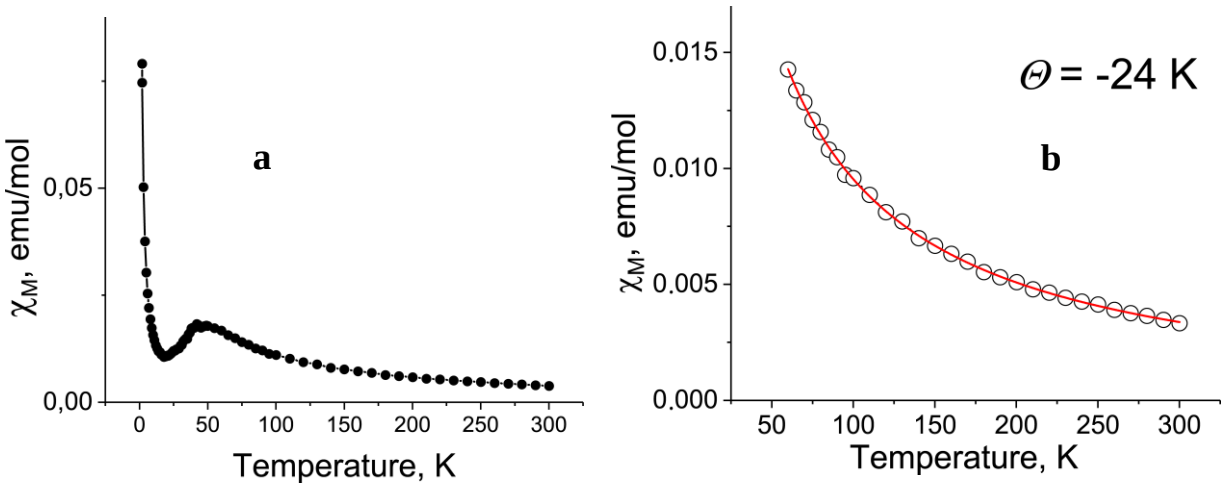

Figure S6. Temperature dependence of molar magnetic susceptibility of **1**: (a) experimental curve approximated by two contributions from 5% of paramagnetic Curie impurities and bulk sample and (b) molar magnetic susceptibility in the 60-300 K range fitted well by the Curie-Weiss law with Weiss temperature of -24K.

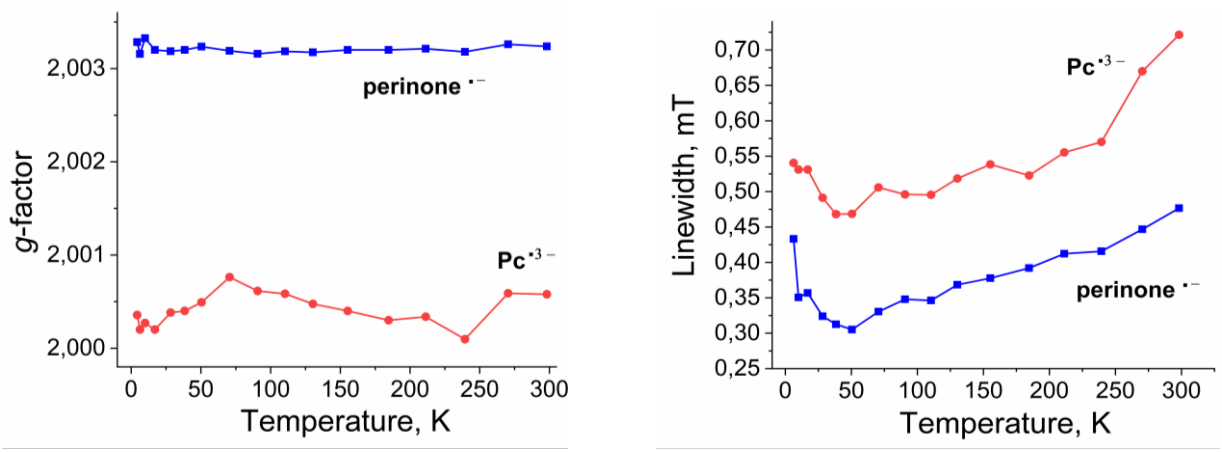

Figure S7. Temperature dependence of *g*-factor and linewidth of lines manifested in the EPR spectra of salt **3.**