Electronic Supporting Information

for

Heteroleptic [1]Zirconametalloarenophanes: Potential Precursors to Metal-enriched Metallopolymers

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General Considerations.

All manipulations were conducted either under an atmosphere of dry argon or *in vacuo* using standard Schlenk line or glovebox techniques. Solvents (toluene, hexane and pentane) were purified by distillation from Na/K alloy under dry argon immediately *prior* to use. C_6D_6 was degassed by three freeze-pump-thaw cycles and stored over molecular sieves. Reagents were dried and purified by standard procedures. NMR spectra were acquired on a Bruker Avance 500 NMR spectrometer. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were referenced to external TMS *via* the residual protons of the solvent (^{1}H) or the solvent itself (^{13}C). Microanalyses (C, H, N) were performed on a Leco Instruments elemental analyzer, type CHNS 932, using V_2O_5 to promote complete combustion. UV-vis spectra were measured on a JASCO V-660 UV-Vis-spectrometer as toluene solutions. $[Cr(\eta^6\text{-}C_6H_5Li)_2]\cdot$tmeda,[1] $[Cr(\eta^5\text{-}C_5H_4Li)(\eta^7\text{-}C_7H_6Li)]\cdot$tmeda,[2] $[Mn(\eta^5\text{-}C_5H_4Li)(\eta^6\text{-}C_6H_5Li)]\cdot$tmeda,[3] and $[Cl_2Zr(\eta^5\text{-}C_5H_4{}^t\text{Bu})_2]$[4] were prepared according to published procedures.

X-ray Diffraction Studies.

The crystal data of **1**-**3** were collected on a Bruker X8APEX diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structures were solved using direct methods, refined with the Shelx software package[5] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealized geometric positions. Compounds **2** and **3** feature severe disorders of the cyclic π ligands attached to chromium and manganese, respectively, and have been refined applying strong constraints and restraints. Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-804814 (**1**), CCDC-804815 (**2**), and CCDC-804816 (**3**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

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Computational Details.

Geometry optimizations on compounds **1-3** were carried out without symmetry restrictions using the GAUSSIAN03 program on a cluster of Linux workstations.[6] Frequency calculations were used to verify that the final geometries represent energy minima. All SCF computations were performed using DFT methods, applying the three hybrid functional B3LYP using using 6–31G(d,p) basis functions sets for non-metals and Stuttgart relativistic, small core ECP basis sets for metals.[7-9] The Wiberg bond indices given in the text were obtained with the NBO 5 program.[10] Illustrations of molecular orbitals were prepared with Molekel 5.4.[11] Excitation energies were calculated using the TD-DFT method included in the GAUSSIAN03 package both employing the B3LYP and the BP86[12,13] functional.

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Experimental Procedures

[Cr(η^6-C_6H_5)$_2$Zr(η^5-$C_5H_4{}^t$Bu)$_2$], 1. In a modification to the literature synthesis,[14] **1** was be obtained by addition of toluene (60 mL) over a period of 15 min to a solid mixture of [Cr(η^6-$C_6H_5Li)_2$·tmeda] (168.15 mg, 0.50 mmol) and [Cl_2Zr(η^5-$C_5H_4{}^t$Bu)$_2$] (242.74 mg, 0.60 mmol) at RT under vigorous stirring. During addition, the color of the reaction mixture changed to dark green. After additional 20 min, all volatiles were removed under reduced pressure, the residue washed hexane (3 x 20 mL), and extracted into toluene (20 ml). After filtration, a dark green filtrate was be obtained, which was concentrated to 3 ml in volume. Storage at −70 °C afforded **1** (82.8 mg, 0.15 mmol, 30%) as a dark greenish, blue solid, which was washed with cold hexane (−30 °C, 5 x 4 mL) and dried *in vacuo*. Crystals suitable for X-ray diffraction were obtained by recrystallization from toluene/hexane (1:1) at RT.

