Supporting Information

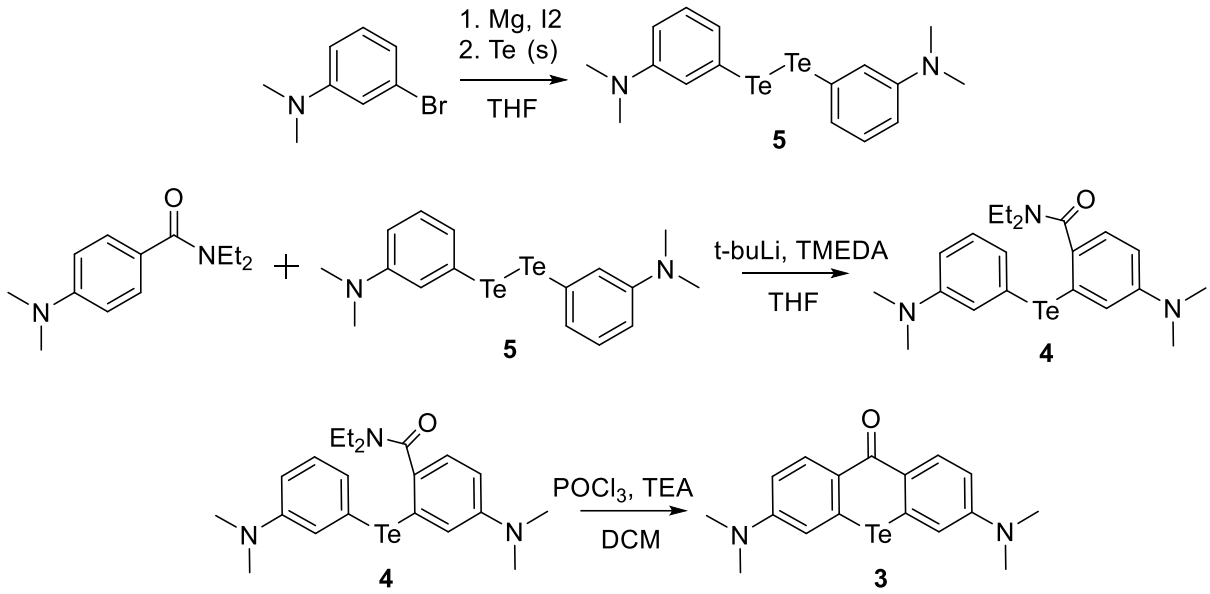
for

Synthesis, photophysical characterization, and aerobic redox reactivity of electron-rich tellurorhodamine photocatalysts

Irving D. Rettig, Kristine M. Halvorsen, Theresa M. McCormick*

Department of Chemistry, Portland State University, Portland, Oregon, 97201, USA
*t.m.mccormick@pdx.edu

Contents



Scheme S1. Synthesis of **3** from intermediates **4** and **5** as previously described in Ref[1].

Table S1. Crystal data and structure refinement for **1A**.

