Thin films of chlorosubstituted vanadyl phthalocyanine: charge transport properties and optical spectroscopy study of structure

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Supporting Information

Thin Films of Chlorosubstituted Vanadyl Phthalocyanine: Charge Transport Properties and Optical Spectroscopy Study of Structure

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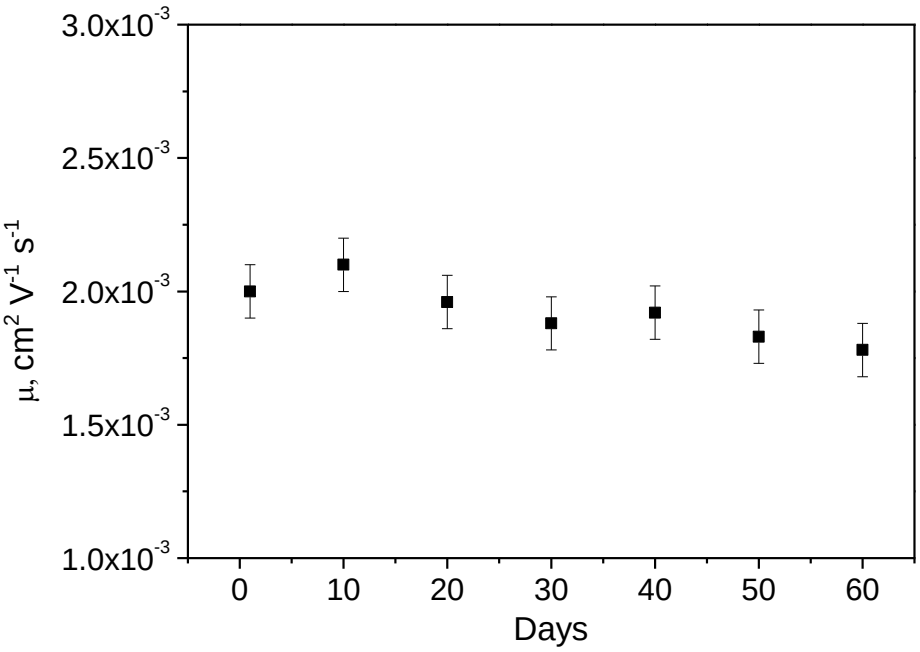

Figure S1. Charge carrier mobility in $VOPcCl_{16}$ organic field-effect thin film transistor upon exposure to air as a function of time.

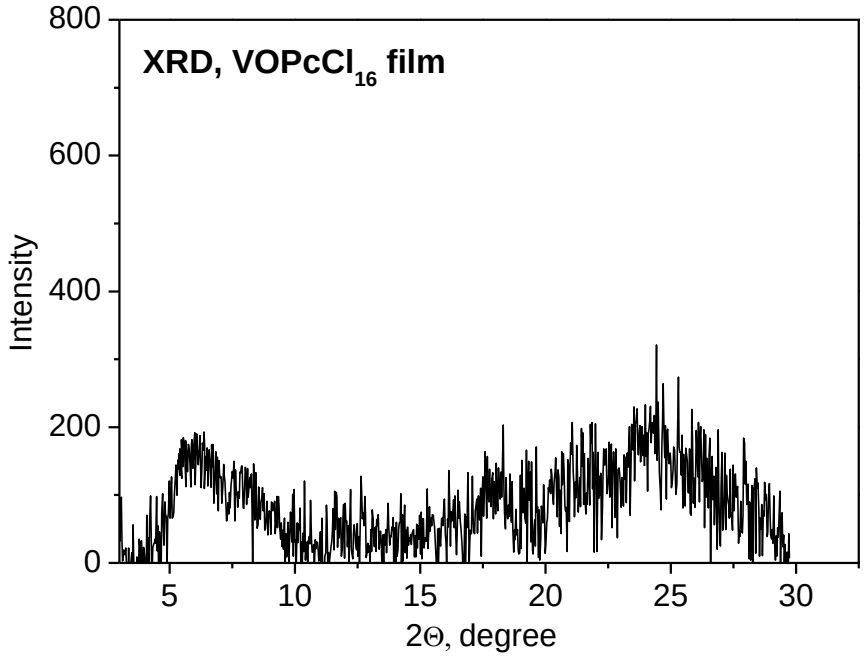

Figure S2. X-ray diffraction pattern of a $VOPcCl_{16}$ film.

