

Supplementary Materials: Synthesis, Spectroscopic Characterization and Photoactivity of Zr(IV) Phthalocyanines Functionalized with Aminobenzoic Acids and Their GO-Based Composites

Leili Tahershamsi, Yuriy Gerasymchuk, Anna Wedzynska, Maciej Ptak, Iryna Tretyakova and Anna Lukowiak

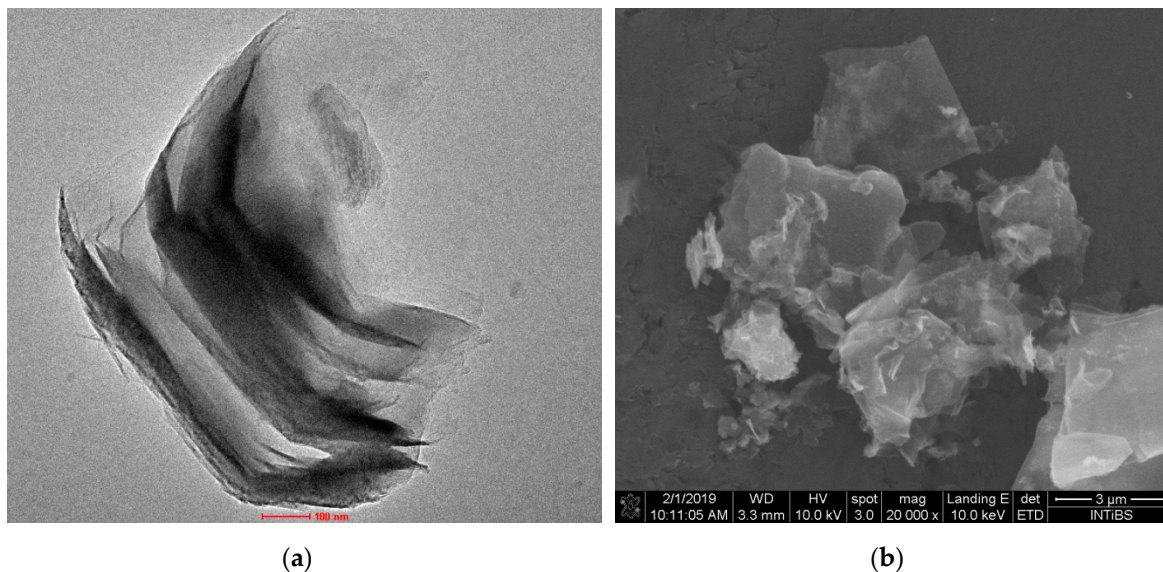


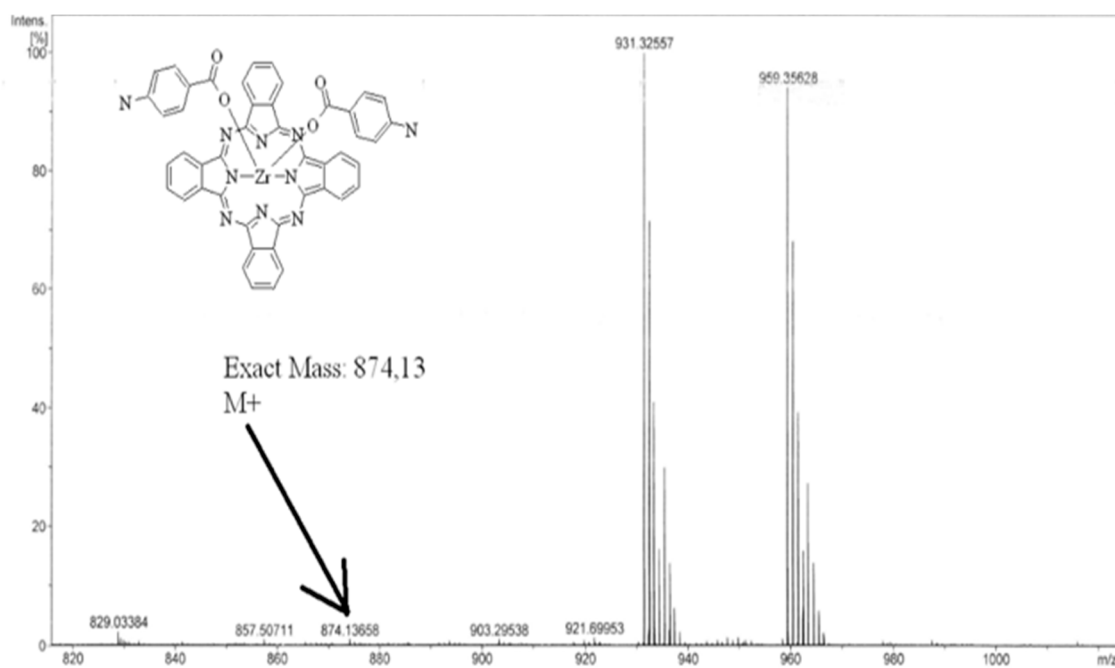
Figure S1. (a) TEM and (b) SEM images of graphite oxide flakes with zirconium(IV) phthalocyanine derivatives. Because the concentration of Pc complexes is very low in the composites, these methods are not informative for characterization of composites (ZrPcs are not seen in the images nor detected by EDS analysis).