Identification code	**1A**	
Empirical formula	C27 H31.08 F6 N2.46 O0.27 P Te	
Formula weight	666.95	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	triclinic	
Space group	*P*-1	
Unit cell dimensions	*a* = 7.8985(2) Å	a = 115.0760(10)°
	b = 13.2724(2) Å	b = 94.431(2)°
	c = 14.3100(2) Å	g = 90.9680(10)°
Volume	1352.64(5) $Å^3$	
Z	2	
Density (calculated)	1.638 Mg/m^3	
Absorption coefficient	9.806 mm^{-1}	
F(000)	667	
Crystal color, morphology	dark green, plate	
Crystal size	0.092 x 0.082 x 0.016 mm^3	
Theta range for data collection	3.425 to 77.739°	
Index ranges	-9 £ *h* £ 10, -16 £ *k* £ 16, -18 £ *l* £ 18	
Reflections collected	45164	
Independent reflections	5689 [*R*(int) = 0.0758]	
Observed reflections	5384	
Completeness to theta = 74.504°	99.7%	
Absorption correction	Multi-scan	
Max. and min. transmission	1.00000 and 0.61756	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5689 / 321 / 398	
Goodness-of-fit on F^2	1.115	
Final *R* indices [*I*>2sigma(*I*)]	*R*1 = 0.0375, *wR*2 = 0.0984	
R indices (all data)	*R*1 = 0.0393, *wR*2 = 0.0999	
Largest diff. peak and hole	1.273 and -1.041 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1A**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Te1	7600(1)	4561(1)	4003(1)	22(1)
N1	5573(4)	2314(3)	-36(2)	30(1)
N2	7486(4)	5405(3)	7979(2)	26(1)
C1	4390(5)	1589(3)	2031(3)	26(1)
C2	4466(5)	1552(3)	1069(3)	28(1)
C3	5467(5)	2360(3)	918(3)	26(1)
C4	6341(4)	3218(3)	1814(3)	25(1)
C5	5339(4)	3006(3)	5805(3)	26(1)
C6	5880(4)	3721(3)	6795(3)	25(1)
C7	6947(4)	4688(3)	7011(3)	24(1)
C8	7402(4)	4862(3)	6148(3)	22(1)
C9	5100(4)	2379(3)	3914(3)	24(1)
C10	6236(4)	3247(3)	2784(3)	22(1)
C11	5265(4)	2425(3)	2947(3)	24(1)
C12	5756(4)	3167(3)	4914(3)	22(1)
C13	6818(4)	4144(3)	5147(2)	20(1)
C14	4203(4)	1341(3)	3861(3)	23(1)
C15	2474(5)	1303(3)	4008(3)	30(1)
C16	1734(5)	317(3)	3959(3)	34(1)
C17	2662(5)	-616(3)	3755(3)	32(1)
C18	4376(5)	-572(3)	3607(3)	28(1)
C19	5165(4)	405(3)	3671(3)	25(1)
C20	6709(5)	3107(3)	-194(3)	34(1)
C21	4503(6)	1519(4)	-928(3)	37(1)
C22	8712(5)	6321(3)	8183(3)	33(1)
C23	7003(5)	5255(4)	8878(3)	32(1)
C24	1411(5)	2305(3)	4233(4)	38(1)
C25	7035(5)	445(3)	3545(3)	31(1)
P1	1404(1)	3445(1)	8025(1)	30(1)
F1	1854(4)	4134(3)	7383(2)	61(1)
F2	993(4)	2840(3)	8735(3)	73(1)

F3	-482(3)	3185(2)	7479(2)	51(1)
F4	2022(5)	2353(3)	7158(3)	78(1)
F5	3316(3)	3713(2)	8579(2)	45(1)
F6	855(4)	4589(3)	8908(2)	56(1)
N3	-820(20)	955(13)	1323(12)	98(4)
C26	-150(30)	192(15)	1235(13)	71(3)
C27	860(30)	-774(15)	999(15)	70(4)
C28	-430(70)	330(30)	-1527(19)	87(8)
C29	-330(40)	718(19)	-375(18)	88(5)
O1	500(20)	-42(19)	-30(15)	87(4)
C30	-130(60)	240(30)	970(20)	76(4)
C31	570(70)	-620(30)	1310(30)	65(5)

Table S3. Bond lengths [Å] and angles [°] for **1A**.