Table S1. The B3LYP/6-311++G(2df,p) optimized geometry of the $VOPcCl_{16}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	2.331031
2	23	0	0.000000	0.000000	0.757308
3	7	0	0.000000	1.975439	0.208666
4	7	0	-1.961186	0.000000	0.118702
5	7	0	0.000000	-1.975439	0.208666
6	7	0	1.961186	0.000000	0.118702
7	7	0	2.360020	2.372104	0.086477
8	7	0	-2.360020	2.372104	0.086477
9	7	0	-2.360020	-2.372104	0.086477
10	7	0	2.360020	-2.372104	0.086477
11	6	0	1.117413	2.764597	0.273058
12	6	0	0.704189	4.147515	0.491723
13	6	0	1.418919	5.325338	0.703257
14	6	0	0.704449	6.512151	0.892521
15	6	0	-0.704449	6.512151	0.892521
16	6	0	-1.418919	5.325338	0.703257
17	6	0	-0.704189	4.147515	0.491723
18	6	0	-1.117413	2.764597	0.273058
19	6	0	-2.730977	1.117732	-0.074475
20	6	0	-4.075137	0.703841	-0.463384
21	6	0	-5.215732	1.418870	-0.827481
22	6	0	-6.368521	0.704431	-1.166518
23	6	0	-6.368521	-0.704431	-1.166518
24	6	0	-5.215732	-1.418870	-0.827481
25	6	0	-4.075137	-0.703841	-0.463384
26	6	0	-2.730977	-1.117732	-0.074475
27	6	0	-1.117413	-2.764597	0.273058
28	6	0	-0.704189	-4.147515	0.491723
29	6	0	-1.418919	-5.325338	0.703257
30	6	0	-0.704449	-6.512151	0.892521
31	6	0	0.704449	-6.512151	0.892521
32	6	0	1.418919	-5.325338	0.703257
33	6	0	0.704189	-4.147515	0.491723
34	6	0	1.117413	-2.764597	0.273058
35	6	0	2.730977	-1.117732	-0.074475
36	6	0	4.075137	-0.703841	-0.463384
37	6	0	5.215732	-1.418870	-0.827481
38	6	0	6.368521	-0.704431	-1.166518
39	6	0	6.368521	0.704431	-1.166518
40	6	0	5.215732	1.418870	-0.827481
41	6	0	4.075137	0.703841	-0.463384
42	6	0	2.730977	1.117732	-0.074475
43	17	0	-7.805482	-1.552922	-1.604626
44	17	0	-7.805482	1.552922	-1.604626
45	17	0	-5.225200	3.139559	-0.890619

46	17	0	-5.225200	-3.139559	-0.890619
47	17	0	-3.139367	-5.337983	0.773342
48	17	0	-1.553374	-7.991941	1.148968
49	17	0	1.553374	-7.991941	1.148968
50	17	0	3.139367	-5.337983	0.773342
51	17	0	5.225200	-3.139559	-0.890619
52	17	0	7.805482	-1.552922	-1.604626
53	17	0	7.805482	1.552922	-1.604626
54	17	0	5.225200	3.139559	-0.890619
55	17	0	-3.139367	5.337983	0.773342
56	17	0	-1.553374	7.991941	1.148968
57	17	0	1.553374	7.991941	1.148968
58	17	0	3.139367	5.337983	0.773342

Table S2. The experimental and calculated (B3LYP/6-311++G(2df,p)) Raman and IR wavenumbers (cm^{-1}) of the $VOPcCl_{16}$.