^{1}H NMR (500 MHz, C_6D_6): δ = 1.40 (s, 18H, ^{t}Bu), 3.80 (m, 4H, *m*−C_6H_5), 4.81 (m, 4H, *o*−C_6H_5), 4.90 (m, 2H, *p*−C_6H_5), 5.50 (m, 4H, $C_5H_4{}^t$Bu), 6.08 (m, 4H, $C_5H_4{}^t$Bu) ppm.
^{13}C {^{1}H} NMR (126 MHz, C_6D_6): δ = 32.96 (*i*−C_tBu), 33.52 (C_tBu), 73.58 (*m*-C_6H_5), 77.46 (*p*-C_6H_5), 92.41 (*o*-C_6H_5), 105.76 ($C_5H_4{}^t$Bu), 106.77 ($C_5H_4{}^t$Bu), 138.22 (*i*−$C_5H_4{}^t$Bu), 173.27 (*i*-C_6H_5) ppm.
Elemental analysis (%) calcd. for $C_{30}H_{36}CrZr$ (539.83): C 66.75, H 6.72; found: C 66.40, H 6.81.
UV-vis: λ = 334 nm, 623 nm (ε = 1553 L/mol^{-1}cm^{-1}).

[Cr(η^5-C_5H_4)(η^7-C_7H_6)Zr(η^5-$C_5H_4{}^t$Bu)$_2$], 2. 2 was prepared by addition of in toluene (120 mL) to a solid mixture of [Cr(η^5-C_5H_4Li)(η^7-C_7H_6Li)·tmeda] (500.00 mg, 1.49 mmol) and [Cl_2Zr(η^5-$C_5H_4{}^t$Bu)$_2$] (691.75 mg, 1.71 mmol) at RT. After complete addition, insolubilities were immediately removed by

filtration and the filtrate concentrated to 10 ml in volume. Storage at −70 °C for 5 days afforded **2** as a dark blue solid (328.40 mg, 0.61 mmol, 41%), which was washed with cold pentane (−35 °C, 3 x 5 mL) and dried *in vacuo*. Crystals for X-ray diffraction were grown from a saturated solution in toluene:hexane (1:1) at −30 °C.

^{1}H NMR (500.13 MHz, C_6D_6): δ = 1.38 (s, 18H, ^{t}Bu), 3.51 (m, 2H, β-C_5H_4), 4.18 (m, 2H, $C_5H_4{}^t$Bu), 4.32 (m, 2H, α-C_5H_4), 5.57 (m, 2H, C_7H_6), 5.68 (m, 4H, $C_5H_4{}^t$Bu), 5.79 (m, 2H, $C_5H_4{}^t$Bu), 6.12 (m, 2H, C_7H_6), 6.22 (m, 2H; C_7H_6) ppm.
^{13}C {^{1}H} NMR (126 MHz, C_6D_6): δ = 32.95 (i−$C_{t\mathrm{Bu}}$), 33.23 ($C_{t\mathrm{Bu}}$), 80.53 (α-C_5H_4), 86.63 (β-C_7H_6), 86.96 (γ-C_7H_6), 89.47 (β-C_5H_4), 100.54 (α-C_7H_6), 105.53 ($C_5H_4{}^t$Bu), 106.76 ($C_5H_4{}^t$Bu), 107.77 ($C_5H_4{}^t$Bu), 139.15 (i-$C_5H_4{}^t$Bu), 159.12 (i-C_5H_4), 174.85 (i-C_7H_6) ppm.
Elemental analysis (%) calcd. for $C_{30}H_{36}CrZr$ (539.83): C 66.75, H 6.72; found: C 66.36, H 6.89.
UV-vis: λ = 342 nm (ε = 5019 L/mol^{-1}cm^{-1}), 603 nm (ε = 2287 L/mol^{-1}cm^{-1}), 750 nm (ε = 1765 L/mol^{-1}cm^{-1}).

[Mn(η^5-C_5H_4)(η^6-C_6H_5)Zr(η^5-$C_5H_4{}^t$Bu)$_2$], 3. **3** was obtained by a procedure analogous to that described above for the synthesis of **2** using [Mn(η^5-C_5H_4Li)(η^6-C_6H_5Li)·pmdta] (191.67 mg, 0.50 mmol) and [Cl_2Zr(η^5-$C_5H_4{}^t$Bu)$_2$] (242.74 mg, 0.60 mmol) in toluene (70 mL). Crystallization at −70 °C for 7 days yielded **3** (108.50 mg, 0.20 mmol, 41%) as a red crystalline material, which was washed with cold pentane (−30 °C, 5 x 3 mL) and dried *in vacuo*. Crystals suitable for X-ray diffraction were obtained by recrystallization from toluene/hexane (1:1) at RT.

