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FOR

Palladium(II) complexes of 2,2'-tellurobis(*N*,*N*-diphenyl acetamide): efficient catalysts for Suzuki-Miyaura coupling at room temperature under air

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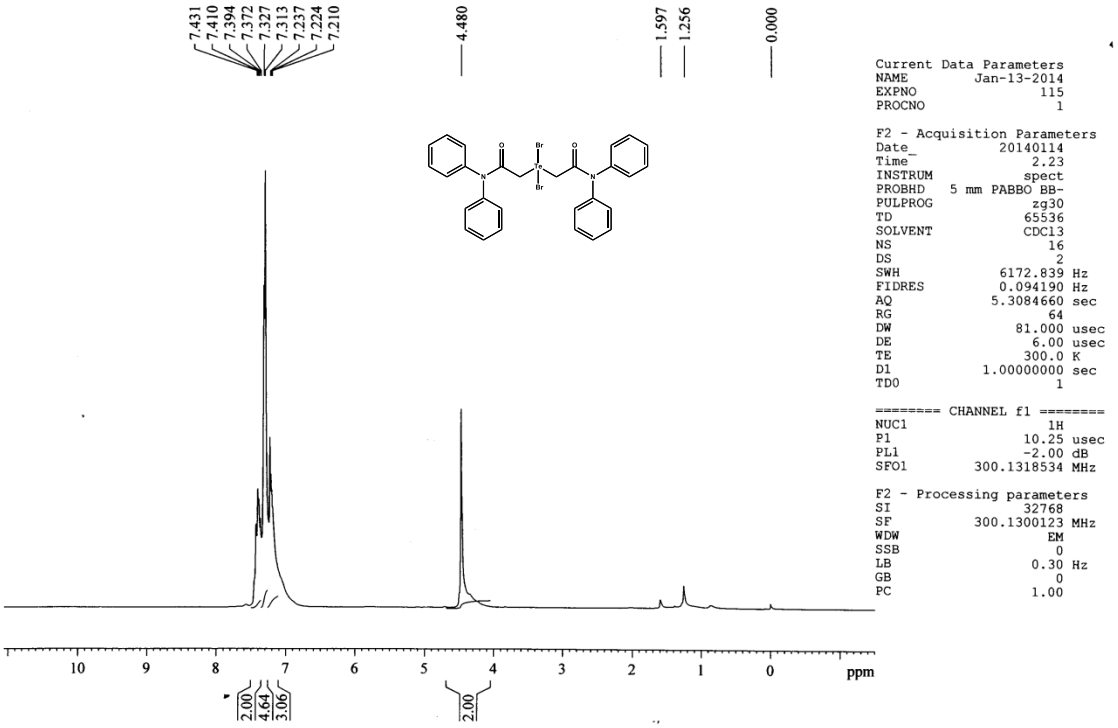


