Supporting Information for

Synthesis and coordination chemistry of pentadienyl ligands derived from (1*R*)-(–)myrtenal

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1. Crystallographic details

Table S1. Crystallographic data

Compound reference	[K(18-crown-6)][**3c**]	**4b**	**4c**	**5a**	**5b**	**5c**	**6a**
Chemical formula	$C_{24}H_{41}KO_6$	$C_{25}H_{28}Zr$	$C_{19}H_{24}Zr$	$C_{23}H_{35}PZr$	$C_{28}H_{37}PZr$	$C_{22}H_{33}PZr$	$C_{25}H_{35}NZr$
Formula Mass	464.67	419.69	343.60	433.70	495.77	419.67	440.76
Crystal system	orthorhombic	monoclinic	orthorhombic	orthorhombic	orthorhombic	triclinic	orthorhombic
a/Å	10.3222(2)	6.5559(2)	10.4927(3)	8.3511(3)	8.1113(3)	8.1222(1)	9.1213(2)
b/Å	14.4954(3)	18.9486(5)	10.9438(3)	13.0443(4)	15.7346(5)	8.1265(1)	13.8169(3)
c/Å	17.0039(4)	15.7614(4)	13.6917(4)	19.7724(6)	18.9910(7)	15.8261(2)	17.9360(4)
α/°	90.00	90.00	90.00	90.00	90.00	90.580(1)	90.00
β/°	90.00	90.924(3)	90.00	90.00	90.00	92.710(1)	90.00
γ/°	90.00	90.00	90.00	90.00	90.00	105.581(1)	90.00
Unit cell volume/Å^3	2544.21(9)	1957.71(9)	1572.22(8)	2153.89(12)	2423.79(15)	1004.81(2)	2260.45(9)
Temperature/K	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
Space group	$P2_12_12_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P1$	$P2_12_12_1$
No. of formula units per unit cell, *Z*	4	4	4	4	4	2	4
Radiation type	Mo Kα	Cu Kα	Mo Kα	Cu Kα	Mo Kα	Cu Kα	Mo Kα
Absorption coefficient, μ/mm^{-1}	0.243	4.611	0.688	4.879	0.532	5.215	0.495
No. of reflections measured	61001	41432	85804	33365	60076	10164	62840
No. of independent reflections	5621	8030	4820	4517	7186	10164	6805
R_{int}	0.0609	0.0528	0.0671	0.0551	0.0875		0.0526
Final R_1 values ($I > 2\sigma(I)$)	0.0349	0.0247	0.0233	0.0257	0.0356	0.0295	0.0249
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0732	0.0588	0.0449	0.0634	0.0620	0.0809	0.0478
Final R_1 values (all data)	0.0382	0.0256	0.0288	0.0268	0.0491	0.0298	0.0307
Final $wR(F^2)$ values (all data)	0.0746	0.0594	0.0467	0.0641	0.0666	0.0811	0.0497
Flack parameter	0.05(3)	-0.019(7)	-0.04(3)	-0.027(10)	-0.03(3)	-0.018(8)	-0.03(2)
Goodness of fit on F^2	1.098	1.024	1.067	1.021	1.031	1.088	1.064
Δρ [e Å^{-3}]	0.206/-0.200	0.409/-0.528	0.369/-0.309	0.329/-0.741	0.536/-0.466	0.925/-1.109	0.323/-0.228