^{1}H NMR (500 MHz, C_6D_6): δ = 1.35 (s, 18H, ^{t}Bu), 3.78 (m, 2H, β-C_5H_4), 4.00 (m, 2H, m-C_6H_5), 4.35 (m, 2H, α-C_5H_4), 4.78 (m, 2H, o-C_6H_5), 5.19 (m, 1H, p-C_6H_5), 5.53 (m, 2H, $C_5H_4{}^t$Bu), 5.58 (m, 2H, $C_5H_4{}^t$Bu), 6.05 (m, 4H, $C_5H_4{}^t$Bu) ppm.
^{13}C {^{1}H} NMR (126 MHz, C_6D_6): δ = 32.92 (i−$C_{t\mathrm{Bu}}$), 33.36 ($C_{t\mathrm{Bu}}$), 72.83 (m-C_6H_5), 73.01 (α-C_5H_4), 77.18 (p-C_6H_5), 83.99 (β-C_5H_4), 88.13 (o-C_6H_5), 105.39 ($C_5H_4{}^t$Bu), 106.15 ($C_5H_4{}^t$Bu), 106.73 ($C_5H_4{}^t$Bu), 138.81 (i−$C_5H_4{}^t$Bu), 158.22 (i−C_5H_4), 164.65 (i-C_6H_5) ppm.
Elemental analysis (%) calcd. for $C_{29}H_{35}MnZr$ (529.75): C 65.75, H 6.66; found: C 64.59, H 6.68.
UV-vis: λ = 365 nm (ε = 2735 L/mol^{-1}cm^{-1}), 462 nm (ε = 1491 L/mol^{-1}cm^{-1}).

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Crystallographic Details for 1:

Data	
Empirical formula	$C_{30}H_{36}CrZr$
Formula weight ($g \cdot mol^{-1}$)	539.81
Temperature (K)	100(2)
Radiation, λ (Å)	$Mo_{K\alpha}$ 0.71073
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	
a (Å)	16.329(3)
b (Å)	19.239(3)
c (Å)	7.3960(12)
α (°)	90.00
β (°)	97.846(7)
γ (°)	90.00
Volume ($Å^3$)	2301.7(6)
Z	4
Calculated density ($Mg \cdot m^{-3}$)	1.558
Absorbtion coefficient (mm^{-1})	0.941
F(000)	1120
Theta range for collection	1.64 to 28.35°
Reflections collected	39152
Independent reflections	2865
Minimum/maximum transmission	0.8301/0.9633
Refinement method	Full-matrix least-squares on F^2
Data / parameters / restrains	2865 / 149 / 0
Goodness-of-fit on F^2	1.045
Final R indices [I>2σ(I)]	R_1 = 0.0255, wR^2 = 0.0693
R indices (all data)	R_1 = 0.0272, wR^2 = 0.0707
Maximum/minimum residual electron density ($e \cdot Å^{-3}$)	1.565 / –0.270

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Crystallographic Details for 2:

Data	
Empirical formula	$C_{30}H_{36}CrZr$
Formula weight (g·mol^{-1})	539.81
Temperature (K)	100(2)
Radiation, λ (Å)	$Mo_{K\alpha}$ 0.71073
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	
a (Å)	16.780(5)
b (Å)	19.128(5)
c (Å)	7.402(2)
α (°)	90.00
β (°)	96.303(14)
γ (°)	90.00
Volume (Å^3)	2361.4(12)
Z	4
Calculated density (Mg·m^{-3})	1.518
Absorbtion coefficient (mm^{-1})	0.918
F(000)	1120
Theta range for collection	1.62 to 28.38°
Reflections collected	39926
Independent reflections	2931
Minimum/maximum transmission	0.8160/0.9642
Refinement method	Full-matrix least-squares on F^2
Data / parameters / restrains	2931 / 185 / 140
Goodness-of-fit on F^2	1.129
Final R indices [I>2σ(I)]	R_1 = 0.0485, wR^2 = 0.1016
R indices (all data)	R_1 = 0.0506, wR^2 = 0.1026
Maximum/minimum residual electron density (e·Å^{-3})	1.159 / –1.124

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Crystallographic Details for 3:

