

Supporting information

Crystalline salts of anionic free-base tetrapyrazinoporphyrazines with alkyl-substituents or an extended π -electron system

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IR spectra

Table S1. IR-spectra (cm⁻¹ in KBr) of starting macrocycles and salts **1-3**.

Components	PPN ⁺	Cryptand	H ₂ TPyzPzMe ₈	1	H ₂ TPyzPzEt ₈	2	H ₂ T(PhnPyz)Pz	3
Macroheterocycle			447w	447w	-	442m	405m	-
			556w	-	540w	534s*	442s	442w
			686m	-	590w	-	498w	-
			696m	-	617w	615w	555s	557w
			748m	752m*	667w	-	592w	-
			802m	791w	694m	692s	613s	613w
			978w	972m	719m	723s*	619m	627w
			1001w	977w	748m	748m	663w	-
			1032m	1031w*	800s	800s	691s	-
			1101w	1074w	953w	942w	706s	706m
			1136s	1115s	1042s	1032m*	725s	723m*
			1184w	1182w	1099m	-	745s	743w
			1207w	1211w	1132s	1115s	758s	754m*
			1233m	-	1179s	1161m	793w	-
			1261m	1261m*	1200s	1202m	804w	804s
			1310w	1300m	1240m	-	824w	-
			1336s	1335m	1261s	1263s	843w	-
			1367w	-	1292s	1294s	866w	878m
			1385s	1385w	1325w	1354w	937s	-
			1441m	1437s*	1383m	1377w	1016m	1020s*
			1504m	-	-	1410m	1040m	-
			1537m	-	1429w	1437s	1065m	-
			1634s	-	1456m	1456m	1090m	-
			1728m	-	1504w	1504w	1113w	-
					1557m	1557w	1146s	-
					1634s	1614m	1184m	1194w
					1674m	-	1223m	1223w
					1732m	1732w	1250m	1261s
					2334w	-	1283m	-
					2359w	2355w	1362s	1360w
					2855m	2855s	1437m	1425m
					2878w	-	1508w	-
					2926s	2926s	1551m	1555w
					2965s	2961s	1605s	-
					3296w	-	1638s	1631m
							1686m	
							1735m	
Cation				501s		501s		523w
				534s		534s*		575w
				548s		548s		-
				692s		692s		-
				723s		723s*		951m
				-		-		-
				-		-		-
				752s*		1032m*		-
				1031w*		1263s*		1103s
				1261m*		1437s*		-
				1437s*		-		-
				1481w		-		1296w
				-		-		1335w
				1587w		1585s		1360w*
								-
								-
								-
								-
								2870s
								-
Solvent				C ₆ H ₄ Cl ₂		C ₆ H ₄ Cl ₂		C ₆ H ₄ Cl ₂
				752m*		1032m*		754m*
				1031w*		1456m*		1454m*
				1456w				

w – weak, m –middle and s – strong intensity. * - bands are coincided

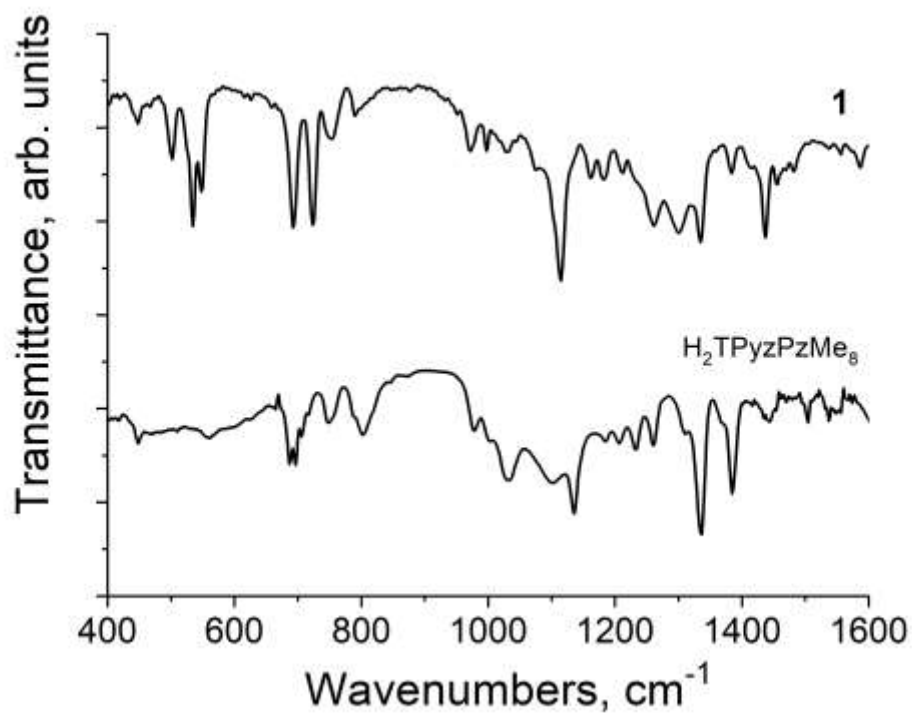


Figure S1. IR spectra of starting H₂TPyzPzMe₈ and salt **1** in KBr pellets prepared in anaerobic condition.