Table S1. IR wavenumbers (cm⁻¹) and relative intensities of observed bands together with proposed assignment for the studied complexes and composites.^a

bis(PABA)ZrPc	bis(PABA)ZrPc/GO	bis(DABA)ZrPc	bis(DABA)ZrPc/GO	Assignment
3618b, 3464b, 3387sh, 3357b, 3220b	3578b, 3451b, 3325s, 3250sh, 3185vw, 3124vw	3592b, 3454sh, 3429b, 3373sh, 3354b, 3228b	3586b, 3426b, 3326b, 3184sh, 3126sh	v(NH ₂) + v(OH)
3081vw, 3060vw, 3051vw, 3032vw, 3015sh, 2946vw, 2924vw, 2842vw, 2841sh	2953w, 2946m, 2933sh, 2928s, 2916m, 2897sh, 2850m	3080vw, 3058vw, 3031vw, 3016vw, 2944sh, 2924w, 2852w	3078vw, 3037w, 2952sh, 2944sh, 2927m, 2917m, 2896sh, 2850m	v(CH) + v(NH ₂)
	1724b, 1612m		1725b, 1612sh	GO
1689vw, 1621m, 1602s, 1584w, 1530w	1647sh, 1626vs, 1576s, 1537w	1654sh, 1624m, 1608m, 1590sh, 1559vw, 1516m	1646m, 1627vs, 1612sh, 1575m, 1537w	v(CO) + v(φ) + δ (NH ₂)
1499m, 1478w, 1466w	1498vw, 1461vw	1498m, 1477w, 1461sh	1495vw, 1458sh	v(CNC) + v(φ) + δ (CH)
1440s, 1421vs, 1403sh, 1392sh	1449w, 1436w, 1417vw, 1388vw	1447sh, 1437m, 1420m, 1398sh, 1391ww	1449w, 1436w, 1417w, 1386w	v(φ) + δ (CH)
1332vs, 1316m	1346vw, 1311w	1332vs, 1318sh	1346vw, 1312w, 1300sh	v(CNC) + δ (ZrN ₄) + v(φ) + v(CN)
1288m, 1207vw	1271vw, 1244m, 1230vw	1288m	1271vw, 1251sh, 1244w, 1230vw	δ (CO) + v(φ) + v(CNC) + δ (CH)
1178m, 1163w, 1142vw, 1119s	1187vw, 1159vw, 1102sh	1193w, 1163w, 1118s	1186vw, 1158vw, 1103sh	δ (CH) + δ (ZrN ₄) + v(φ)
1074vs	1088m, 1070vw	1075vs	1088m, 1068w, 1062w	δ (CH) + δ (φ) + ρ (ZrN ₄)
	1068b		1070b, 983b	GO
1004vw, 954vw	1051vw, 1045vw, 968vw	1002vw, 993vw, 957sh, 955vw, 946sh	1051w, 1046w, 968vw	δ (CH) + δ (φ) + ρ (ZrN ₄)
894m, 878sh, 873w, 870w, 851w, 847w	904vw, 893w, 843vw	894m, 878vw, 868vw, 854vw	903vw, 892w, 843vw	γ (CH) + δ (φ) + δ (CNC) + δ (CN)
827w, 820sh, 797sh789m, 785sh, 775m, 748s		830vw, 804m, 786sh, 783w, 777w, 749m		γ (CH) + δ (ZrN ₄) + γ (φ)
735vs, 727sh, 704w	736vw	735vs, 727w, 724sh, 695vw	732vw	δ (φ) + δ (CNC) + γ (φ)
678w, 648sh, 640m, 633m	658w, 641m	675vw, 643vw, 631w, 598vw, 585vw	669sh, 664w, 654sh, 641w	γ (φ) + γ (CH) + δ (CNC) + ρ (ZrN ₄)
568vw, 505w	537vw	568w, 505w	537vw	δ (φ) + γ (CH) + δ (CNC) + ρ (ZrN ₄)
439w	447vw, 418vw	465w, 440w	417vw	δ (CNC) + ρ (ZrN ₄) + γ (φ) + γ (CH)