Data	
Empirical formula	$C_{29}H_{35}MnZr$
Formula weight (g·mol^{-1})	529.73
Temperature (K)	100(2)
Radiation, λ (Å)	$Mo_{K\alpha}$ 0.71073
Crystal system	Monoclinic
Space group	*C*2/*c*
Unit cell dimensions	
a (Å)	16.367(7)
b (Å)	19.183(8)
c (Å)	7.386(3)
α (°)	90.00
β (°)	97.165(11)
γ (°)	90.00
Volume (Å^3)	2300.9(18)
Z	4
Calculated density (Mg·m^{-3})	1.529
Absorbtion coefficient (mm^{-1})	1.016
F(000)	1096
Theta range for collection	1.64 to 25.91°
Reflections collected	5075
Independent reflections	2201
Minimum/maximum transmission	0.7175/0.9605
Refinement method	Full-matrix least-squares on F^2
Data / parameters / restrains	2201 / 173 / 171
Goodness-of-fit on F^2	1.071
Final R indices [I>2σ(I)]	R_1 = 0.0599, wR^2 = 0.1609
R indices (all data)	R_1 = 0.0640, wR^2 = 0.1643
Maximum/minimum residual electron density (e·Å^{-3})	1.790 / –2.372

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Density Functional Theory (DFT) Calculations on 1-3.

Optimized Geometry of 1 (no imaginary frequency):

SCF energy (zero point corrected) = -1298.426326 a.u.

1	24	0	0.000582	2.577240	-0.000001
2	6	0	-1.067546	1.084010	1.114437
3	6	0	-2.003370	1.881638	0.362305
4	1	0	-2.657620	1.409781	-0.355752
5	6	0	-2.029405	3.298256	0.408000
6	1	0	-2.695998	3.844858	-0.252917
7	6	0	-1.128189	3.999350	1.241857
8	1	0	-1.091867	5.084051	1.227119
9	6	0	-0.252789	3.262326	2.072201
10	1	0	0.461886	3.781724	2.704245
11	6	0	-0.241056	1.845829	2.019572
12	1	0	0.509829	1.349801	2.622003
13	40	0	-0.000146	-0.643464	0.000018
14	6	0	-2.377671	-1.743323	-0.691781
15	6	0	-2.060285	-0.767378	-1.684917
16	1	0	-2.640025	0.113532	-1.916620
17	6	0	-0.889554	-1.172265	-2.376722
18	1	0	-0.414540	-0.655668	-3.197742
19	6	0	-0.453336	-2.393130	-1.809504
20	1	0	0.410242	-2.964697	-2.120010
21	6	0	-1.361477	-2.736169	-0.775577
22	1	0	-1.311384	-3.632559	-0.172976
23	6	0	-3.676094	-1.912236	0.103059
24	6	0	-4.489848	-3.034303	-0.593075
25	1	0	-4.716895	-2.768001	-1.630576
26	1	0	-5.438252	-3.198237	-0.068632
27	1	0	-3.939280	-3.980192	-0.602468
28	6	0	-4.534496	-0.634762	0.119340
29	1	0	-4.752450	-0.278356	-0.893105
30	1	0	-4.049160	0.169013	0.676277
31	1	0	-5.494130	-0.843918	0.604132
32	6	0	-3.394395	-2.331561	1.561377
33	1	0	-4.337136	-2.484509	2.098429
34	1	0	-2.823158	-1.559386	2.085898
35	1	0	-2.835061	-3.271834	1.612846
36	6	0	1.068043	1.083521	-1.114406
37	6	0	2.004226	1.880750	-0.362294
38	1	0	2.658282	1.408631	0.355767
39	6	0	2.030889	3.297356	-0.408022
40	1	0	2.697727	3.843674	0.252882
41	6	0	1.129982	3.998834	-1.241888
42	1	0	1.094142	5.083551	-1.227171
43	6	0	0.254254	3.262180	-2.072214
44	1	0	-0.460193	3.781883	-2.704267
45	6	0	0.241892	1.845690	-2.019556
46	1	0	-0.509216	1.349990	-2.621977
47	6	0	2.376884	-1.744379	0.691777
48	6	0	2.059932	-0.768296	1.684915
49	1	0	2.640066	0.112353	1.916622
50	6	0	0.889033	-1.172669	2.376733
51	1	0	0.414257	-0.655861	3.197759
52	6	0	0.452273	-2.393341	1.809516

53	1	0	-0.411555	-2.964528	2.120024
54	6	0	1.360255	-2.736779	0.775582
55	1	0	1.309760	-3.633143	0.172976
56	6	0	3.675226	-1.913858	-0.103077
57	6	0	4.488492	-3.036295	0.593032
58	1	0	4.715675	-2.770105	1.630532
59	1	0	5.436813	-3.200644	0.068571
60	1	0	3.937504	-3.981939	0.602424
61	6	0	4.534199	-0.636767	-0.119347
62	1	0	4.752306	-0.280463	0.893100
63	1	0	4.049224	0.167226	-0.676284
64	1	0	5.493740	-0.846350	-0.604136
65	6	0	3.393323	-2.333034	-1.561397
66	1	0	4.335990	-2.486365	-2.098472
67	1	0	2.822398	-1.560609	-2.085887
68	1	0	2.833594	-3.273071	-1.612875

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Optimized Geometry of 2 (no imaginary frequency):

SCF energy (zero point corrected) = -1298.406159 a.u.