Experimental wavenumbers		Calculated wavenumbers	Calculated IR intensities	Sym-metry	Assignment
Raman	IR				
	205	209	1.82	B_2	O-V-N_α, N_β, C_γ and C_δ out-of-plane motions
	222	218	0.0879	A_1	C_β-C_γ-Cl, C_γ-C_δ-Cl, $C_{\beta'}$-$C_{\gamma'}$-Cl, $C_{\gamma'}$-$C_{\delta'}$-Cl, N_α-N_β
223		229	0	A_2	N_α-V-N_α, C_β-C_γ-Cl, C_γ-C_δ-Cl, $C_{\beta'}$-$C_{\gamma'}$-Cl, $C_{\gamma'}$-$C_{\delta'}$-Cl, N_α-V=O
	236	235	0.12	A_1	C_γ-C_δ-Cl, $C_{\gamma'}$-$C_{\delta'}$-Cl, N_α-V-N_α
238		235	0.06	B_1	$C_{\beta'}$-$C_{\gamma'}$-Cl, $C_{\gamma'}$-$C_{\delta'}$-Cl, N_α-V-N_α
	259	254	0.61	A_1	V-N_α, N_α, C_γ and C_δ out-of-plane motions
	276	271	2.21	B_1	$N_{\alpha'}$, N_β out-of-plane motions, V-$N_{\alpha'}$
290		284	1.87	B_2	N_α-V=O, N_α out-of-plane motions
298	294	297	0. 39	B_2	V-N_α, N_α-V=O, C_β-C_γ-C_δ, $C_{\beta'}$-$C_{\gamma'}$-Cl
	310	304	0.09	B_1	V-$N_{\alpha'}$, $N_{\alpha'}$-V=O, $C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$, C_β-C_γ-Cl
320		332	0.01	A_1	$C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$, C_β-C_γ-C_δ, V-N_α, V-$N_{\alpha'}$
334	330	340	9.78	B_2	benzene ring deformations (OP), N_α-V=O
		342	8.25	B_1	benzene ring deformations (OP), $N_{\alpha'}$-V=O
349	343		0.60	B_1	$N_{\alpha'}$-V=O, benzene ring deformations (IP)
		350	0.37	B_2	N_α-V=O, benzene ring deformations (IP)
369	365	375	3.92	B_1	$C_{\gamma'}$ and C_β out-of-plane motions, $N_{\alpha'}$-V=O, $N_{\alpha'}$-V
374	374	377	4.29	B_2	C_γ and $C_{\beta'}$ out-of-plane motions, N_α-V=O, N_α-V
	384	378	2.23	A_1	N_β, $C_{\beta'}$, C_β out-of-plane motions
420	417	391	1.37	B_1	V- $N_{\alpha'}$, $N_{\alpha'}$-V=O, C_β-C_γ-C_δ
		393	2.45	B_2	V- N_α, N_α-V=O, $C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$
456	462	455	5.68	A_1	macroring breathing, V-N_α, V-$N_{\alpha'}$
	506	506	59.42	B_1	V- $N_{\alpha'}$, benzene def., N_β-C_α-C_β, N_β-$C_{\alpha'}$-$C_{\beta'}$, $C_{\delta'}$-Cl
		508	64.96	B_2	V- N_α, benzene def., N_β-C_α-C_β, N_β-$C_{\alpha'}$-$C_{\beta'}$, C_δ-Cl
519		516	0.14	A_1	macroring breathing, V-N_α, V-$N_{\alpha'}$
541	543	560	5.39	B_2	isoindole out-of-plane def.
		563	0.04	B_1	isoindole out-of-plane def.
590		593	0	A_2	isoindole def.
	606	610	29.45	B_1	C_γ-Cl, C_β-C_β-C_γ, $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, $C_{\gamma'}$-Cl, V-$N_{\alpha'}$
		612	23.04	B_2	$C_{\gamma'}$-Cl, $C_{\beta'}$-$C_{\beta'}$-$C_{\gamma'}$, C_α-N_α-C_α, C_γ-Cl, V-N_α