Figure S1. ^{1}H NMR of L1

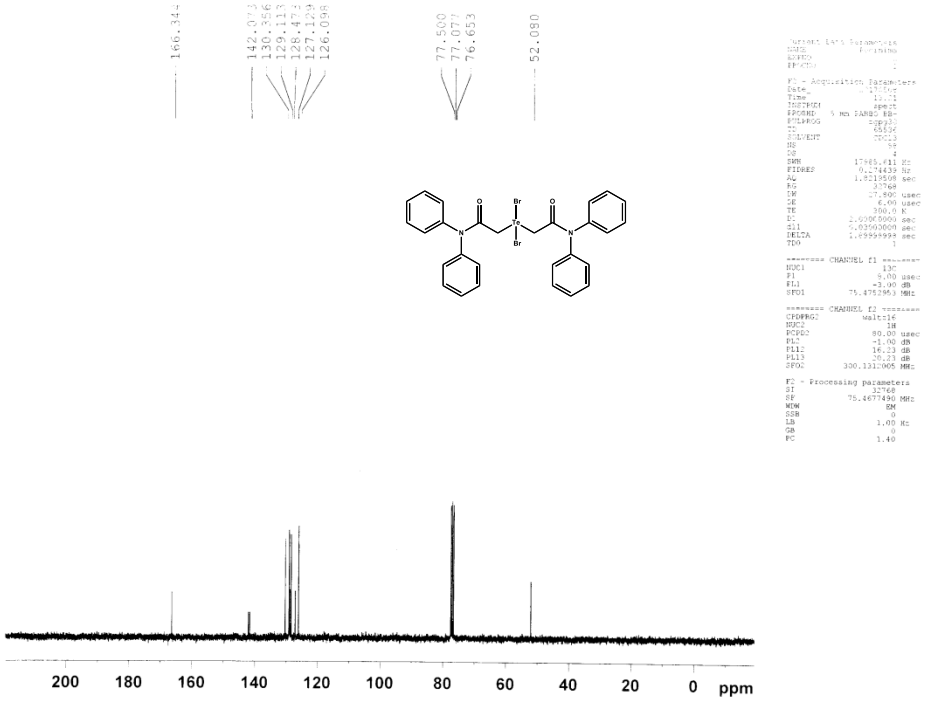


Figure S2. ^{13}C{^{1}H} NMR of L1

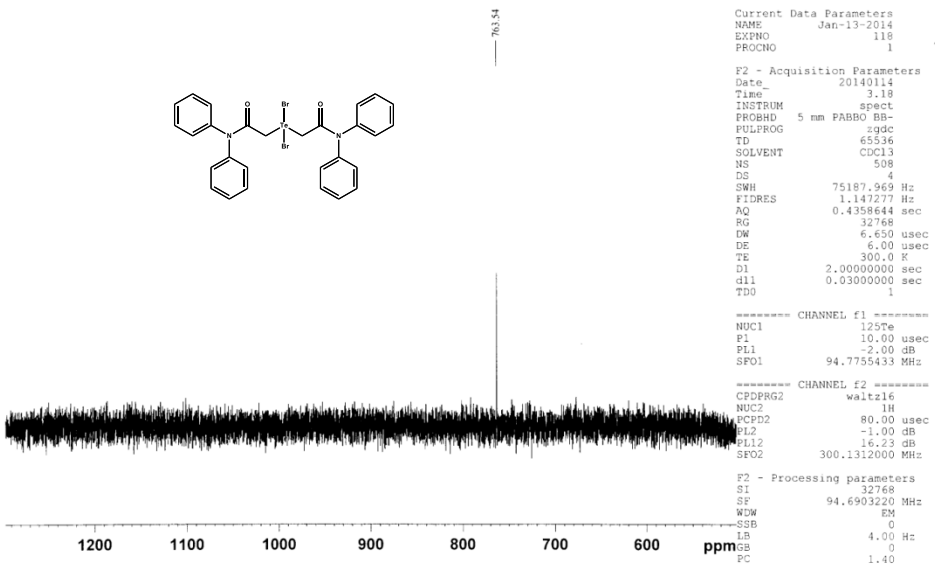


Figure S3. ^{125}Te{^{1}H} NMR of L1

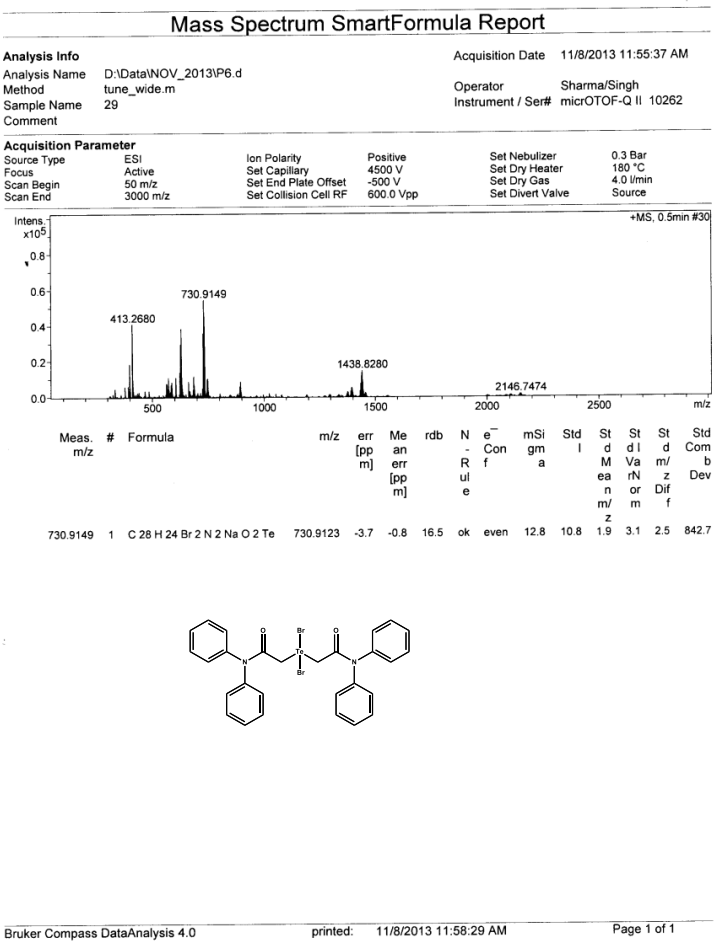


Figure S4. Mass Spectrum of L1

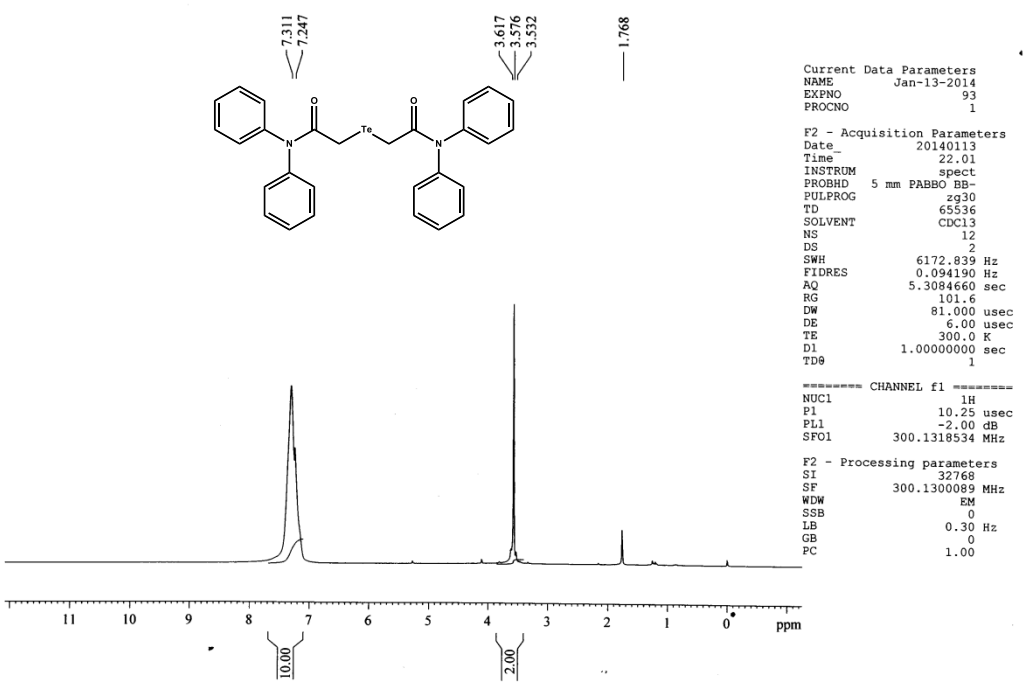


Figure S5. ^{1}H NMR of L2

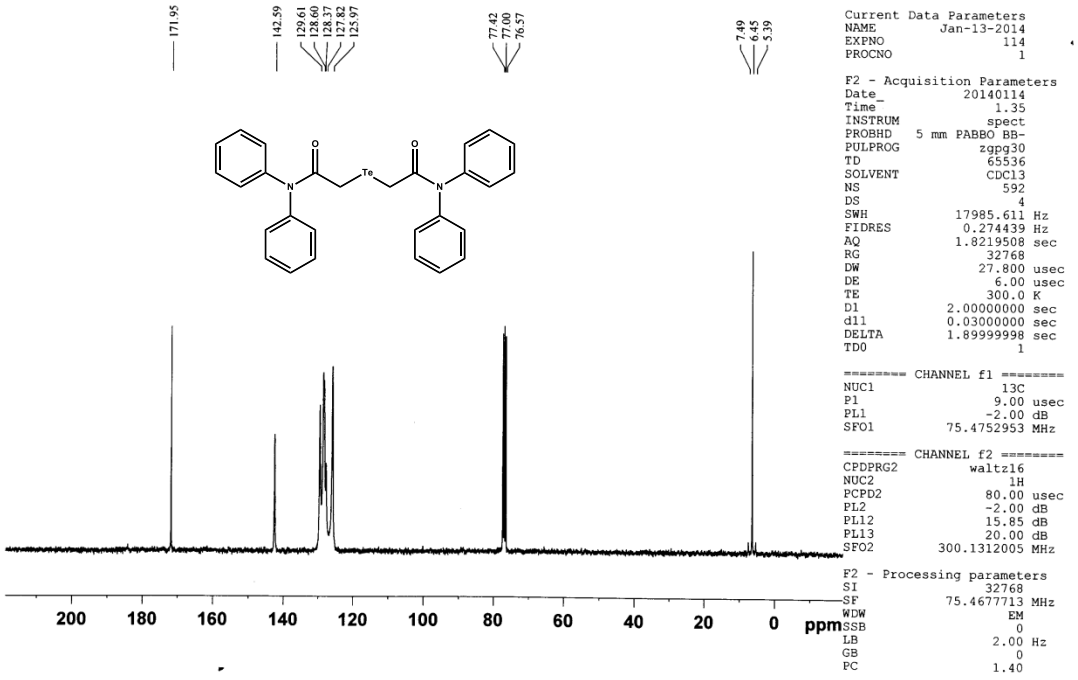


Figure S6. ^{13}C{^{1}H} NMR of L2

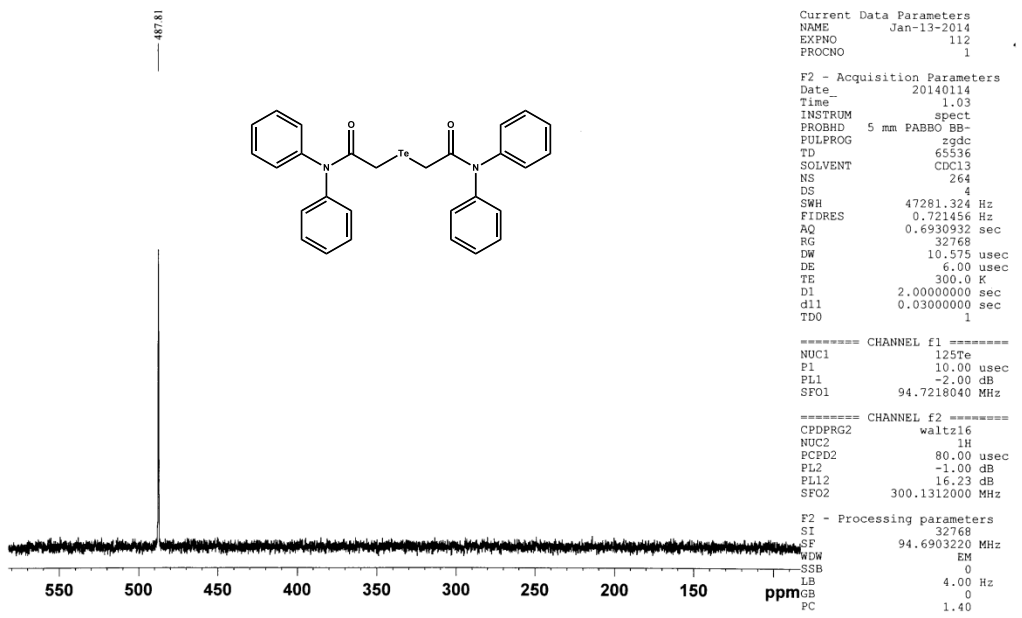


Figure S7. $^{125}Te\{^{1}H\}$ NMR of L2

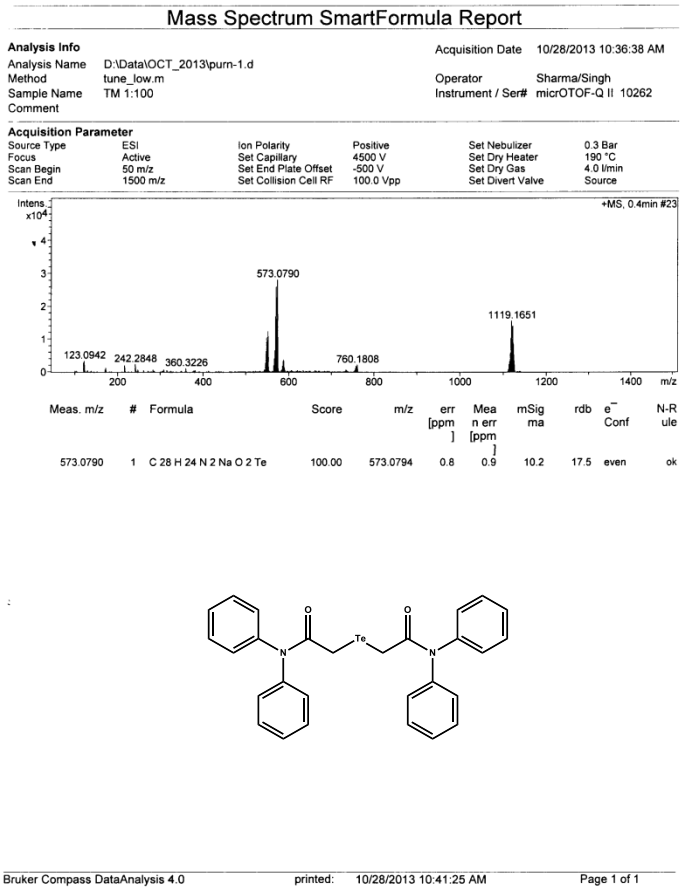


Figure S8. Mass Spectrum of L2

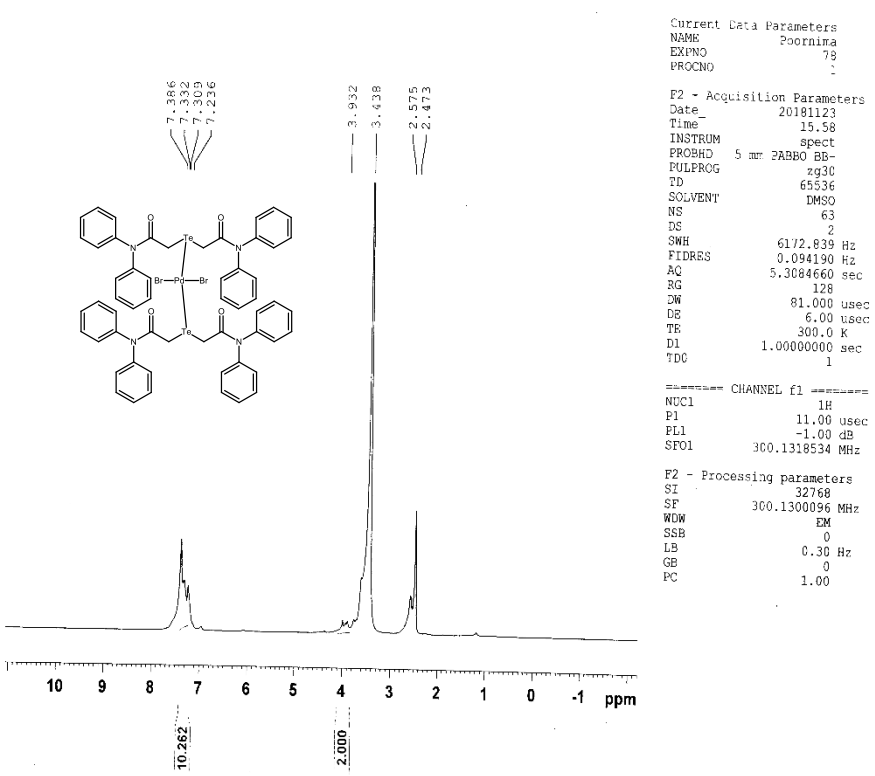


Figure S9. ^{1}H NMR of C1

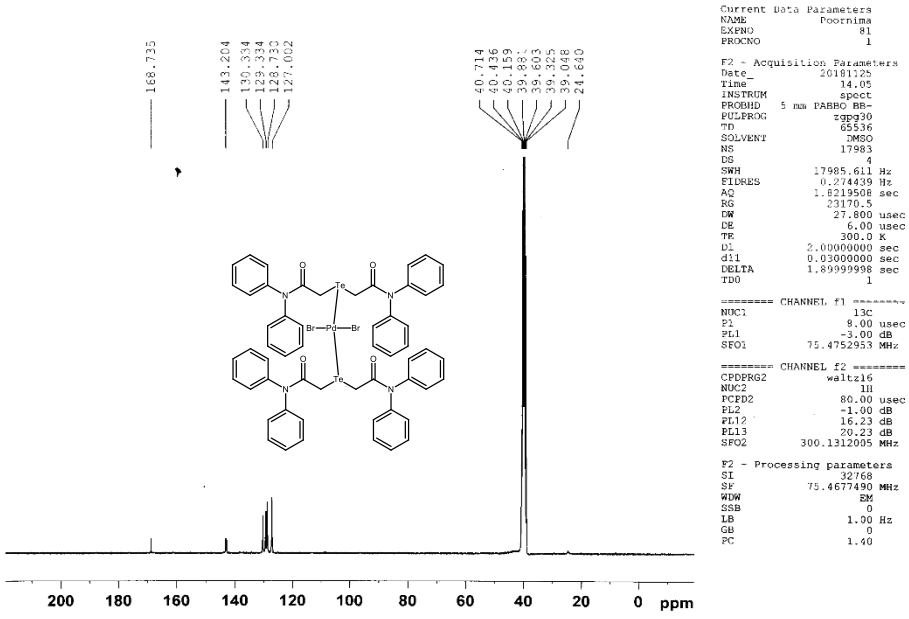


Figure S10. ^{13}C{^{1}H} NMR of C1

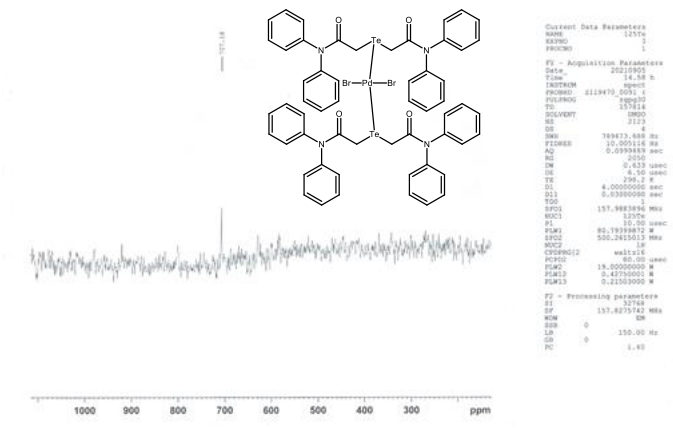


Figure S11. $^{125}Te\{^{1}H\}$ NMR of C1

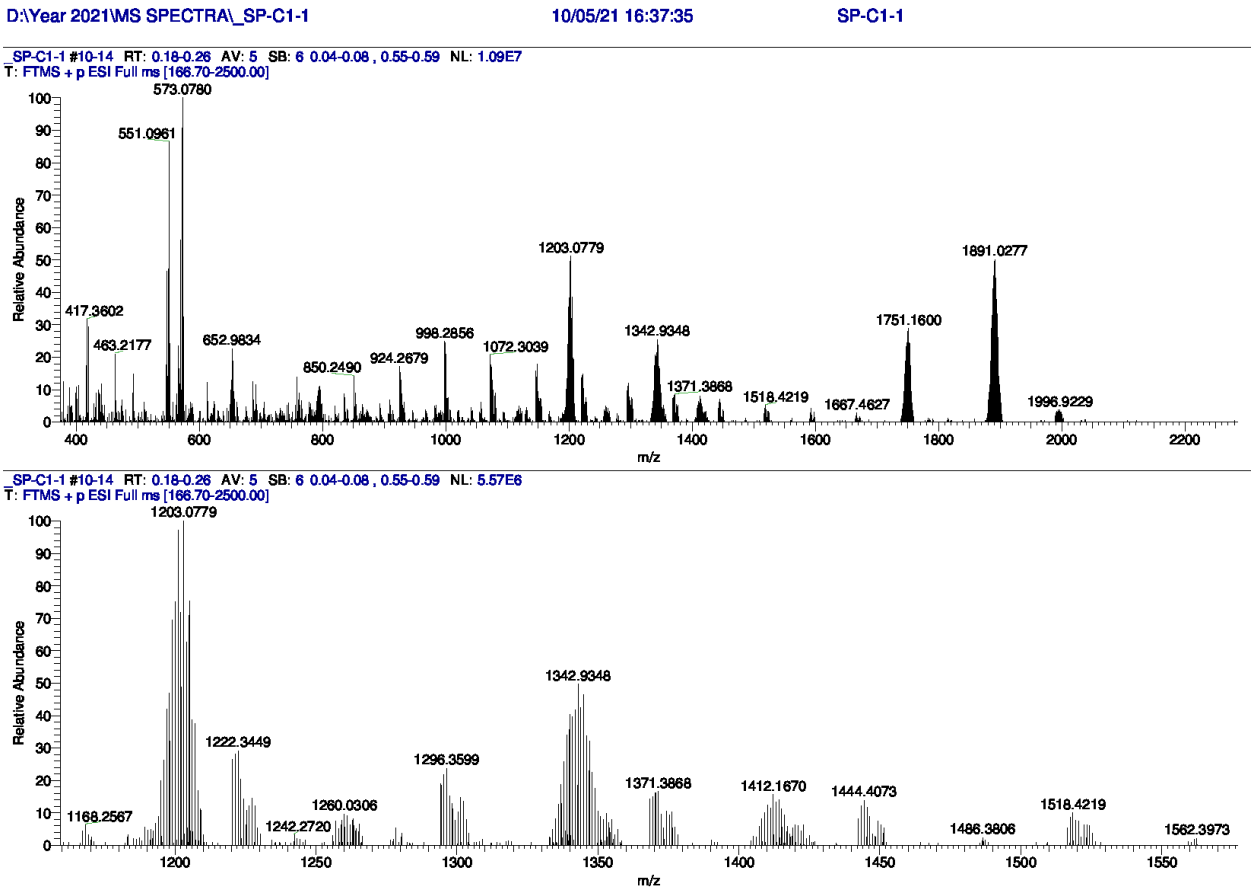


Figure S12. Mass Spectrum of C1

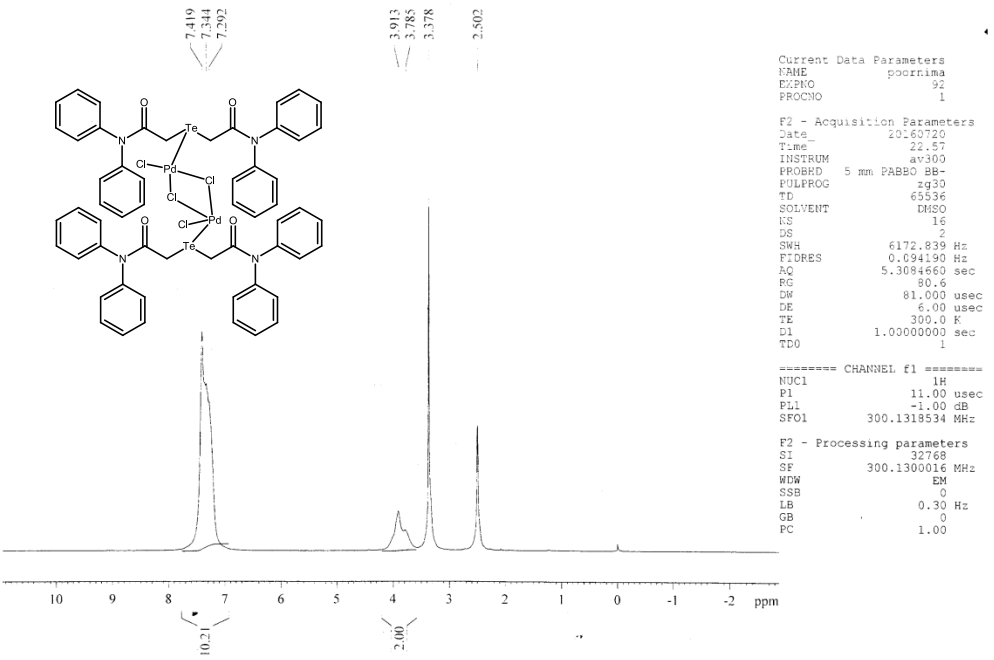


Figure S13. ^{1}H NMR of C2

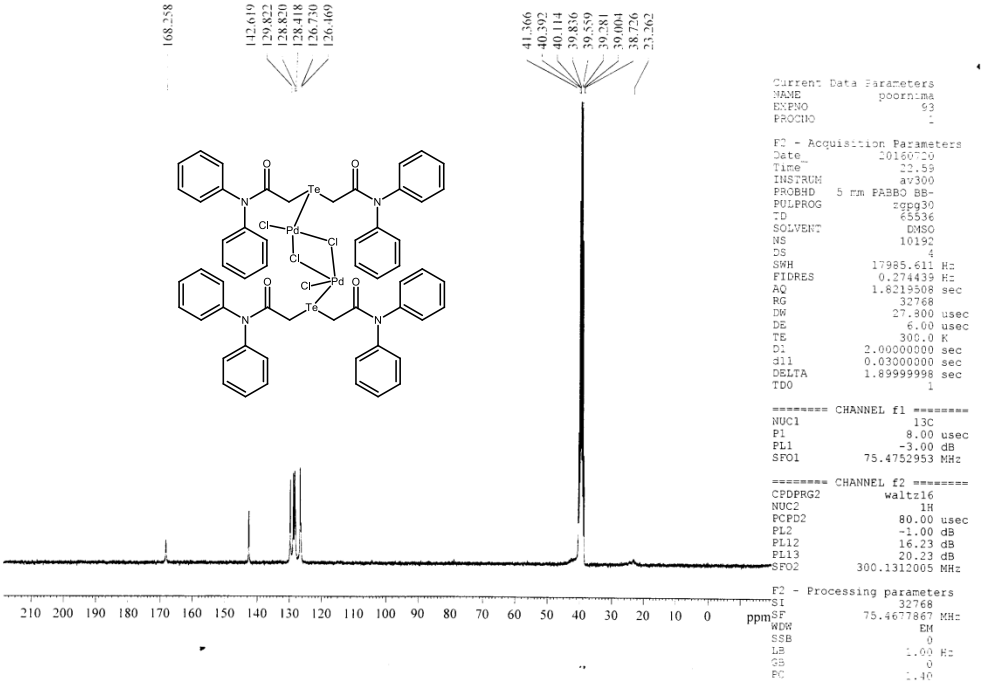


Figure S14. ^{13}C{^{1}H} NMR of C2

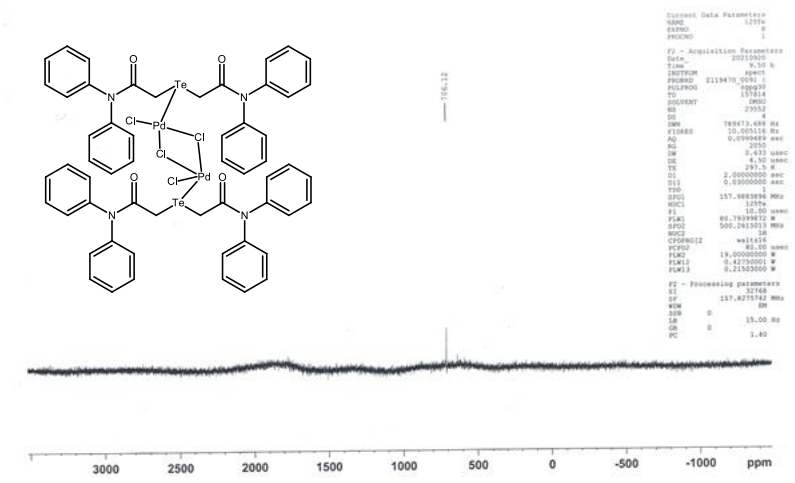


Figure 15. $^{125}Te\{^{1}H\}$ NMR of C2

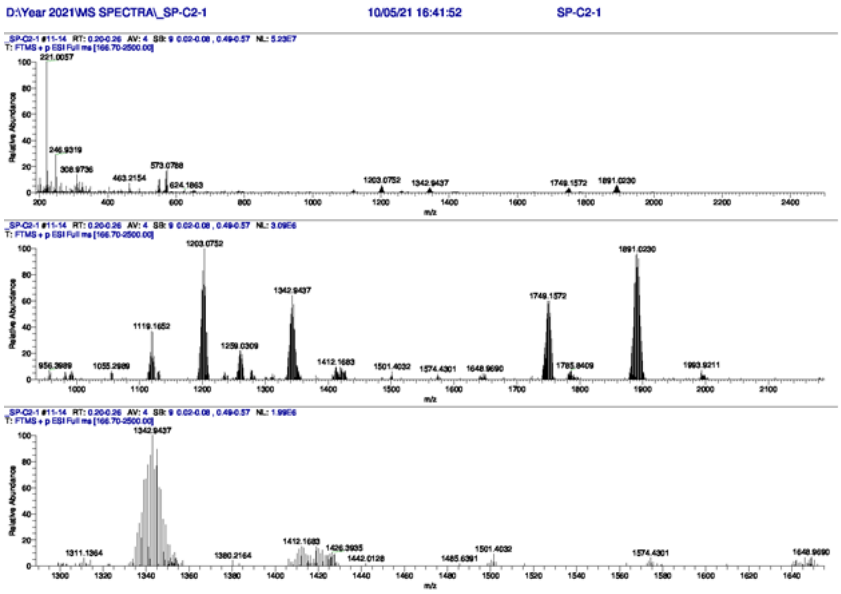


Figure S16. Mass Spectrum of C2

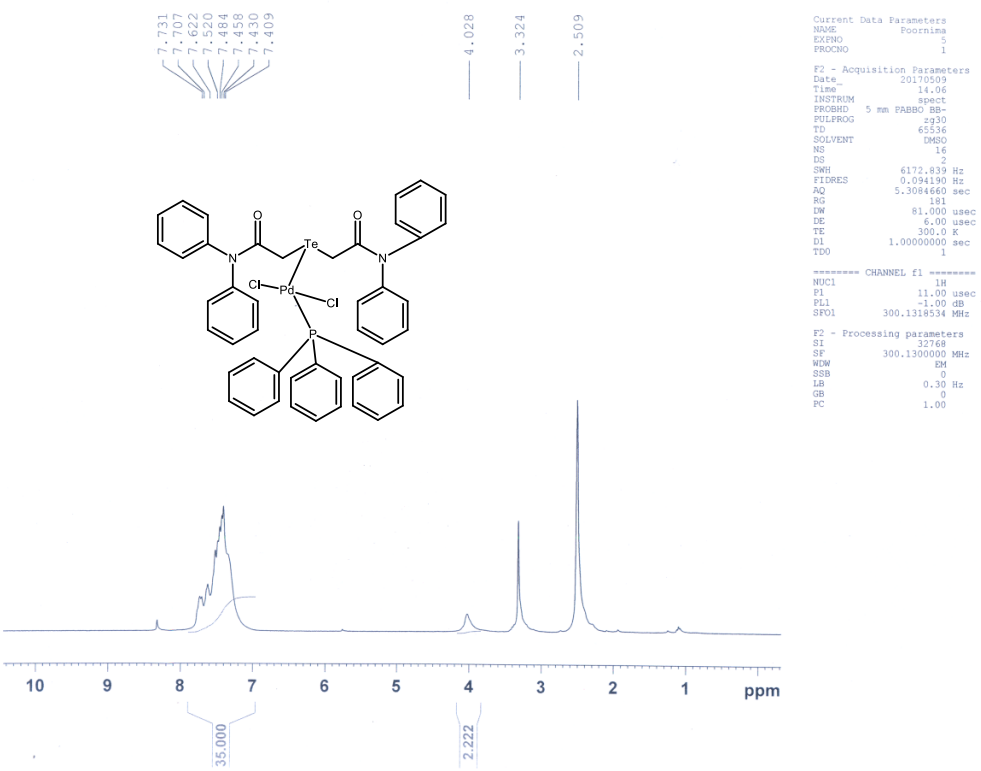


Figure S17. ^{1}H NMR of C3

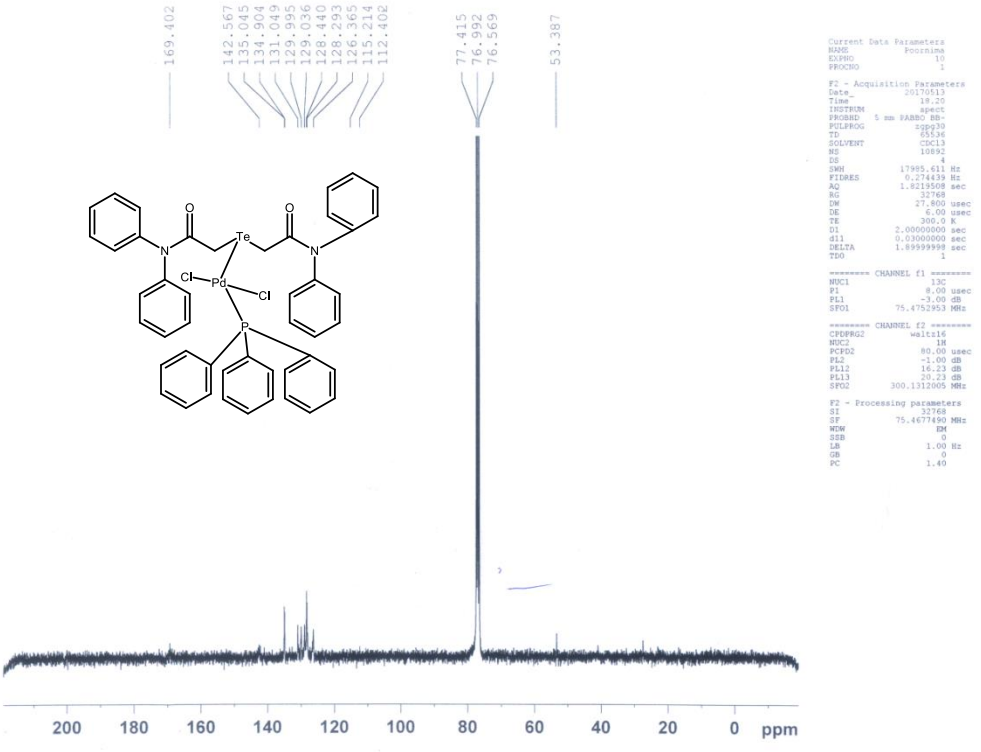


Figure S18. ^{13}C{^{1}H} NMR of C3

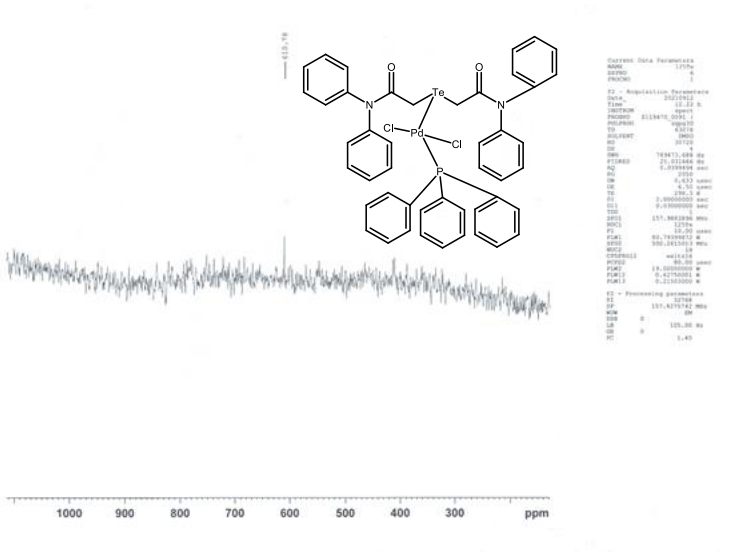