1	24	0	-1.086119	-2.334525	-0.077001
2	6	0	0.552760	-1.341762	-1.130021
3	6	0	-0.436596	-1.774107	-2.099495
4	1	0	-1.034631	-1.124617	-2.725121
5	6	0	-0.569545	-3.185670	-2.081429
6	1	0	-1.245128	-3.774198	-2.690159
7	6	0	0.346884	-3.691344	-1.117022
8	1	0	0.493238	-4.733528	-0.860738
9	6	0	1.028004	-2.583301	-0.551289
10	1	0	1.761296	-2.671436	0.236739
11	6	0	-1.427525	-0.599232	1.127275
12	6	0	-0.919019	-1.640268	1.971273
13	1	0	-0.026277	-1.408438	2.538014
14	6	0	-1.191239	-3.029821	2.003309
15	1	0	-0.473367	-3.611067	2.579885
16	6	0	-2.070221	-3.800041	1.213470
17	1	0	-1.934061	-4.877463	1.262752
18	6	0	-3.003452	-3.330049	0.266202
19	1	0	-3.506467	-4.085309	-0.332356
20	6	0	-3.254832	-1.988531	-0.088429
21	1	0	-3.936243	-1.859630	-0.927941
22	6	0	-2.574574	-0.807195	0.294206
23	1	0	-2.858894	0.028163	-0.326857
24	40	0	0.279294	0.597525	0.041625
25	6	0	-1.396976	2.624890	-0.652643
26	6	0	-1.522046	1.630098	-1.668317
27	1	0	-2.425774	1.102100	-1.933786
28	6	0	-0.280511	1.487016	-2.337878
29	1	0	-0.069006	0.823249	-3.163021
30	6	0	0.636883	2.383628	-1.739769
31	1	0	1.668004	2.525016	-2.031440
32	6	0	-0.045378	3.070455	-0.702293
33	1	0	0.381073	3.845856	-0.080815
34	6	0	-2.501292	3.326496	0.144274
35	6	0	-2.697585	4.729186	-0.487722
36	1	0	-1.779385	5.322355	-0.439073

37	1	0	-3.484772	5.278215	0.041609
38	1	0	-2.989000	4.647841	-1.540032
39	6	0	-2.102761	3.496993	1.625830
40	1	0	-1.960533	2.523937	2.106511
41	1	0	-2.887506	4.035558	2.168730
42	1	0	-1.178067	4.074274	1.732489
43	6	0	-3.846790	2.580259	0.080889
44	1	0	-4.167548	2.407505	-0.951311
45	1	0	-4.622163	3.182116	0.566390
46	1	0	-3.803210	1.620513	0.598373
47	6	0	2.905430	0.528799	0.688611
48	6	0	2.194198	-0.236507	1.661279
49	1	0	2.319571	-1.293065	1.847308
50	6	0	1.334635	0.627439	2.391659
51	1	0	0.689582	0.354717	3.214050
52	6	0	1.478171	1.930376	1.859797
53	1	0	0.962292	2.816929	2.202346
54	6	0	2.433068	1.864963	0.812519
55	1	0	2.778175	2.707654	0.229242
56	6	0	4.136401	0.125625	-0.128504
57	6	0	5.362208	0.802934	0.538307
58	1	0	5.268975	1.893376	0.535371
59	1	0	6.280200	0.539562	0.000634
60	1	0	5.472614	0.478338	1.578175
61	6	0	4.031795	0.611079	-1.589695
62	1	0	3.177308	0.149977	-2.093924
63	1	0	4.940560	0.344696	-2.140839
64	1	0	3.924170	1.699635	-1.647920
65	6	0	4.370890	-1.395245	-0.130936
66	1	0	4.445814	-1.795208	0.885966
67	1	0	5.314312	-1.619932	-0.639866
68	1	0	3.574016	-1.923069	-0.657138

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Optimized Geometry of 3 (no imaginary frequency):

SCF energy (zero point corrected) = -1277.091597 a.u.