610		629	0.21	B_1	C_{γ}-Cl, C_{γ} out-of-plane motions
		628	0.77	B_2	$C_{\gamma'}$-Cl, $C_{\gamma'}$ out-of-plane motions
	646	630	0.59	A_1	C_{β}-C_{γ}-C_{δ}
648		640	0	A_2	$C_{\gamma'}$-Cl, C_{γ}-Cl, $C_{\delta'}$-Cl, C_{δ}-Cl, C_{α}-C_{β}-C_{γ}, $C_{\alpha'}$-$C_{\beta'}$-$C_{\gamma'}$
658	670	648	1.22	B_1	C_{γ}-C_{δ}-Cl, C_{β}-C_{γ}-Cl, C_{α}-C_{β}-C_{γ}, C_{α}-N_{β}-$C_{\alpha'}$
		650	1.49	B_2	$C_{\gamma'}$-$C_{\delta'}$-Cl, $C_{\beta'}$-$C_{\gamma'}$-Cl, $C_{\alpha'}$-$C_{\beta'}$-$C_{\gamma'}$, C_{α}-N_{β}-$C_{\alpha'}$
684		683	0.05	A_1	C_{α}-N_{β}-C_{α}, macroring def.
704		707	0	A_2	$N_{\alpha'}$- $C_{\alpha'}$-N_{β}, N_{α}-C_{α}-N_{β}, isoindole def., C_{γ}-Cl, $C_{\gamma'}$-Cl
719		722	0	A_2	C_{γ}, C_{γ}, C_{δ}, $C_{\delta'}$, C_{β}, $C_{\beta'}$ out-of-plane motions
742		741	0.15	A_1	C_{α}-N_{α}-C_{α}, $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, V-$N_{\alpha'}$, V-N_{α}
	747	756	57.79	B_2	macroring def.
757	755	758	73.44	B_1	macroring def.
		767	19.70	B_2	C_{α} out-of-plane motions, $C_{\alpha'}$-$C_{\beta'}$-$C_{\gamma'}$
	764	769	50.73	B_1	$C_{\alpha'}$ out-of-plane motions, C_{α}-C_{β}-C_{γ}
776	772	776	154.29	B_1	$C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, V-$N_{\alpha'}$, $C_{\gamma'}$-Cl, C_{α}-C_{β}-C_{β}
782	778	776	217.02	B_2	C_{α}-N_{α}-C_{α}, V-N_{α}, C_{γ}-Cl, $C_{\alpha'}$-$C_{\beta'}$-$C_{\beta'}$
805		783	1.97	A_1	V-N_{α}, N_{α}-C_{α}-N_{α}, inner ring breathing, N_{α}-V=O
820	819	812	7.30	A_1	macroring breathing, $C_{\delta'}$-Cl, C_{δ}-Cl, C_{γ}-Cl, $C_{\gamma'}$-Cl
	947	946	183.29	B_2	C_{β}-C_{γ}-C_{δ}, C_{γ}-Cl, isoindole def.
		949	177.53	B_1	$C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$, $C_{\gamma'}$-Cl, isoindole def.
962		954	2.42	A_1	C_{α}-N_{α}-C_{α}, $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, V-N_{α}, V-$N_{\alpha'}$, C_{β}-C_{γ}-C_{δ}, C_{γ}-Cl, $C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$, $C_{\gamma'}$-Cl
	970	958	11.75	B_1	C_{γ}-C_{δ}-C_{δ}, C_{δ}-Cl, C_{α}-C_{β}, N_{α}-C_{α}-N_{β}, $C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$, $C_{\gamma'}$-Cl
		958	11.41	B_2	$C_{\gamma'}$-$C_{\delta'}$-$C_{\delta'}$, $C_{\delta'}$-Cl, $C_{\alpha'}$-$C_{\beta'}$, $N_{\alpha'}$-$C_{\alpha'}$-N_{β}, C_{β}-C_{γ}-C_{δ}, C_{γ}-Cl
976		978	0	A_2	C_{α}-N_{β}-$C_{\alpha'}$, $C_{\gamma'}$-$C_{\delta'}$-$C_{\delta'}$, C_{γ}-C_{δ}-C_{δ}, $C_{\delta'}$-Cl, C_{δ}-Cl
1012	1007	1073	131.58	A_1	V=O
1080		1084	0	A_2	C_{α}-N_{α}, benzene deformations, $C_{\delta'}$-Cl, C_{δ}-Cl, $C_{\gamma'}$-Cl, C_{γ}-Cl
1100	1082	1101	115.34	B_2	$C_{\alpha'}$-$N_{\alpha'}$, benzene deformations, $C_{\delta'}$-Cl, $C_{\gamma'}$-Cl, C_{α}-N_{α}-C_{α}
	1088	1109	111.62	B_1	C_{α}-N_{α}, benzene deformations, C_{δ}-Cl, C_{γ}-Cl, $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$
	1139	1146	401.77	B_2	$C_{\alpha'}$-$N_{\alpha'}$, $C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$, $C_{\delta'}$-Cl, $C_{\gamma'}$-Cl, $C_{\alpha'}$-N_{β}, benzene breathing
1150	1146	1148	504.92	B_1	C_{α}-N_{α}, C_{β}-C_{γ}-C_{δ}, C_{δ}-Cl, C_{γ}-Cl, C_{α}-N_{β}, benzene breathing
1172		1187	0.02	A_1	Benzene def., C_{α}-N_{α}-C_{α}, C_{δ}-Cl, C_{γ}-Cl, $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, $C_{\delta'}$-Cl, $C_{\gamma'}$-Cl, macroring breathing
1190	1184	1191	25.49	A_1	Benzene def., C_{α}-N_{α}-C_{α}, C_{δ}-Cl, C_{γ}-Cl, $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, $C_{\delta'}$-Cl, $C_{\gamma'}$-Cl, macroring breathing
	1192	1201	491.74	B_2	C_{α}-N_{α}-C_{α}, isoindole def., C_{δ}-Cl, C_{γ}-Cl, benzene breathing
1206	1208	1202	470.09	B_1	$C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, isoindole def., $C_{\delta'}$-Cl, $C_{\gamma'}$-Cl, benzene breathing
	1267	1281	152.67	B_2	C_{δ}-C_{δ}, C_{β}-C_{β}, C_{β}-C_{γ}-C_{δ}, N_{β}-C_{α}-C_{β}
	1273	1283	174.81	B_1	$C_{\delta'}$-$C_{\delta'}$, $C_{\beta'}$-$C_{\beta'}$, $C_{\beta'}$-$C_{\gamma'}$-$C_{\delta'}$, N_{β}-$C_{\alpha'}$-$C_{\beta'}$
1290	1292	1304	125.81	B_2	C_{β}-C_{β}, C_{δ}-C_{δ}, isoindole def.
		1305	172.65	B_1	$C_{\beta'}$-$C_{\beta'}$, $C_{\delta'}$-$C_{\delta'}$, isoindole def.
1302		1314	1.91	A_1	C_{α}-N_{α}-C_{α}, C_{γ}-C_{δ}, $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$, $C_{\gamma'}$-$C_{\delta'}$
	1302	1314	495.44	B_2	C_{α}-N_{α}, C_{α}-C_{β}, Pyrrole def., C_{α}-N_{α}-C_{α}
		1315	400.45	B_1	$C_{\alpha'}$-$N_{\alpha'}$, $C_{\alpha'}$-$C_{\beta'}$, Pyrrole def., $C_{\alpha'}$-$N_{\alpha'}$-$C_{\alpha'}$
1320	1313	1333	8.87	A_1	isoindole def.
	1366	1383	7.13	A_1	macroring def.
1386	1390	1386	205.56	B_2	$C_{\alpha'}$-$C_{\beta'}$, $C_{\gamma'}$-$C_{\delta'}$, isoindole def.