Figure S19. $^{125}Te\{^{1}H\}$ NMR of C3

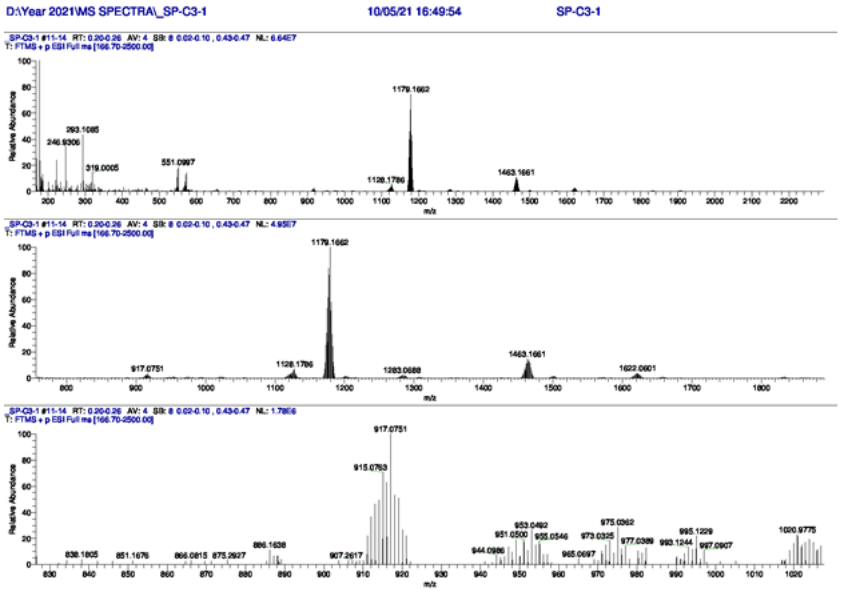


Figure S20. Mass Spectrum of C3

Table S1
Crystal Data and Structure Refinement Details for Ligands (L1, L2) and Complexes (C1, C2, C3)

	L1	**L2**	**C1**	**C2**	**C3**
Empirical formula	$C_{28}H_{24}Br_2N_2O_2Te$	$C_{28}H_{24}N_2O_2Te$	$C_{56}H_{48}Br_{1.29}Cl_{0.71}N_4O_4PdTe_2$ [+ solvent]	$C_{56}H_{48}Cl_4N_4O_4Pd_2Te_2$	$C_{46}H_{39}Cl_2N_2O_2PPdTe.2(CH_2Cl_2)$ [+ solvent]
Formula mass (g mol^{-1})	707.89	548.09	1330.74	1450.78	1157.51
Temperature (K)	299(2)	293(2)	293(2)	298(2)	298(2)
Wavelenth, λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic	Monoclinic
Crystal size (mm^3)	0.36 x 0.29 x 0.15	0.33 x 0.31 x 0.30	0.31 x 0.29 x 0.28	0.32 x 0.31 x 0.30	0.33 x 0.31 x 0.29
Space group	C 2/c	P -1	P -1	$P2_1/n$	$P2_1/c$
a (Å)	17.4421(13)	9.448(2)	11.649(2)	12.665(2)	13.32(2)
b (Å)	8.7369(6)	10.736(2)	12.518(3)	16.115(3)	23.67(5)
c (Å)	18.3468(13)	13.107(3)	12.546(3)	14.020(2)	16.79(3)
α (deg)	90	73.175(4)	98.174(4)	90	90
β (deg)	94.406(2)	72.501(4)	106.150(3)	93.688(4)	106.18(2)
γ (deg)	90	79.615(4)	112.524(3)	90	90
V ($Å^3$)	2787.6(3)	1207.3(4)	1558.2(6)	2855.5(8)	5084(16)
Z	4	2	1	2	4
ρ_{calcd} (Mg m^{-3})	1.687	1.508	1.433	1.687	1.512
Absorption coefficient (mm^{-1})	3.961	1.259	2.113	1.865	1.312
F(000)	1376	548.0	656.8	1416	2304
h, k, l ranges collected	–24→23	–12→12	–13→13	–17→17	–17→17