2. Packing diagram of 4b

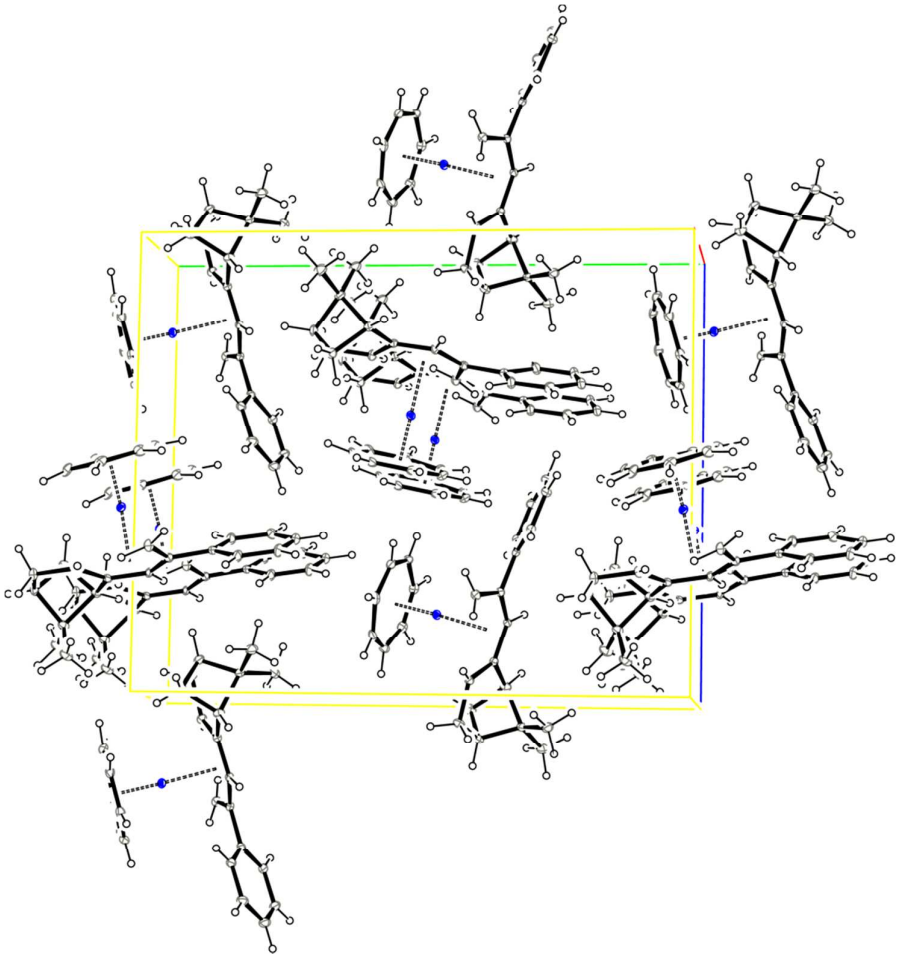


Figure S1. Packing diagram of **4b**.

3. ORTEP diagrams of 5b and 5c

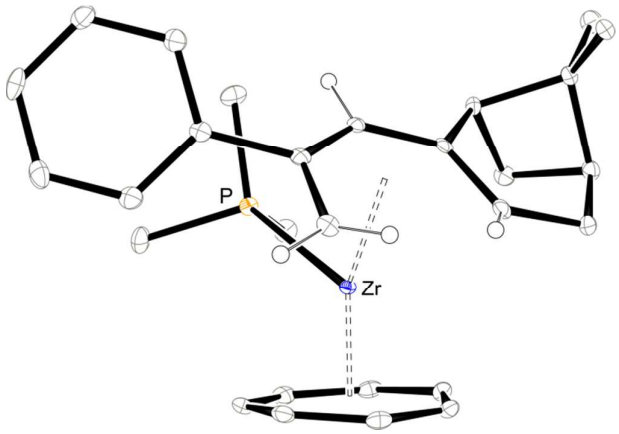


Figure S2. ORTEP diagram of the half-open trozircene **5b** with thermal displacement parameters drawn at 30% probability. Hydrogen atoms, with the exception of those connected to C1-C5, were omitted for clarity.