Te(1)-C(10)	2.077(3)	C(16)-C(17)	1.383(6)
Te(1)-C(13)	2.069(3)	C(17)-H(17)	0.9500
N(1)-C(3)	1.351(5)	C(17)-C(18)	1.391(5)
N(1)-C(20)	1.471(5)	C(18)-H(18)	0.9500
N(1)-C(21)	1.455(5)	C(18)-C(19)	1.394(5)
N(2)-C(7)	1.336(5)	C(19)-C(25)	1.504(5)
N(2)-C(22)	1.456(5)	C(20)-H(20A)	0.9800
N(2)-C(23)	1.460(5)	C(20)-H(20B)	0.9800
C(1)-H(1)	0.9500	C(20)-H(20C)	0.9800
C(1)-C(2)	1.363(5)	C(21)-H(21A)	0.9800
C(1)-C(11)	1.424(5)	C(21)-H(21B)	0.9800
C(2)-H(2)	0.9500	C(21)-H(21C)	0.9800
C(2)-C(3)	1.419(5)	C(22)-H(22A)	0.9800
C(3)-C(4)	1.420(5)	C(22)-H(22B)	0.9800
C(4)-H(4)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(10)	1.382(5)	C(23)-H(23A)	0.9800
C(5)-H(5)	0.9500	C(23)-H(23B)	0.9800
C(5)-C(6)	1.358(5)	C(23)-H(23C)	0.9800
C(5)-C(12)	1.439(5)	C(24)-H(24A)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24B)	0.9800
C(6)-C(7)	1.428(5)	C(24)-H(24C)	0.9800
C(7)-C(8)	1.419(5)	C(25)-H(25A)	0.9800
C(8)-H(8)	0.9500	C(25)-H(25B)	0.9800
C(8)-C(13)	1.379(5)	C(25)-H(25C)	0.9800
C(9)-C(11)	1.427(5)	P(1)-F(1)	1.599(3)
C(9)-C(12)	1.417(5)	P(1)-F(2)	1.586(3)
C(9)-C(14)	1.509(5)	P(1)-F(3)	1.589(3)
C(10)-C(11)	1.430(5)	P(1)-F(4)	1.572(3)
C(12)-C(13)	1.433(4)	P(1)-F(5)	1.610(3)
C(14)-C(15)	1.401(5)	P(1)-F(6)	1.604(3)
C(14)-C(19)	1.404(5)	N(3)-C(26)	1.114(9)
C(15)-C(16)	1.396(5)	C(26)-C(27)	1.451(10)
C(15)-C(24)	1.515(5)	C(27)-H(27A)	0.9800
C(16)-H(16)	0.9500	C(27)-H(27B)	0.9800