	–12→11	–14→13	–14→14	–21→21	–30→31
	–25→25	–17→17	–14→14	–18→18	–21→21
Reflection collected	31200	14354	15045	35428	60756
Independent reflections	3921 [R(int) = 0.0776]	6060 [R(int) = 0.0265]	5486 [R(int) = 0.0398]	7259 [R(int) = 0.0772]	12752 [R(int) = 0.1188]
θ range (°)	2.227–29.592	1.68–28.39	2.547–22.215	1.93–28.52	2.384–21.621
Completeness to θ_{max}(%)	100	99.8	99.5	97.4	99.9
Absorption correction	Semi-empirical from equivalents				
Max., min. transmission	0.543, 0.268	0.683, 0.669	0. 0.553, 0.525	0.568, 0.558	0.684, 0.655
Refinement method	Full-matrix least-squares on F2				
Data/restraints /parameters	3921 / 0 / 159	6060 / 0 / 298	5486 / 0 / 317	7259 / 0 / 325	12752 / 7 / 544
Goodness of fit on F^2	0.932	0.985	1.120	0.982	0.902
Final *R* indices ($I > 2\sigma(I)$)	R1 = 0.0337, wR2 = 0.1115	R1 = 0.0369, wR2 = 0.0776	R1 =0.0553, wR2 = 0.1290	R1 = 0.0397, wR2 = 0.0706	R1 = 0.0588, wR2 = 0.1298
R indices (all data)	R1 = 0.0492, wR2 = 0.1301	R1 = 0.0559, wR2 = 0.0840	R1 = 0.0695, wR2 = 0.1345	R1 = 0.0795, wR2 = 0.0823	R1 = 0.1251, wR2 = 0.1480
Largest diff peak/hole (e $Å^{-3}$)	0.715/ –1.094	0.600/–0.264	1.09/ –1.25	0.969 /–0.905	0.85 /–1.18
Extinction coefficient	–	–	–	–	–

Intermolecular Structures of L1, L2, C1, C2 and C3

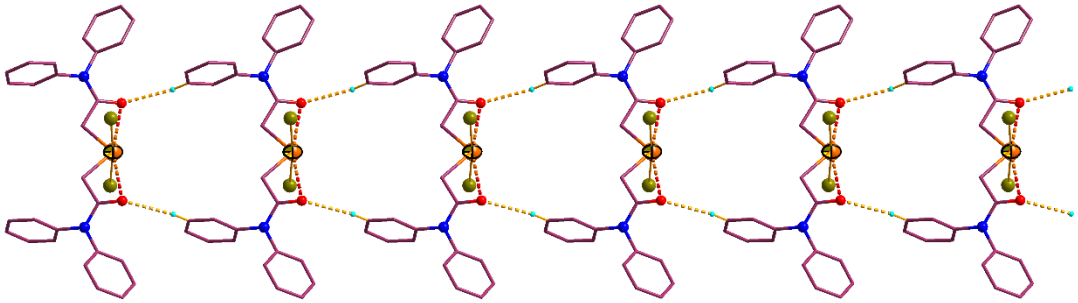


Figure S21. Supramolecular Structure due to C–H···O Interactions in the Crystal Lattice of **L1**.