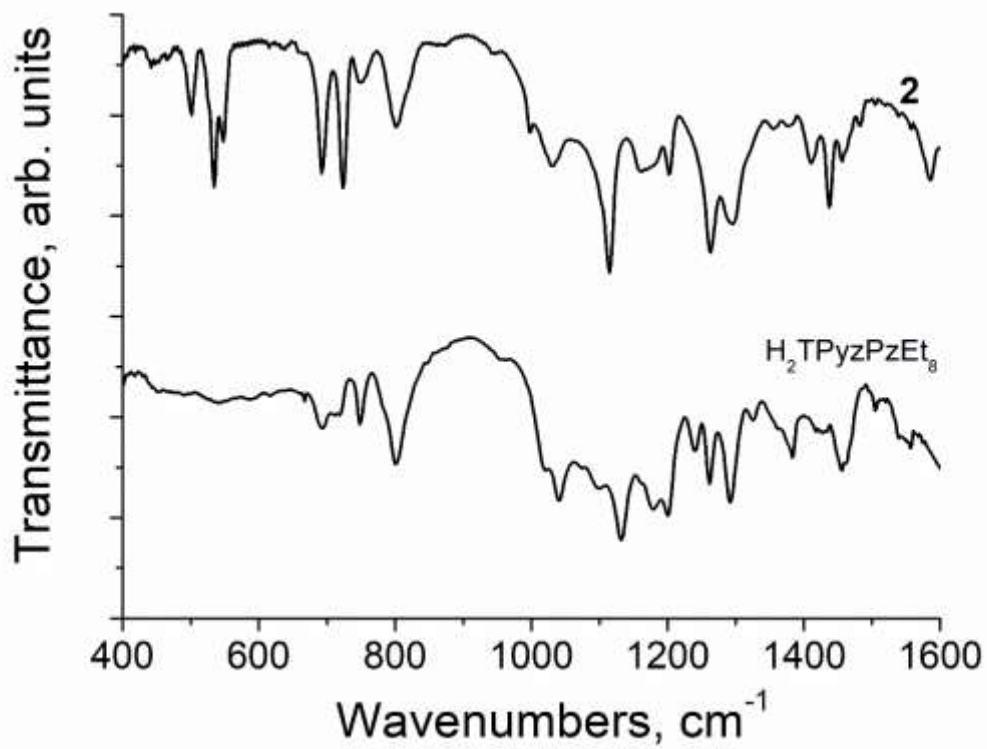


Figure S2. IR spectra of starting H₂TPyzPzEt₈ and salt **2** in KBr pellets prepared in anaerobic condition.

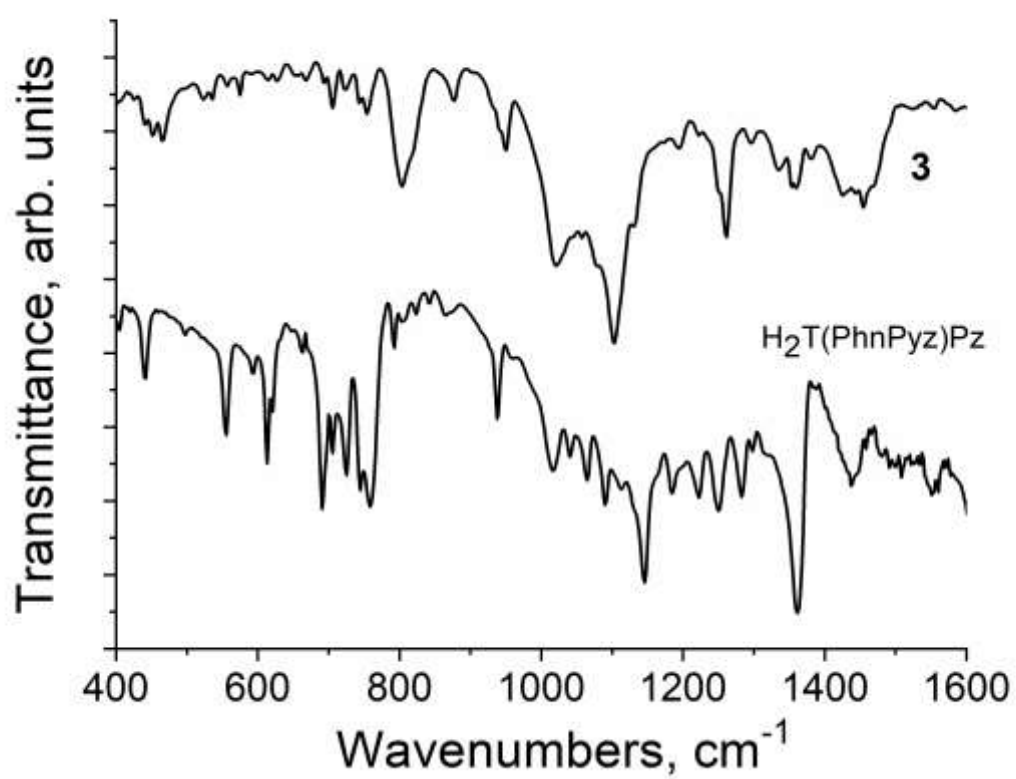


Figure S3. IR spectra of starting H₂T(PhnPyz)Pz and salt 3 in KBr pellets prepared in anaerobic condition.