C(27)-H(27C)	0.9800	C(12)-C(5)-H(5)	118.2
C(28)-H(28A)	0.9800	C(5)-C(6)-H(6)	119.6
C(28)-H(28B)	0.9800	C(5)-C(6)-C(7)	120.9(3)
C(28)-H(28C)	0.9800	C(7)-C(6)-H(6)	119.6
C(28)-C(29)	1.500(15)	N(2)-C(7)-C(6)	121.8(3)
C(29)-H(29A)	0.9900	N(2)-C(7)-C(8)	121.2(3)
C(29)-H(29B)	0.9900	C(8)-C(7)-C(6)	117.0(3)
C(29)-O(1)	1.444(15)	C(7)-C(8)-H(8)	119.1
O(1)-C(30)	1.454(15)	C(13)-C(8)-C(7)	121.7(3)
C(30)-H(30A)	0.9900	C(13)-C(8)-H(8)	119.1
C(30)-H(30B)	0.9900	C(11)-C(9)-C(14)	116.2(3)
C(30)-C(31)	1.518(15)	C(12)-C(9)-C(11)	127.7(3)
C(31)-H(31A)	0.9800	C(12)-C(9)-C(14)	116.1(3)
C(31)-H(31B)	0.9800	C(4)-C(10)-Te(1)	115.6(2)
C(31)-H(31C)	0.9800	C(4)-C(10)-C(11)	122.6(3)
C(13)-Te(1)-C(10)	95.29(13)	C(11)-C(10)-Te(1)	121.8(2)
C(3)-N(1)-C(20)	120.8(3)	C(1)-C(11)-C(9)	118.9(3)
C(3)-N(1)-C(21)	121.0(3)	C(1)-C(11)-C(10)	114.6(3)
C(21)-N(1)-C(20)	118.1(3)	C(9)-C(11)-C(10)	126.6(3)
C(7)-N(2)-C(22)	121.1(3)	C(9)-C(12)-C(5)	119.0(3)
C(7)-N(2)-C(23)	122.1(3)	C(9)-C(12)-C(13)	126.2(3)
C(22)-N(2)-C(23)	116.6(3)	C(13)-C(12)-C(5)	114.8(3)
C(2)-C(1)-H(1)	118.2	C(8)-C(13)-Te(1)	115.6(2)
C(2)-C(1)-C(11)	123.6(3)	C(8)-C(13)-C(12)	122.1(3)
C(11)-C(1)-H(1)	118.2	C(12)-C(13)-Te(1)	122.3(2)
C(1)-C(2)-H(2)	119.5	C(15)-C(14)-C(9)	121.8(3)
C(1)-C(2)-C(3)	121.0(3)	C(15)-C(14)-C(19)	120.5(3)
C(3)-C(2)-H(2)	119.5	C(19)-C(14)-C(9)	117.8(3)
N(1)-C(3)-C(2)	121.3(3)	C(14)-C(15)-C(24)	121.7(3)
N(1)-C(3)-C(4)	121.7(3)	C(16)-C(15)-C(14)	118.6(3)
C(2)-C(3)-C(4)	117.1(3)	C(16)-C(15)-C(24)	119.8(3)
C(3)-C(4)-H(4)	119.5	C(15)-C(16)-H(16)	119.3
C(10)-C(4)-C(3)	121.0(3)	C(17)-C(16)-C(15)	121.5(4)
C(10)-C(4)-H(4)	119.5	C(17)-C(16)-H(16)	119.3
C(6)-C(5)-H(5)	118.2	C(16)-C(17)-H(17)	120.2
C(6)-C(5)-C(12)	123.5(3)	C(16)-C(17)-C(18)	119.6(3)

C(18)-C(17)-H(17)	120.2	H(24B)-C(24)-H(24C)	109.5
C(17)-C(18)-H(18)	119.8	C(19)-C(25)-H(25A)	109.5
C(17)-C(18)-C(19)	120.5(3)	C(19)-C(25)-H(25B)	109.5
C(19)-C(18)-H(18)	119.8	C(19)-C(25)-H(25C)	109.5
C(14)-C(19)-C(25)	121.1(3)	H(25A)-C(25)-H(25B)	109.5
C(18)-C(19)-C(14)	119.4(3)	H(25A)-C(25)-H(25C)	109.5
C(18)-C(19)-C(25)	119.5(3)	H(25B)-C(25)-H(25C)	109.5
N(1)-C(20)-H(20A)	109.5	F(1)-P(1)-F(5)	89.45(16)
N(1)-C(20)-H(20B)	109.5	F(1)-P(1)-F(6)	87.61(18)
N(1)-C(20)-H(20C)	109.5	F(2)-P(1)-F(1)	175.9(2)
H(20A)-C(20)-H(20B)	109.5	F(2)-P(1)-F(3)	91.69(17)
H(20A)-C(20)-H(20C)	109.5	F(2)-P(1)-F(5)	88.45(15)
H(20B)-C(20)-H(20C)	109.5	F(2)-P(1)-F(6)	88.9(2)
N(1)-C(21)-H(21A)	109.5	F(3)-P(1)-F(1)	90.41(17)
N(1)-C(21)-H(21B)	109.5	F(3)-P(1)-F(5)	179.78(16)
N(1)-C(21)-H(21C)	109.5	F(3)-P(1)-F(6)	90.48(15)
H(21A)-C(21)-H(21B)	109.5	F(4)-P(1)-F(1)	90.6(2)
H(21A)-C(21)-H(21C)	109.5	F(4)-P(1)-F(2)	92.9(2)
H(21B)-C(21)-H(21C)	109.5	F(4)-P(1)-F(3)	91.53(17)
N(2)-C(22)-H(22A)	109.5	F(4)-P(1)-F(5)	88.64(17)
N(2)-C(22)-H(22B)	109.5	F(4)-P(1)-F(6)	177.3(2)
N(2)-C(22)-H(22C)	109.5	F(6)-P(1)-F(5)	89.35(15)
H(22A)-C(22)-H(22B)	109.5	N(3)-C(26)-C(27)	171(2)
H(22A)-C(22)-H(22C)	109.5	C(26)-C(27)-H(27A)	109.5
H(22B)-C(22)-H(22C)	109.5	C(26)-C(27)-H(27B)	109.5
N(2)-C(23)-H(23A)	109.5	C(26)-C(27)-H(27C)	109.5
N(2)-C(23)-H(23B)	109.5	H(27A)-C(27)-H(27B)	109.5
N(2)-C(23)-H(23C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(23A)-C(23)-H(23B)	109.5	H(27B)-C(27)-H(27C)	109.5
H(23A)-C(23)-H(23C)	109.5	H(28A)-C(28)-H(28B)	109.5
H(23B)-C(23)-H(23C)	109.5	H(28A)-C(28)-H(28C)	109.5
C(15)-C(24)-H(24A)	109.5	H(28B)-C(28)-H(28C)	109.5
C(15)-C(24)-H(24B)	109.5	C(29)-C(28)-H(28A)	109.5
C(15)-C(24)-H(24C)	109.5	C(29)-C(28)-H(28B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(29)-C(28)-H(28C)	109.5
H(24A)-C(24)-H(24C)	109.5	C(28)-C(29)-H(29A)	108.9