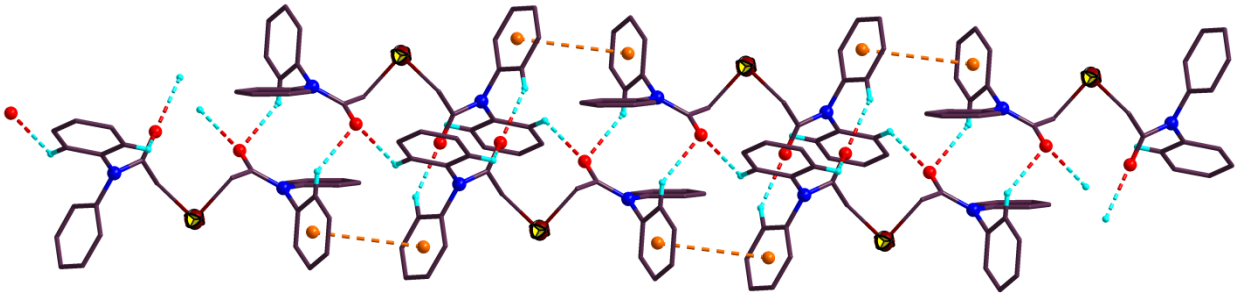


Figure S22. π–π and C–H···O Interactions in the Crystal Lattice of **L2**.

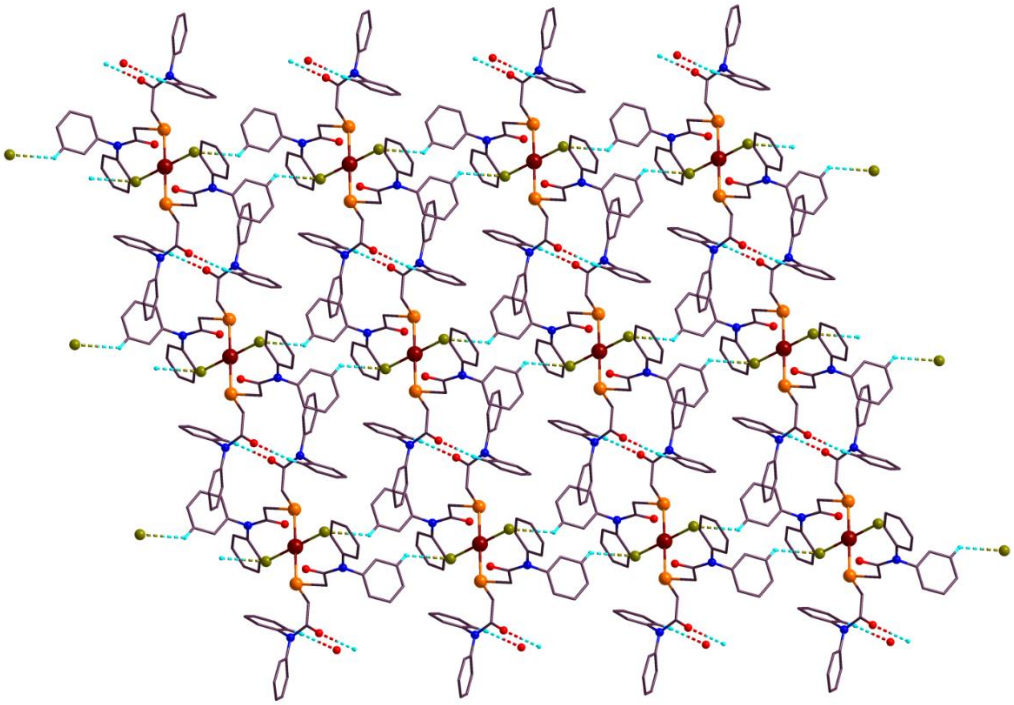


Figure S23. Supramolecular Structure due to Intermolecular C–H···O and C–H···Br Interactions in **C1**.

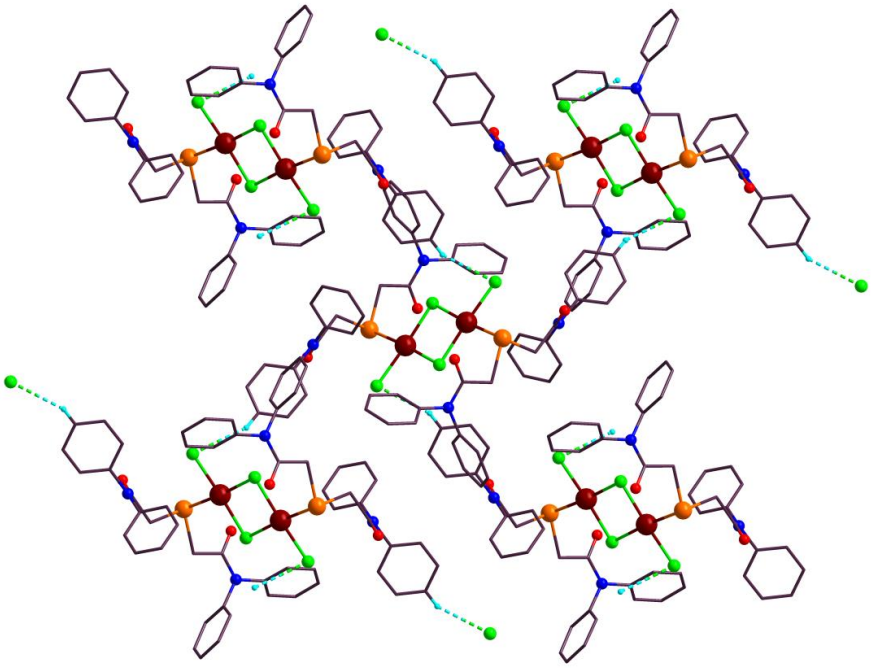


Figure S24. Supramolecular Structure due to Intermolecular C–H···Cl Interactions in the Crystal of **C2**.

Table S2

Selected bond lengths [Å] and bond angles [°]

Compounds	Bond length [Å]		Bond angle [°]	
L1	Te(1)-C(14)	2.121(3)	C(14)-Te(1)-C(14)#1	91.15(16)
	Te(1)-C(14)#1	2.121(3)	C(14)-Te(1)-Br(1)	85.19(9)
	Te(1)-Br(1)	2.6629(5)	C(14)#1-Te(1)-Br(1)	91.18(9)
	Te(1)-Br(1)#1	2.6629(5)	C(14)-Te(1)-Br(1)#1	91.17(9)
	O(1)-C(13)	1.219(4)	C(14)#1-Te(1)-Br(1)#1	85.18(9)
	N(1)-C(13)	1.355(3)	Br(1)-Te(1)-Br(1)#1	174.80(2)
	N(1)-C(6)	1.439(3)	C(13)-N(1)-C(6)	119.6(2)
	N(1)-C(7)	1.452(3)	C(13)-N(1)-C(7)	121.1(2)
	C(6)-C(1)	1.376(4)	C(6)-N(1)-C(7)	119.2(2)
	C(6)-C(5)	1.387(4)	C(1)-C(6)-C(5)	120.1(3)
	C(13)-C(14)	1.513(4)	C(1)-C(6)-N(1)	119.3(3)
	C(7)-C(12)	1.365(4)	C(5)-C(6)-N(1)	120.6(3)
	C(7)-C(8)	1.375(4)	O(1)-C(13)-N(1)	123.8(3)
	C(8)-C(9)	1.380(5)	O(1)-C(13)-C(14)	119.2(3)
	C(1)-C(2)	1.381(5)	N(1)-C(13)-C(14)	117.0(2)
	C(9)-C(10)	1.353(7)	C(12)-C(7)-C(8)	120.4(3)
	C(5)-C(4)	1.384(6)	C(12)-C(7)-N(1)	120.9(3)
	C(4)-C(3)	1.362(7)	C(8)-C(7)-N(1)	118.6(3)
	C(10)-C(11)	1.373(6)	C(13)-C(14)-Te(1)	104.65(18)
	C(12)-C(11)	1.389(5)	C(7)-C(8)-C(9)	119.4(4)
	C(3)-C(2)	1.369(6)	C(6)-C(1)-C(2)	119.4(3)
			C(10)-C(9)-C(8)	120.9(4)
			C(4)-C(5)-C(6)	118.8(4)
			C(3)-C(4)-C(5)	121.5(4)
			C(9)-C(10)-C(11)	119.7(4)
			C(7)-C(12)-C(11)	119.4(4)
			C(4)-C(3)-C(2)	119.1(4)
			C(3)-C(2)-C(1)	121.1(4)
			C(10)-C(11)-C(12)	120.2(4)
L2	Te(1)-C(14)	2.149(3)	C(14)-Te(1)-C(15)	91.93(11)
	Te(1)-C(15)	2.150(3)	C(13)-N(1)-C(6)	122.2(2)
	N(1)-C(13)	1.381(4)	C(13)-N(1)-C(12)	121.1(2)
	N(1)-C(6)	1.434(4)	C(6)-N(1)-C(12)	116.7(2)
	N(1)-C(7)	1.444(3)	C(11)-C(12)-C(7)	120.3(2)
	C(12)-C(11)	1.369(4)	C(11)-C(12)-N(1)	119.1(2)
	C(12)-C(7)	1.375(4)	C(7)-C(12)-N(1)	120.6(2)
	C(6)-C(1)	1.376(4)	C(1)-C(6)-C(5)	119.2(3)
	C(6)-C(5)	1.377(4)	C(1)-C(6)-N(1)	119.0(2)
	C(17)-C(18)	1.373(4)	C(5)-C(6)-N(1)	121.7(3)
	C(17)-C(22)	1.381(4)	C(18)-C(17)-C(22)	119.5(3)
	C(17)-N(2)	1.437(3)	C(18)-C(17)-N(2)	121.3(2)
	C(15)-C(16)	1.498(4)	C(22)-C(17)-N(2)	119.2(2)
	C(11)-C(10)	1.371(4)	C(16)-C(15)-Te(1)	109.37(17)
	C(1)-C(2)	1.380(4)	C(12)-C(11)-C(10)	120.0(3)
	C(7)-C(8)	1.380(4)	C(6)-C(1)-C(2)	120.7(3)
	O(2)-C(16)	1.218(3)	C(12)-C(7)-C(8)	119.1(3)
	C(24)-C(23)	1.371(4)	C(23)-C(24)-C(25)	120.2(3)
	C(24)-C(25)	1.383(4)	C(16)-N(2)-C(23)	122.9(2)