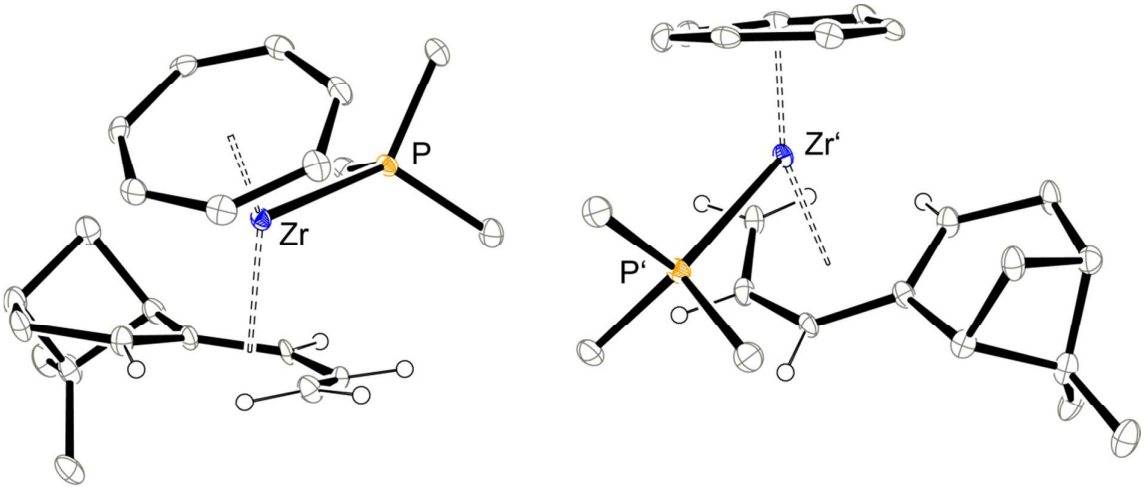


Figure S3. ORTEP diagrams of the half-open trozircene **5c** with thermal displacement parameters drawn at 30% probability. Two independent molecules in the asymmetric unit. Hydrogen atoms, with the exception of those connected to C1-C5, were omitted for clarity.

4. Computational details

All computations were performed using the density functional method B97D as implemented in the Gaussian09 program.[1] For all elements (C, H and K) the all-electron triple-ζ basis set (6-311G**) was used.[2]

Energies of the optimized structures

Compound	E(0 K)[a] [Ha]	H(298 K)[b] [Ha]	G(298 K)[b] [Ha]
U-3a (gas phase)	-1106.269799	-1106.253432	-1106.311610
U-3a (solvent continuum)	-1106.293447	-1106.276866	-1106.335506
U'-3a (gas phase)	-1106.269757	-1106.253641	-1106.310777
U'-3a (solvent continuum)	-1106.292663	-1106.276274	-1106.334185
S-3a (gas phase)	-1106.262114	-1106.245952	-1106.303454
S-3a (solvent continuum)	-1106.285998	-1106.269763	-1106.327527
S'-3a (gas phase)	-1106.262479	-1106.246434	-1106.303376
S'-3a (solvent continuum)	-1106.285589	-1106.269402	-1106.326863
W-3a (gas phase)	-1106.256084	-1106.239975	-1106.297569
W-3a (solvent continuum)	-1106.281066	-1106.264801	-1106.322777
W'-3a (gas phase)	-1106.256888	-1106.240963	-1106.297637
W'-3a (solvent continuum)	-1106.280102	-1106.263732	-1106.322445
U-3b (gas phase)	-1297.852535	-1297.833262	-1297.898828
U-3b (solvent continuum)	-1297.877871	-1297.858327	-1297.924538
U'-3b (gas phase)	-1297.852176	-1297.832977	-1297.898199
U'-3b (solvent continuum)	-1297.876934	-1297.857526	-1297.923298
S-3b (gas phase)	-1297.849074	-1297.829757	-1297.895053
S-3b (solvent continuum)	-1297.873518	-1297.853948	-1297.920280
S'-3b (gas phase)	-1297.848821	-1297.829491	-1297.894903
S'-3b (solvent continuum)	-1297.866596	-1297.846903	-1297.914201
W-3b (gas phase)	-1297.841769	-1297.822248	-1297.888735
W-3b (solvent continuum)	-1297.869255	-1297.849511	-1297.917001
W'-3b (gas phase)	-1297.841910	-1297.822697	-1297.887553

W'-3b (solvent continuum)	-1297.868617	-1297.848999	-1297.915052
U-3c (gas phase)	-1066.999064	-1066.984377	1067.038613
U-3c (solvent continuum)	-1067.023431	-1067.008504	-1067.063217
U'-3c (gas phase)	-1066.999157	-1066.984682	-1067.037988
U'-3c (solvent continuum)	-1067.022392	-1067.007722	-1067.061558
S-3c (gas phase)	-1066.993221	-1066.979403	-1067.032686
S-3c (solvent continuum)	-1067.018258	-1067.003164	-1067.058610
S'-3c (gas phase)	-1066.991160	-1066.976839	-1067.029710
S'-3a (solvent continuum)	-1067.011868	-1066.997112	-1067.051300
W-3c (gas phase)	-1066.989473	-1066.974559	-1067.029623
W-3c (solvent continuum)	-1067.016272	-1067.000949	-1067.057384
W'-3c (gas phase)	-1066.990326	-1066.975648	-1067.029660
W'-3c (solvent continuum)	-1067.016530	-1067.001397	-1067.057376

[a]DFT energy incl. ZPE. [b]standard conditions T = 298.15 K and p = 1 atm.

5. References

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(2) Cao, X.; Dolg, M. *J. Chem. Phys.* **2001**, *115*, 7348.