C(28)-C(29)-H(29B)	108.9	H(30A)-C(30)-H(30B)	109.0
H(29A)-C(29)-H(29B)	107.7	C(31)-C(30)-H(30A)	110.9
O(1)-C(29)-C(28)	113(2)	C(31)-C(30)-H(30B)	110.9
O(1)-C(29)-H(29A)	108.9	C(30)-C(31)-H(31A)	109.5
O(1)-C(29)-H(29B)	108.9	C(30)-C(31)-H(31B)	109.5
C(29)-O(1)-C(30)	102.8(19)	C(30)-C(31)-H(31C)	109.5
O(1)-C(30)-H(30A)	110.9	H(31A)-C(31)-H(31B)	109.5
O(1)-C(30)-H(30B)	110.9	H(31A)-C(31)-H(31C)	109.5
O(1)-C(30)-C(31)	104.1(19)	H(31B)-C(31)-H(31C)	109.5

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1A**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te1	25(1)	22(1)	20(1)	8(1)	2(1)	-4(1)
N1	37(2)	30(2)	22(1)	10(1)	-1(1)	-4(1)
N2	25(1)	32(2)	20(1)	10(1)	2(1)	1(1)
C1	27(2)	24(2)	27(2)	11(1)	-2(1)	-4(1)
C2	30(2)	24(2)	26(2)	9(1)	-4(1)	-1(1)
C3	29(2)	26(2)	24(2)	11(1)	2(1)	4(1)
C4	26(2)	22(2)	22(2)	7(1)	0(1)	-4(1)
C5	26(2)	26(2)	28(2)	14(1)	3(1)	-1(1)
C6	23(2)	30(2)	26(2)	15(1)	4(1)	1(1)
C7	22(2)	26(2)	25(2)	11(1)	1(1)	3(1)
C8	20(2)	24(2)	23(2)	10(1)	1(1)	-1(1)
C9	22(2)	23(2)	25(2)	10(1)	1(1)	2(1)
C10	21(2)	23(2)	20(2)	6(1)	-1(1)	-1(1)
C11	23(2)	21(2)	24(2)	7(1)	-1(1)	-2(1)
C12	20(1)	23(2)	24(2)	11(1)	3(1)	-1(1)
C13	20(1)	23(2)	18(1)	10(1)	6(1)	3(1)
C14	26(2)	21(2)	22(2)	9(1)	0(1)	-2(1)
C15	28(2)	27(2)	35(2)	13(2)	2(1)	-1(1)
C16	26(2)	32(2)	46(2)	17(2)	4(2)	-4(1)
C17	35(2)	24(2)	38(2)	16(2)	0(2)	-6(1)
C18	35(2)	21(2)	27(2)	12(1)	-1(1)	-1(1)
C19	27(2)	25(2)	22(2)	10(1)	0(1)	-1(1)
C20	43(2)	37(2)	25(2)	15(2)	4(2)	-4(2)
C21	48(2)	36(2)	23(2)	9(2)	-3(2)	-5(2)
C22	36(2)	33(2)	23(2)	7(2)	-2(1)	-6(2)
C23	34(2)	41(2)	24(2)	15(2)	4(1)	3(2)
C24	28(2)	25(2)	59(3)	15(2)	6(2)	0(2)
C25	28(2)	29(2)	37(2)	14(2)	4(2)	3(1)
P1	29(1)	30(1)	32(1)	15(1)	1(1)	1(1)
F1	70(2)	74(2)	60(2)	48(2)	8(2)	7(2)
F2	48(2)	103(3)	107(3)	84(2)	-2(2)	-13(2)