	N(2)-C(16)	1.375(3)	C(16)-N(2)-C(17)	120.1(2)
	N(2)-C(23)	1.436(3)	C(23)-N(2)-C(17)	117.0(2)
	C(23)-C(28)	1.386(4)	O(2)-C(16)-N(2)	121.4(3)
	C(28)-C(27)	1.374(4)	O(2)-C(16)-C(15)	121.2(2)
	C(27)-C(26)	1.367(5)	N(2)-C(16)-C(15)	117.4(2)
	C(25)-C(26)	1.375(5)	C(24)-C(23)-C(28)	119.6(3)
	C(19)-C(20)	1.373(5)	C(24)-C(23)-N(2)	119.8(2)
	C(19)-C(18)	1.386(4)	C(28)-C(23)-N(2)	120.6(3)
	C(14)-C(13)	1.494(4)	C(27)-C(28)-C(23)	119.4(3)
	C(8)-C(9)	1.358(5)	C(26)-C(27)-C(28)	121.4(3)
	C(21)-C(20)	1.365(5)	C(26)-C(25)-C(24)	120.3(3)
	C(21)-C(22)	1.381(4)	C(27)-C(26)-C(25)	119.1(3)
	C(9)-C(10)	1.374(5)	C(20)-C(19)-C(18)	119.9(3)
	C(5)-C(4)	1.387(5)	C(13)-C(14)-Te(1)	109.79(19)
	C(4)-C(3)	1.365(5)	C(9)-C(8)-C(7)	120.8(3)
	C(2)-C(3)	1.356(5)	C(20)-C(21)-C(22)	120.8(3)
	O(1)-C(13)	1.213(3)	C(21)-C(22)-C(17)	119.7(3)
			C(21)-C(20)-C(19)	119.8(3)
			C(17)-C(18)-C(19)	120.4(3)
			C(8)-C(9)-C(10)	119.8(3)
			C(11)-C(10)-C(9)	120.1(3)
			C(6)-C(5)-C(4)	119.0(3)
			C(3)-C(4)-C(5)	121.3(3)
			C(3)-C(2)-C(1)	120.2(3)
			C(2)-C(3)-C(4)	119.5(3)
			O(1)-C(13)-N(1)	122.2(3)
			O(1)-C(13)-C(14)	119.9(3)
			N(1)-C(13)-C(14)	117.9(2)
C1	Pd(1)-Te(1)	2.5652(5)	C(14)-Te(1)-Pd(1)	105.79(18)
	Te(1)-C(14)	2.122(6)	C(14)-Te(1)-C(15)	91.9(2)
	Te(1)-C(15)	2.162(6)	C(15)-Te(1)-Pd(1)	98.32(17)
	Pd(1)-Br(1)#1	2.411(4)	Te(1)-Pd(1)-Te(1)#1	180.00
	Pd(1)-Br(1)	2.411(4)	Br(1)#1-Pd(1)-Te(1)	84.51(12)
	Pd(1)-Cl(1)	2.30(2)	Br(1)-Pd(1)-Te(1)	95.50(11)
	Pd(1)-Cl(1)#1	2.30(2)	Cl(1)-Pd(1)-Te(1)	96.3(6)
	O(1)-C(13)	1.233(8)	Cl(1)#1-Pd(1)-Te(1)	83.7(6)
	O(2)-C(16)	1.224(7)	Cl(1)#1-Pd(1)-Cl(1)	180.00(17)
	N(1)-C(6)	1.443(8)	C(7)-N(1)-C(6)	116.9(5)
	N(1)-C(7)	1.425(8)	C(13)-N(1)-C(6)	121.7(6)
	N(1)-C(13)	1.352(8)	C(13)-N(1)-C(7)	121.3(5)
	N(2)-C(16)	1.363(8)	C(16)-N(2)-C(17)	122.5(5)
	N(2)-C(17)	1.441(8)	C(16)-N(2)-C(23)	120.0(5)
	N(2)-C(23)	1.431(8)	C(23)-N(2)-C(17)	117.4(5)
	C(1)-C(2)	1.383(10)	C(6)-C(1)-C(2)	119.2(8)
	C(1)-C(6)	1.374(10)	C(3)-C(2)-C(1)	120.3(8)
	C(2)-C(3)	1.350(12)	C(4)-C(3)-C(2)	120.7(8)
	C(3)-C(4)	1.342(12)	C(3)-C(4)-C(5)	120.8(9)
	C(4)-C(5)	1.365(11)	C(4)-C(5)-C(6)	119.5(8)
	C(5)-C(6)	1.383(10)	C(1)-C(6)-N(1)	121.8(6)
	C(7)-C(8)	1.363(9)	C(1)-C(6)-C(5)	119.6(7)
	C(7)-C(12)	1.368(9)	C(5)-C(6)-N(1)	118.4(6)
	C(8)-C(9)	1.405(11)	C(8)-C(7)-N(1)	121.1(6)
	C(9)-C(10)	1.340(12)	C(8)-C(7)-C(12)	120.3(7)
	C(10)-C(11)	1.377(11)	C(12)-C(7)-N(1)	118.5(6)
	C(11)-C(12)	1.359(10)	C(7)-C(8)-C(9)	118.2(8)

	C(13)-C(14)	1.503(9)	C(10)-C(9)-C(8)	121.0(8)
	C(15)-C(16)	1.516(9)	C(9)-C(10)-C(11)	120.0(8)
	C(17)-C(18)	1.374(10)	C(12)-C(11)-C(10)	119.5(8)
	C(17)-C(22)	1.347(9)	C(11)-C(12)-C(7)	120.9(7)
	C(18)-C(19)	1.370(11)	O(1)-C(13)-N(1)	123.6(6)
	C(19)-C(20)	1.361(13)	O(1)-C(13)-C(14)	119.9(6)
	C(20)-C(21)	1.333(13)	N(1)-C(13)-C(14)	116.6(6)
	C(21)-C(22)	1.393(11)	C(13)-C(14)-Te(1)	108.0(4)
	C(23)-C(24)	1.390(9)	C(16)-C(15)-Te(1)	106.0(4)
	C(23)-C(28)	1.348(10)	O(2)-C(16)-N(2)	122.6(6)
	C(24)-C(25)	1.349(11)	O(2)-C(16)-C(15)	120.4(6)
	C(25)-C(26)	1.352(13)	N(2)-C(16)-C(15)	116.9(5)
	C(26)-C(27)	1.353(14)	C(18)-C(17)-N(2)	120.7(6)
	C(27)-C(28)	1.400(12)	C(22)-C(17)-N(2)	119.3(7)
			C(22)-C(17)-C(18)	120.0(7)
			C(19)-C(18)-C(17)	118.2(8)
			C(20)-C(19)-C(18)	121.7(9)
			C(21)-C(20)-C(19)	120.1(8)
			C(20)-C(21)-C(22)	119.2(8)
			C(17)-C(22)-C(21)	120.8(8)
			C(24)-C(23)-N(2)	120.8(6)
			C(28)-C(23)-N(2)	120.2(6)
			C(28)-C(23)-C(24)	118.9(7)
			C(25)-C(24)-C(23)	120.1(8)
			C(24)-C(25)-C(26)	120.5(8)
			C(25)-C(26)-C(27)	121.5(9)
			C(26)-C(27)-C(28)	117.9(9)
			C(23)-C(28)-C(27)	121.2(8)
C2	Te(1)-C(14)	2.138(4)	C(14)-Te(1)-Pd(1)	96.61(11)
	Te(1)-C(15)	2.129(4)	C(15)-Te(1)-Pd(1)	104.69(10)
	Te(1)-Pd(1)	2.4982(5)	C(15)-Te(1)-C(14)	90.36(15)
	Pd(1)-Cl(1)	2.2766(11)	Cl(1)-Pd(1)-Te(1)	83.36(3)
	Pd(1)-Cl(2)	2.3035(11)	Cl(2)-Pd(1)-Te(1)	96.54(3)
	Pd(1)-Cl(2)#1	2.4148(11)	Cl(2)-Pd(1)-Te(1)#1	175.61(3)
	O(1)-C(13)	1.224(4)	Cl(2)-Pd(1)-Cl(1)	92.81(4)
	O(2)-C(16)	1.215(5)	Cl(2)-Pd(1)-Cl(1)	176.11(5)
	N(1)-C(1)	1.446(5)	C(7)-N(1)-C(1)	117.1(3)
	N(1)-C(7)	1.446(5)	C(13)-N(1)-C(1)	124.9(3)
	N(1)-C(13)	1.350(5)	C(13)-N(1)-C(7)	117.9(3)
	N(2)-C(16)	1.359(5)	C(17)-N(2)-C(16)	122.9(3)
	N(2)-C(17)	1.440(5)	C(23)-N(2)-C(16)	119.8(4)
	N(2)-C(23)	1.446(5)	C(23)-N(2)-C(17)	117.3(3)
	C(1)-C(2)	1.357(7)	C(2)-C(1)-N(1)	119.9(5)
	C(1)-C(6)	1.344(7)	C(6)-C(1)-N(1)	119.5(5)
	C(2)-C(3)	1.390(8)	C(6)-C(1)-C(2)	120.6(5)
	C(3)-C(4)	1.377(13)	C(3)-C(2)-C(1)	118.3(7)
	C(4)-C(5)	1.313(14)	C(4)-C(3)-C(2)	120.5(9)
	C(5)-C(6)	1.383(10)	C(5)-C(4)-C(3)	119.6(9)
	C(7)-C(8)	1.368(6)	C(6)-C(5)-C(4)	120.7(11)
	C(7)-C(12)	1.375(6)	C(5)-C(6)-C(1)	120.3(8)
	C(8)-C(9)	1.377(7)	C(8)-C(7)-N(1)	119.8(4)
	C(9)-C(10)	1.356(8)	C(12)-C(7)-N(1)	119.9(4)
	C(10)-C(11)	1.357(8)	C(12)-C(7)-C(8)	120.3(4)
	C(11)-C(12)	1.392(7)	C(9)-C(8)-C(7)	120.0(5)
	C(13)-C(14)	1.503(5)	C(10)-C(9)-C(8)	120.0(6)