1	40	0	-0.020384	-0.554852	-0.017752
2	25	0	0.082587	2.546112	0.063116
3	6	0	-1.051275	1.125956	1.129884
4	6	0	-1.928332	2.090484	0.488270
5	1	0	-2.641913	1.872803	-0.292056
6	6	0	-1.668197	3.402302	0.970528
7	1	0	-2.154705	4.313101	0.644139
8	6	0	-0.635482	3.305317	1.946560
9	1	0	-0.195913	4.129083	2.495129
10	6	0	-0.275664	1.934679	2.056852
11	1	0	0.513721	1.574704	2.702839
12	6	0	1.117504	1.166381	-1.095003
13	6	0	2.049826	1.919899	-0.291740
14	1	0	2.701191	1.407298	0.399851
15	6	0	2.047325	3.335466	-0.223481
16	1	0	2.682364	3.835504	0.501642
17	6	0	1.129969	4.086294	-0.994321
18	1	0	1.053837	5.161441	-0.872705
19	6	0	0.276820	3.399608	-1.889140
20	1	0	-0.466342	3.950396	-2.457958
21	6	0	0.290861	1.984100	-1.951635

22	1	0	-0.464486	1.528262	-2.578771
23	6	0	2.302041	-1.750758	0.678325
24	6	0	1.240246	-2.694780	0.757224
25	1	0	1.148762	-3.586955	0.153083
26	6	0	0.346354	-2.309893	1.790643
27	1	0	-0.544590	-2.840340	2.096911
28	6	0	0.839885	-1.112595	2.362346
29	1	0	0.386582	-0.568820	3.177779
30	6	0	2.029348	-0.763816	1.674023
31	1	0	2.650183	0.086930	1.911596
32	6	0	3.590993	-1.968666	-0.118725
33	6	0	4.382266	-3.093526	0.598176
34	1	0	4.621561	-2.809339	1.628119
35	1	0	5.323421	-3.292251	0.072687
36	1	0	3.808693	-4.025141	0.632019
37	6	0	3.290779	-2.413706	-1.565620
38	1	0	2.704093	-3.338090	-1.593877
39	1	0	4.226401	-2.606060	-2.102312
40	1	0	2.740925	-1.637374	-2.106858
41	6	0	4.476219	-0.710502	-0.169766
42	1	0	3.998636	0.093122	-0.734174
43	1	0	5.424486	-0.948042	-0.663730
44	1	0	4.716148	-0.340782	0.832865
45	6	0	-2.445402	-1.514465	-0.710867
46	6	0	-1.480979	-2.554097	-0.828699
47	1	0	-1.472046	-3.468384	-0.251110
48	6	0	-0.563597	-2.228578	-1.861469
49	1	0	0.267177	-2.835218	-2.194957
50	6	0	-0.942020	-0.971671	-2.390632
51	1	0	-0.446176	-0.457086	-3.200647
52	6	0	-2.083712	-0.525186	-1.674327
53	1	0	-2.614339	0.396457	-1.862223
54	6	0	-3.744162	-1.632404	0.091438
55	6	0	-4.613521	-2.707555	-0.611397
56	1	0	-4.830768	-2.421803	-1.645838
57	1	0	-5.567036	-2.828892	-0.084759
58	1	0	-4.110623	-3.679585	-0.630359
59	6	0	-3.473963	-2.079889	1.543404
60	1	0	-2.956625	-3.044730	1.580915
61	1	0	-4.420080	-2.197335	2.083419
62	1	0	-2.866939	-1.339123	2.072432
63	6	0	-4.538691	-0.314926	0.123799
64	1	0	-4.001950	0.462606	0.670077
65	1	0	-5.498342	-0.477265	0.626184
66	1	0	-4.757281	0.051355	-0.885088

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Calculated UV-visible parameters of 1-3 applying the B3LYP functional (TD DFT).

	1	**2**	**3**[c]	
λ_{calcd} [nm]	542.12	587.01	460.02	494.71
f[a]	0.0084	0.0012	0.0002	0.0003
transitions[b]	119→122 121*→122 121*→140	121*→122 121*→123 121*→124 121*→129 121*→130 121*→133 121*→135	117→124 117→127 117→128 117→130 118*→119 118*→125 118*→129 118*→131	116→122 116→125 116→129 116→131 118*→124 118*→127 118*→128 118*→130

[a] Oscillator strengths. [b] MO´s involved in lowest-energy excitation. HOMO marked with an asterisk. [c] Two transitions are found for the lowest-energy excitation with similar oscillator strengths.

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