F3	38(1)	36(1)	65(2)	12(1)	-18(1)	0(1)
F4	73(2)	48(2)	71(2)	-11(2)	-10(2)	28(2)
F5	27(1)	68(2)	46(1)	30(1)	3(1)	0(1)
F6	44(2)	56(2)	45(2)	1(1)	0(1)	8(1)
N3	114(10)	101(8)	78(8)	38(7)	2(7)	5(7)
C26	82(7)	78(6)	50(7)	26(6)	6(6)	-23(5)
C27	72(9)	67(7)	53(9)	9(7)	9(7)	-26(5)
C28	116(18)	73(17)	65(11)	28(11)	-3(13)	-41(15)
C29	124(11)	74(9)	62(9)	29(7)	-3(9)	-35(9)
O1	115(8)	80(6)	58(6)	24(5)	2(7)	-37(7)
C30	90(7)	76(7)	56(7)	25(6)	2(7)	-25(6)
C31	67(11)	63(10)	54(11)	15(9)	3(10)	-18(9)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **1A**.

	x	y	z	U(eq)
H1	3715	1025	2094	31
H2	3840	976	490	33
H4	7007	3781	1745	30
H5	4649	2365	5694	31
H6	5544	3577	7352	30
H8	8129	5490	6264	27
H16	567	286	4068	41
H17	2131	-1282	3716	38
H18	5015	-1213	3463	33
H20A	7846	3128	142	52
H20B	6261	3851	108	52
H20C	6777	2870	-938	52
H21A	4783	760	-1049	56
H21B	4702	1641	-1541	56
H21C	3305	1622	-795	56
H22A	8196	6846	7942	49
H22B	9717	6029	7814	49
H22C	9049	6705	8929	49
H23A	5809	4983	8759	49
H23B	7153	5969	9493	49
H23C	7723	4713	8987	49
H24A	1901	2782	3944	57
H24B	1399	2727	4984	57
H24C	246	2055	3917	57
H25A	7478	-290	3388	47
H25B	7635	998	4189	47
H25C	7210	651	2977	47
H27A	1680	-789	515	105
H27B	110	-1453	683	105
H27C	1464	-733	1639	105

H28A	-1566	453	-1776	130
H28B	-226	-466	-1860	130
H28C	426	750	-1700	130
H29A	303	1453	-37	106
H29B	-1491	815	-151	106
H30A	-1392	202	912	91
H30B	284	1005	1474	91
H31A	-223	-1281	1036	98
H31B	707	-311	2065	98
H31C	1673	-836	1035	98

Table S6. Torsion angles [°] for **1A**.