	C(15)-C(16)	1.501(5)	C(11)-C(10)-C(9)	120.6(6)
	C(17)-C(18)	1.371(6)	C(12)-C(11)-C(10)	120.4(6)
	C(17)-C(22)	1.381(6)	C(11)-C(12)-C(7)	118.7(5)
	C(18)-C(19)	1.387(7)	N(1)-C(13)-O(1)	122.1(4)
	C(19)-C(20)	1.353(9)	C(14)-C(13)-O(1)	120.2(4)
	C(19)-C(20)	1.353(9)	C(14)-C(13)-N(1)	117.7(4)
	C(20)-C(21)	1.350(9)	C(13)-C(14)-Te(1)	110.4(3)
	C(21)-C(22)	1.398(7)	C(16)-C(15)-Te(1)	106.7(3)
	C(23)-C(24)	1.360(6)	N(2)-C(16)-O(2)	123.7(4)
	C(23)-C(28)	1.341(6)	C(15)-C(16)-O(2)	119.7(4)
	C(24)-C(25)	1.375(6)	C(15)-C(16)-N(2)	116.5(4)
	C(25)-C(26)	1.366(7)	C(18)-C(17)-N(2)	119.2(4)
	C(26)-C(27)	1.347(7)	C(22)-C(17)-N(2)	120.3(4)
	C(27)-C(28)	1.385(7)	C(22)-C(17)-C(18)	120.5(5)
			C(19)-C(18)-C(17)	119.1(6)
			C(20)-C(19)-C(18)	121.3(7)
			C(21)-C(20)-C(19)	119.3(7)
			C(22)-C(21)-C(20)	121.7(6)
			C(21)-C(22)-C(17)	118.0(5)
			C(24)-C(23)-N(2)	119.9(4)
			C(28)-C(23)-N(2)	120.5(4)
			C(28)-C(23)-C(24)	119.6(4)
			C(25)-C(24)-C(23)	120.8(5)
			C(26)-C(25)-C(24)	119.4(5)
			C(27)-C(26)-C(25)	119.6(5)
			C(28)-C(27)-C(26)	120.5(6)
			C(27)-C(28)-C(23)	120.1(5)
C3	Te(1)-Pd(1)	2.586(4)	C(14)-Te(1)-Pd(1)	100.5(2)
	Te(1)-C(14)	2.188(7)	C(15)-Te(1)-Pd(1)	100.1(2)
	Te(1)-C(15)	2.183(6)	C(15)-Te(1)-C(14)	93.9(2)
	Pd(1)-Cl(1)	2.378(3)	Cl(1)-Pd(1)-Te(1)	88.98(12)
	Pd(1)-Cl(2)	2.383(4)	Cl(1)-Pd(1)-Cl(2)	90.99(13)
	Pd(1)-P(1)	2.290(3)	Cl(2)-Pd(1)-Te(1)	175.43(5)
	P(1)-C(29)	1.854(7)	P(1)-Pd(1)-Te(1)	93.21(12)
	P(1)-C(35)	1.839(7)	P(1)-Pd(1)-Cl(1)	174.76(6)
	P(1)-C(41)	1.840(7)	P(1)-Pd(1)-Cl(2)	87.20(13)
	O(1)-C(13)	1.243(6)	C(29)-P(1)-Pd(1)	110.5(2)
	O(2)-C(16)	1.243(7)	C(35)-P(1)-Pd(1)	119.1(2)
	N(1)-C(6)	1.453(7)	C(35)-P(1)-C(29)	103.3(3)
	N(1)-C(7)	1.458(7)	C(35)-P(1)-C(41)	103.6(3)
	N(1)-C(13)	1.379(7)	C(41)-P(1)-Pd(1)	111.6(2)
	N(2)-C(16)	1.392(8)	C(41)-P(1)-C(29)	107.9(3)
	N(2)-C(17)	1.481(8)	C(6)-N(1)-C(7)	117.7(5)
	N(2)-C(23)	1.469(8)	C(13)-N(1)-C(6)	120.0(5)
	C(1)-C(2)	1.405(10)	C(13)-N(1)-C(7)	122.2(5)
	C(1)-C(6)	1.382(8)	C(16)-N(2)-C(17)	123.2(5)
	C(2)-C(3)	1.374(10)	C(16)-N(2)-C(23)	119.1(5)
	C(3)-C(4)	1.376(11)	C(23)-N(2)-C(17)	117.4(5)
	C(4)-C(5)	1.437(10)	C(6)-C(1)-C(2)	120.6(7)
	C(5)-C(6)	1.387(9)	C(3)-C(2)-C(1)	119.7(7)
	C(7)-C(8)	1.416(9)	C(2)-C(3)-C(4)	121.2(8)
	C(7)-C(12)	1.406(9)	C(3)-C(4)-C(5)	119.1(8)
	C(8)-C(9)	1.392(10)	C(6)-C(5)-C(4)	119.5(7)
	C(9)-C(10)	1.381(12)	C(1)-C(6)-N(1)	121.5(6)
	C(10)-C(11)	1.412(11)	C(1)-C(6)-C(5)	119.9(6)

	C(11)-C(12)	1.406(10)	C(5)-C(6)-N(1)	118.6(5)
	C(13)-C(14)	1.538(8)	C(8)-C(7)-N(1)	119.8(6)
	C(15)-C(16)	1.543(8)	C(12)-C(7)-N(1)	123.2(5)
	C(17)-C(18)	1.380(9)	C(12)-C(7)-C(8)	117.0(6)
	C(17)-C(22)	1.353(8)	C(9)-C(8)-C(7)	120.9(8)
	C(18)-C(19)	1.397(9)	C(10)-C(9)-C(8)	121.0(8)
	C(19)-C(20)	1.369(11)	C(9)-C(10)-C(11)	120.1(8)
	C(20)-C(21)	1.406(12)	C(12)-C(11)-C(10)	118.2(8)
	C(21)-C(22)	1.399(10)	C(7)-C(12)-C(11)	122.5(7)
	C(23)-C(24)	1.417(10)	O(1)-C(13)-N(1)	124.1(5)
	C(23)-C(28)	1.371(11)	O(1)-C(13)-C(14)	119.7(5)
	C(24)-C(25)	1.401(10)	N(1)-C(13)-C(14)	116.2(5)
	C(25)-C(26)	1.361(15)	C(13)-C(14)-Te(1)	104.8(4)
	C(26)-C(27)	1.393(17)	C(16)-C(15)-Te(1)	105.4(4)
	C(27)-C(28)	1.433(14)	O(2)-C(16)-N(2)	123.3(5)
	C(29)-C(30)	1.436(8)	O(2)-C(16)-C(15)	120.1(6)
	C(29)-C(34)	1.401(9)	C(28)-C(23)-C(24)	120.1(7)
	C(30)-C(31)	1.383(9)	C(25)-C(24)-C(23)	122.1(9)
	C(31)-C(32)	1.400(11)	C(26)-C(25)-C(24)	114.5(12)
	C(32)-C(33)	1.410(11)	C(25)-C(26)-C(27)	127.7(13)
	C(33)-C(34)	1.402(10)	C(26)-C(27)-C(28)	115.4(13)
	C(35)-C(36)	1.422(8)	C(23)-C(28)-C(27)	120.2(10)
	C(35)-C(40)	1.407(8)	C(30)-C(29)-P(1)	119.5(5)
	C(36)-C(37)	1.426(9)	C(34)-C(29)-P(1)	121.6(5)
	C(37)-C(38)	1.380(10)	C(34)-C(29)-C(30)	118.8(6)
	C(38)-C(39)	1.395(11)	C(31)-C(30)-C(29)	120.6(6)
	C(39)-C(40)	1.427(9)	C(30)-C(31)-C(32)	121.1(7)
	C(41)-C(42)	1.382(9)	C(31)-C(32)-C(33)	118.2(7)
	C(41)-C(46)	1.414(9)	C(36)-C(35)-P(1)	120.8(5)
	C(42)-C(43)	1.399(10)	C(40)-C(35)-P(1)	121.7(5)
	C(43)-C(44)	1.375(11)	C(40)-C(35)-C(36)	117.5(6)
	C(44)-C(45)	1.407(11)	C(35)-C(36)-C(37)	121.1(6)
	C(45)-C(46)	1.410(10)	C(38)-C(37)-C(36)	120.0(7)
			C(37)-C(38)-C(39)	120.2(7)
			C(38)-C(39)-C(40)	120.2(7)
			C(35)-C(40)-C(39)	120.9(7)
			C(42)-C(41)-P(1)	124.4(6)
			C(42)-C(41)-C(46)	117.4(6)
			C(46)-C(41)-P(1)	118.2(5)
			C(41)-C(42)-C(43)	122.4(8)
			C(44)-C(43)-C(42)	119.7(8)
			C(43)-C(44)-C(45)	120.6(8)
			C(44)-C(45)-C(46)	118.6(8)
			C(45)-C(46)-C(41)	121.3(7)

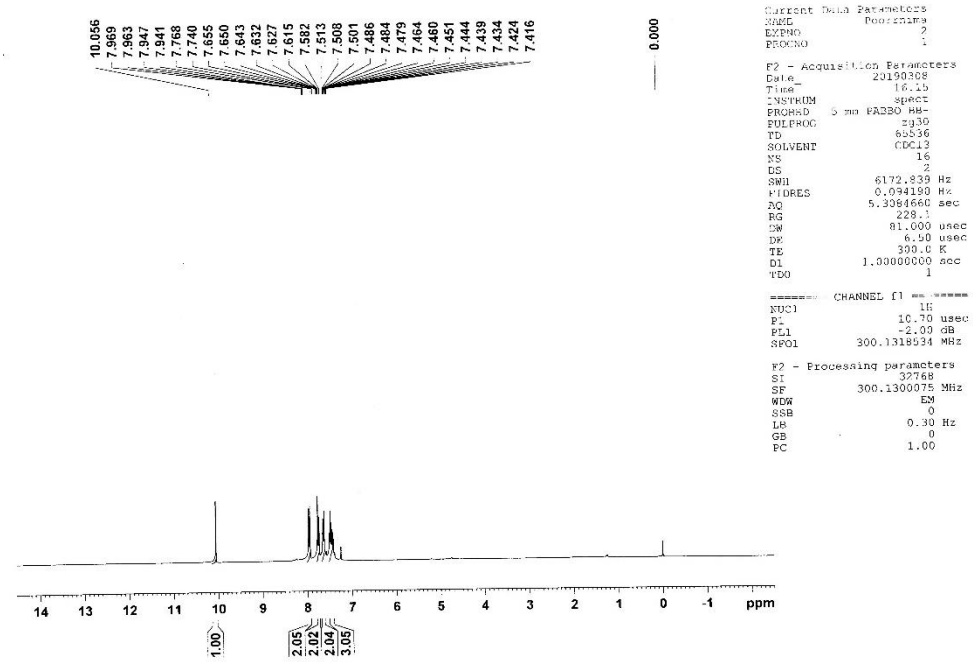
Table S3.

Parametric details of D–H···A interactions.

	D–H···A	d(D–H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (°)	Symmetry operation
L1	C(11)–H(11)···O1	0.93	2.610	3.499(4)	160.3	1-x, y, 1/2-z
L2	C(7)–H(7)···O1	0.93	2.478	3.225(5)	137.5	-x,1-y,-z
	C(22)–H(22)···O1	0.93	2.642	3.305(4)	128.8	-x,1-y,-z
	C(28)–H(28)···O2	0.93	2.569	3.412(4)	150.9	-x,1-y,-z
C1	C(11)–H(11)···Br(1)	0.93	3.035	3.726(2)	132.5	1-x, 2-y,1-z
	C(18)–H(18)···O(2)	0.93	2.583	3.425(2)	150.7	2-x, 2-y, 2-z
C2	C(10)–H(10)···Cl(1)	0.93	2.843	3.713(7)	156.1	2-x,1-y,1-z

C−C couplin reaction:[2]

4−Phenylbenzaldehyde:

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EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
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Time                   16.15
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                     228.1
DW                  81.000 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.70 usec
PL1                     -2.00 dB
SFO1             300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF               300.1300075 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
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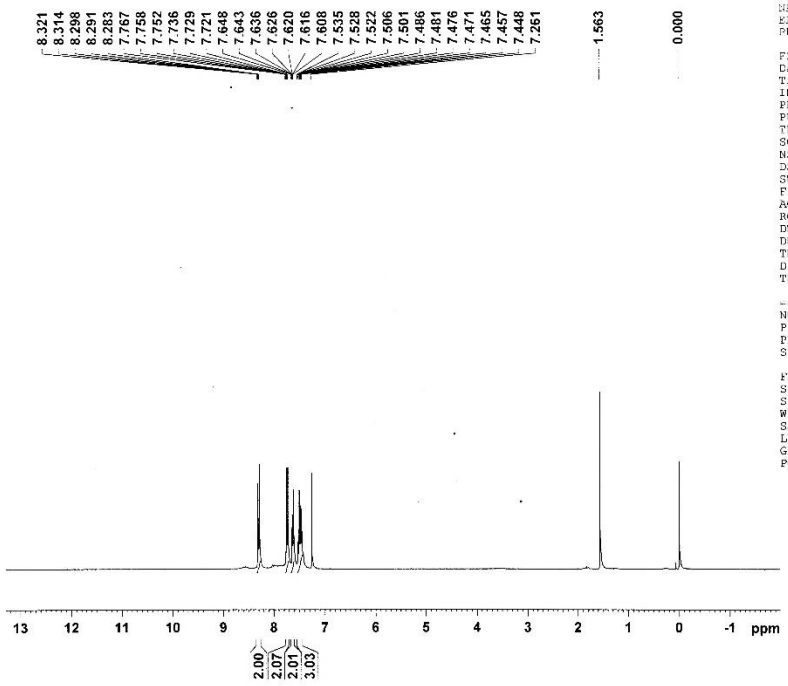
4−Nitrobiphenyl:

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Current Data Parameters
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EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190308
Time                   16.35
INSTRUM                spect
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PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                     456.1
DW                  81.000 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.70 usec
PL1                     -2.00 dB
SFO1             300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF               300.1300062 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
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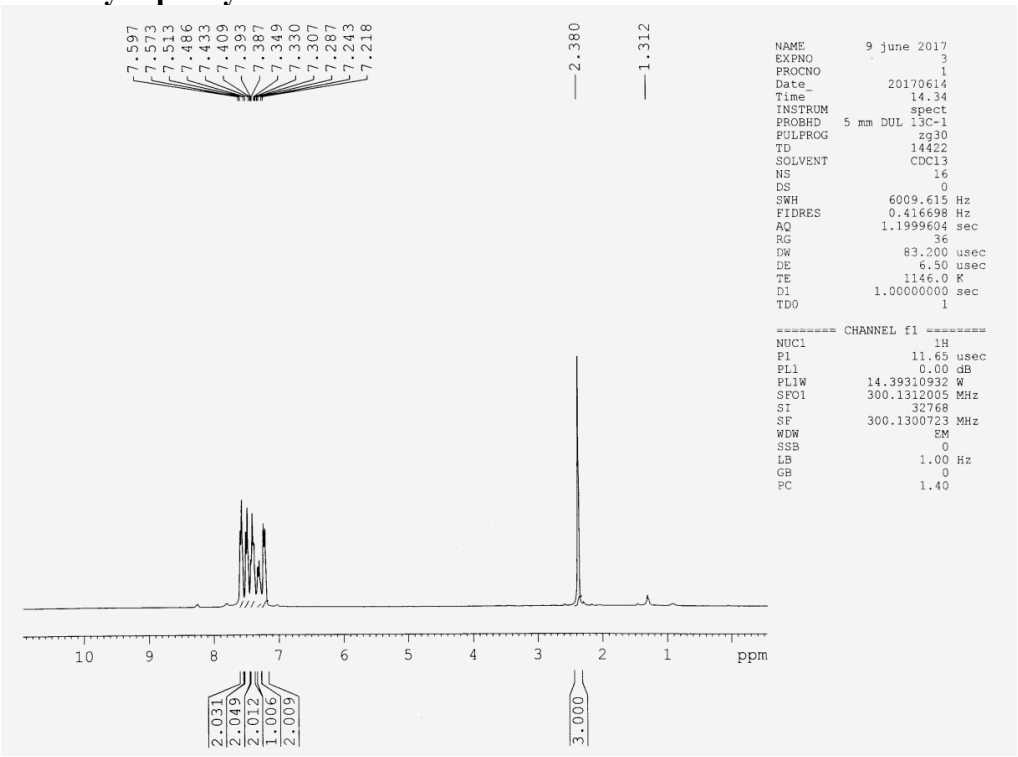
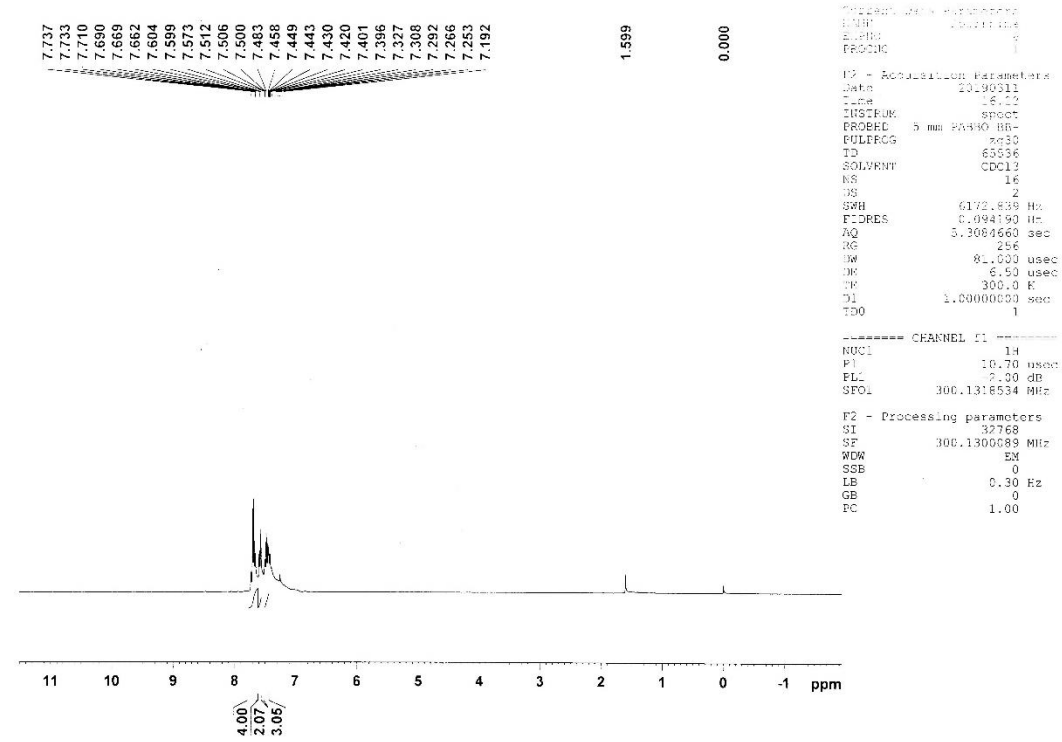
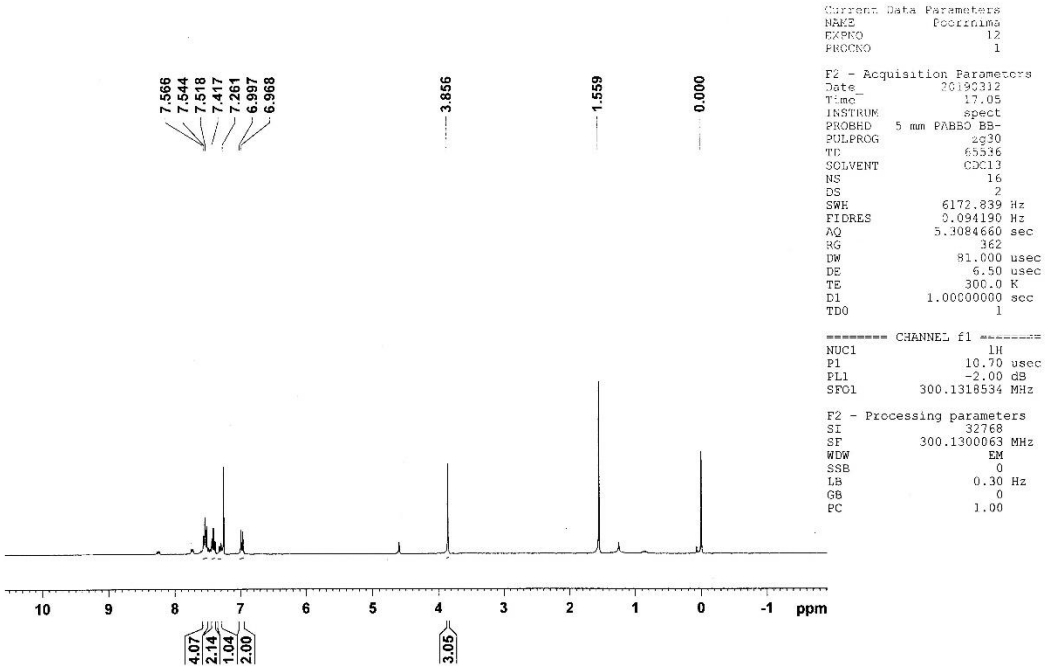
4−Methylbiphenyl:



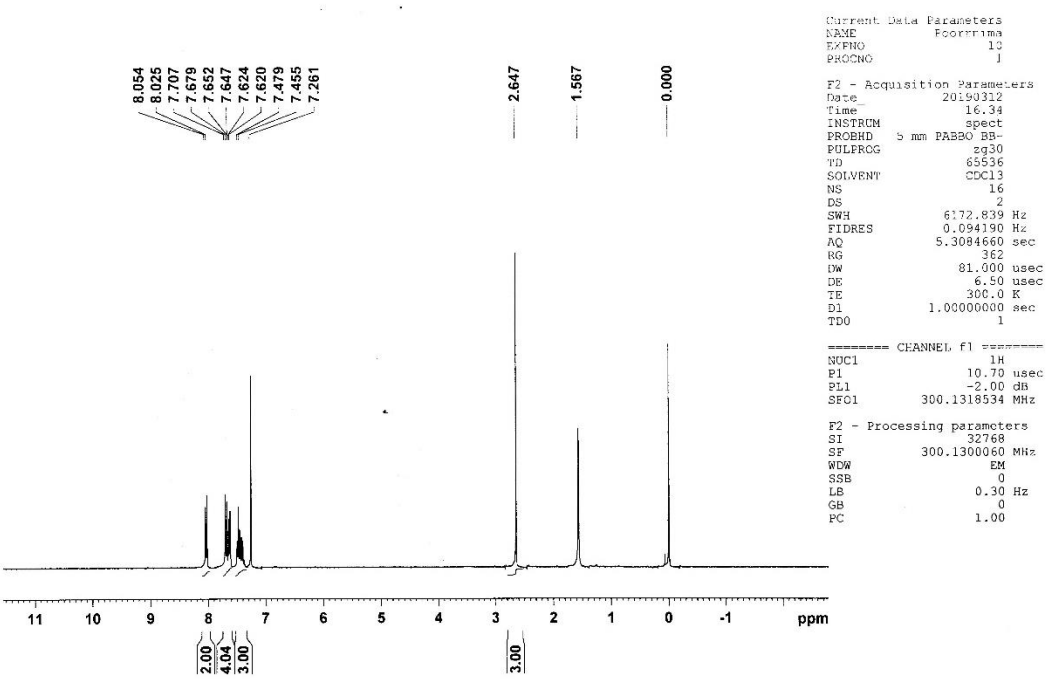
4−Phenylbenzonitrile:



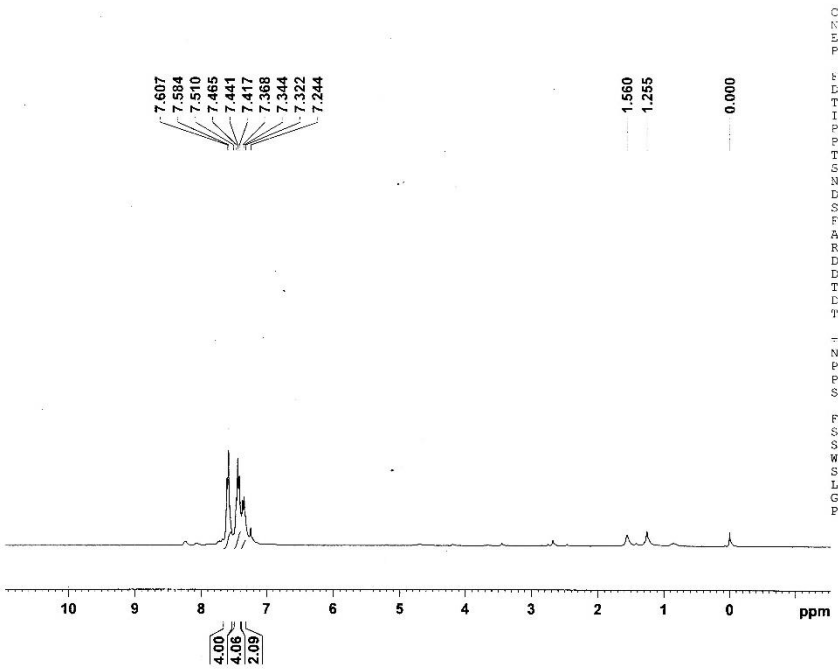
4−Methoxybiphenyl:



4−Acetylbiphenyl:



Biphenyl:

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Current Data Parameters
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PROCNO                      1

F2 - Acquisition Parameters
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Time                   16.41
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                      362
DW                   81.000 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.70 usec
PL1                   -2.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300107 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

References

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