1393		1386	199.49	B_1	C_α-C_β, C_γ-C_δ, isoindole def.
1422		1463	0.56	B_2	$C_{\alpha'}$-N_β, C_α-C_β, C_β-C_β
1439	1437	1467	1.90	B_1	C_α-N_β, $C_{\alpha'}$-$C_{\beta'}$, $C_{\beta'}$-$C_{\beta'}$
1473		1494	0	A_2	$C_{\alpha'}$-N_β, C_α-N_β, $C_{\alpha'}$-$C_{\beta'}$, C_α-C_β
	1482	1506	57.66	B_1	$C_{\alpha'}$-N_β, $C_{\alpha'}$-$C_{\beta'}$, C_α-N_β, C_α-N_α-C_α
	1497	1510	40.34	B_2	C_α-N_β, C_α-C_β, C_γ-C_δ
1500		1513	0.14	A_1	C_α-N_β, $C_{\alpha'}$-N_β, $C_{\alpha'}$-$C_{\beta'}$, C_α-C_β
1517		1536	0.40	A_1	C_β-C_β, $C_{\beta'}$-$C_{\beta'}$, C_δ-C_δ, $C_{\delta'}$-$C_{\delta'}$, C_α-N_α, $C_{\alpha'}$-$N_{\alpha'}$
	1519	1539	11.54	B_2	C_β-C_β, C_δ-C_δ, C_β-C_γ
		1539	12.34	B_1	$C_{\beta'}$-$C_{\beta'}$, $C_{\delta'}$-$C_{\delta'}$, $C_{\beta'}$-$C_{\gamma'}$
1535		1561	0	A_2	C_β-C_γ, $C_{\beta'}$-$C_{\gamma'}$, C_α-C_β, $C_{\alpha'}$-$C_{\beta'}$, C_α-N_β, $C_{\alpha'}$-N_β
	1537	1562	23.09	B_2	C_β-C_γ, C_γ-C_δ, C_α-C_β, C_α-N_α
1542		1562	23.80	B_1	$C_{\beta'}$-$C_{\gamma'}$, $C_{\gamma'}$-$C_{\delta'}$, $C_{\alpha'}$-$C_{\beta'}$, $C_{\alpha'}$-$N_{\alpha'}$
1565		1562	0	A_2	C_β-C_γ, $C_{\beta'}$-$C_{\gamma'}$, C_γ-C_δ, $C_{\gamma'}$-$C_{\delta'}$, C_α-N_α, $C_{\alpha'}$-$N_{\alpha'}$
	1563	1563	14.99	A_1	C_α-N_β, $C_{\alpha'}$-N_β