Te1-C10-C11-C1	179.3(2)	C12-C9-C11-C1	-174.9(3)
Te1-C10-C11-C9	-0.4(5)	C12-C9-C11-C10	4.7(6)
N1-C3-C4-C10	-179.3(3)	C12-C9-C14-C15	86.0(4)
N2-C7-C8-C13	-178.3(3)	C12-C9-C14-C19	-93.2(4)
C1-C2-C3-N1	178.7(3)	C14-C9-C11-C1	8.6(5)
C1-C2-C3-C4	-1.6(5)	C14-C9-C11-C10	-171.7(3)
C2-C1-C11-C9	-179.7(3)	C14-C9-C12-C5	-8.2(5)
C2-C1-C11-C10	0.6(5)	C14-C9-C12-C13	172.3(3)
C2-C3-C4-C10	1.1(5)	C14-C15-C16-C17	-1.0(6)
C3-C4-C10-Te1	179.9(3)	C15-C14-C19-C18	1.3(5)
C3-C4-C10-C11	0.3(5)	C15-C14-C19-C25	-178.0(3)
C4-C10-C11-C1	-1.2(5)	C15-C16-C17-C18	0.8(6)
C4-C10-C11-C9	179.1(3)	C16-C17-C18-C19	0.4(6)
C5-C6-C7-N2	179.7(3)	C17-C18-C19-C14	-1.5(5)
C5-C6-C7-C8	0.2(5)	C17-C18-C19-C25	177.9(3)
C5-C12-C13-Te1	179.9(2)	C19-C14-C15-C16	-0.1(6)
C5-C12-C13-C8	0.7(5)	C19-C14-C15-C24	178.9(4)
C6-C5-C12-C9	-178.9(3)	C20-N1-C3-C2	-175.6(4)
C6-C5-C12-C13	0.7(5)	C20-N1-C3-C4	4.8(6)
C6-C7-C8-C13	1.2(5)	C21-N1-C3-C2	7.7(6)
C7-C8-C13-Te1	179.1(3)	C21-N1-C3-C4	-171.9(4)
C7-C8-C13-C12	-1.7(5)	C22-N2-C7-C6	173.6(3)
C9-C12-C13-Te1	-0.5(5)	C22-N2-C7-C8	-7.0(5)
C9-C12-C13-C8	-179.7(3)	C23-N2-C7-C6	-0.8(5)
C9-C14-C15-C16	-179.3(3)	C23-N2-C7-C8	178.6(3)
C9-C14-C15-C24	-0.3(6)	C24-C15-C16-C17	180.0(4)
C9-C14-C19-C18	-179.4(3)	C28-C29-O1-C30	-158(4)
C9-C14-C19-C25	1.2(5)	C29-O1-C30-C31	174(3)
C11-C1-C2-C3	0.8(6)		
C11-C9-C12-C5	175.4(3)		
C11-C9-C12-C13	-4.2(6)		
C11-C9-C14-C15	-97.1(4)		
C11-C9-C14-C19	83.6(4)		
C12-C5-C6-C7	-1.2(6)		

Table S7. Crystal data and structure refinement for **1B**.