Key: vs, very strong; s, strong; m, medium; w, weak; vw, very weak; b, broad; φ , ring; v, stretching vibration; ρ , rocking vibration; δ , deformational or in-plane bending vibration; γ , out-of-plane vibration.

(a)



(b)

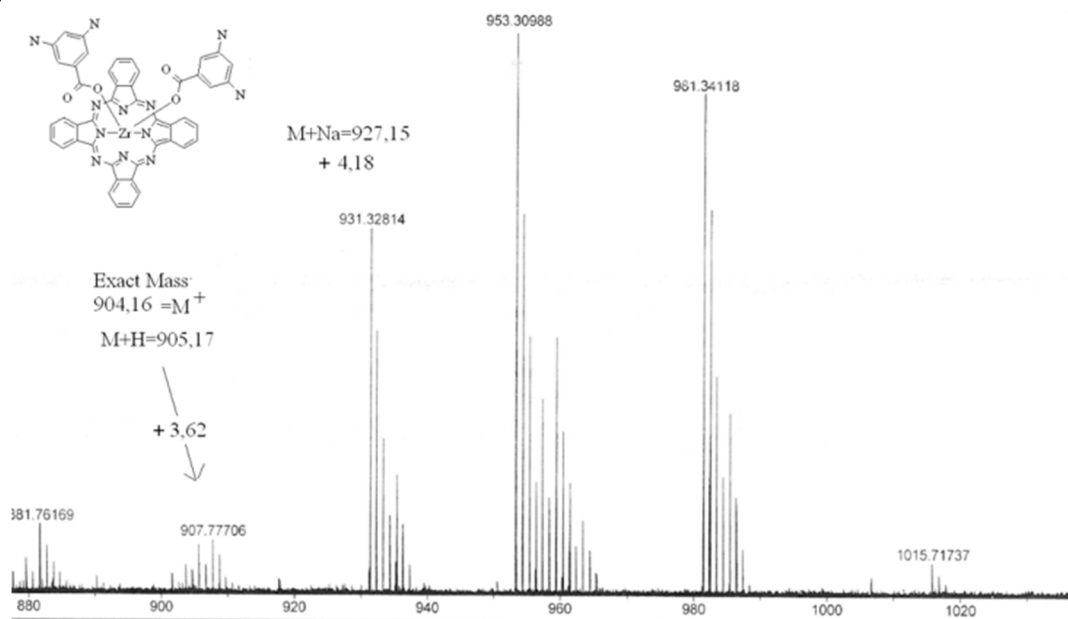


Figure S2. Mass spectra of (a) bis(PABA)ZrPc and (b) bis(DABA)ZrPc.