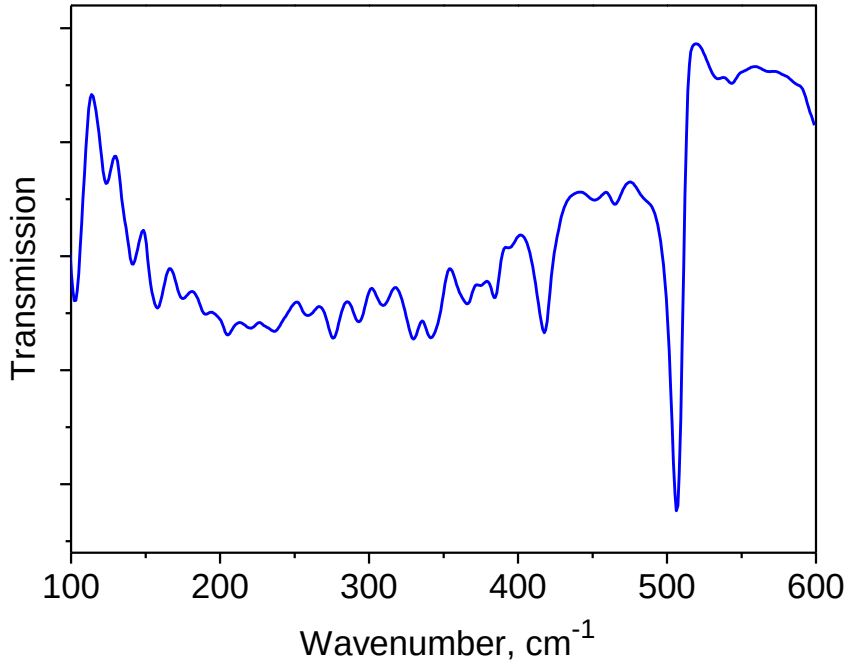

Figure S3. The experimental far IR spectra of $VOPcCl_{16}$.