Identification code	**1B**	
Empirical formula	C26 H29 F6 N2 P Te	
Formula weight	642.08	
Temperature	99.99(10) K	
Wavelength	1.54184 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.08690(10) Å	a = 90°
	b = 20.1974(2) Å	b = 100.5010(10)°
	c = 15.9300(2) Å	g = 90°
Volume	2558.34(5) Å^3	
Z	4	
Density (calculated)	1.667 Mg/m^3	
Absorption coefficient	10.330 mm^{-1}	
F(000)	1280	
Crystal color, morphology	dark green, block	
Crystal size	0.183 x 0.133 x 0.125 mm^3	
Theta range for data collection	3.571 to 77.854°	
Index ranges	-7 £ h £ 10, -25 £ k £ 25, -19 £ l £ 20	
Reflections collected	43625	
Independent reflections	5404 [R(int) = 0.0572]	
Observed reflections	5219	
Completeness to theta = 74.504°	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	1.00000 and 0.42674	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5404 / 0 / 333	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0974	
R indices (all data)	R1 = 0.0366, wR2 = 0.0983	
Largest diff. peak and hole	1.891 and -1.345 e.Å^{-3}	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1B**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Te1	8067(1)	4423(1)	5129(1)	18(1)
N1	6691(3)	6984(1)	4593(2)	20(1)
N2	6934(3)	1847(1)	4491(2)	23(1)
C1	7096(3)	5808(1)	4723(2)	16(1)
C2	6345(3)	6370(1)	4286(2)	16(1)
C3	5196(3)	6257(1)	3506(2)	20(1)
C4	4887(4)	5635(1)	3198(2)	18(1)
C5	5010(3)	3215(1)	3160(2)	19(1)
C6	5382(4)	2590(1)	3444(2)	22(1)
C7	6523(3)	2474(1)	4219(2)	20(1)
C8	7199(3)	3032(1)	4689(2)	19(1)
C9	5240(3)	4428(1)	3247(2)	16(1)
C10	6755(3)	5176(1)	4415(2)	16(1)
C11	5633(3)	5052(1)	3622(2)	15(1)
C12	5702(3)	3796(1)	3606(2)	16(1)
C13	6811(3)	3668(1)	4395(2)	16(1)
C14	4301(4)	4424(1)	2340(2)	16(1)
C15	2547(4)	4413(1)	2132(2)	18(1)
C16	1776(4)	4385(1)	1270(2)	20(1)
C17	2702(4)	4362(1)	618(2)	21(1)
C18	4454(4)	4384(1)	844(2)	22(1)
C19	5266(4)	4413(1)	1687(2)	21(1)
C20	7936(4)	7089(2)	5364(2)	24(1)
C21	6062(4)	7574(2)	4111(2)	28(1)
C22	8246(4)	1742(2)	5233(2)	32(1)
C23	6467(4)	1288(2)	3914(2)	29(1)
C24	1485(4)	4427(2)	2816(2)	26(1)
C25	1854(5)	4299(2)	-302(2)	31(1)
C26	7159(4)	4425(2)	1911(2)	33(1)
P1	9942(1)	8066(1)	7632(1)	28(1)
F1	9176(3)	7343(1)	7652(2)	53(1)

F2	10720(3)	8790(1)	7615(2)	49(1)
F3	11780(2)	7786(1)	8017(2)	44(1)
F4	9624(3)	8195(1)	8584(1)	46(1)
F5	8113(3)	8345(2)	7252(2)	53(1)
F6	10279(3)	7944(1)	6687(1)	45(1)

Table S9. Bond lengths [Å] and angles [°] for **1B**.

Te(1)-C(10)	2.072(3)	C(16)-C(17)	1.388(4)
Te(1)-C(13)	2.071(3)	C(17)-C(18)	1.398(5)
N(1)-C(2)	1.343(4)	C(17)-C(25)	1.505(4)
N(1)-C(20)	1.455(4)	C(18)-H(18)	0.9500
N(1)-C(21)	1.458(4)	C(18)-C(19)	1.384(5)
N(2)-C(7)	1.361(4)	C(19)-C(26)	1.508(4)
N(2)-C(22)	1.453(4)	C(20)-H(20A)	0.9800
N(2)-C(23)	1.461(4)	C(20)-H(20B)	0.9800
C(1)-H(1)	0.9500	C(20)-H(20C)	0.9800
C(1)-C(2)	1.411(4)	C(21)-H(21A)	0.9800
C(1)-C(10)	1.377(4)	C(21)-H(21B)	0.9800
C(2)-C(3)	1.428(4)	C(21)-H(21C)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22A)	0.9800
C(3)-C(4)	1.355(4)	C(22)-H(22B)	0.9800
C(4)-H(4)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(11)	1.435(4)	C(23)-H(23A)	0.9800
C(5)-H(5)	0.9500	C(23)-H(23B)	0.9800
C(5)-C(6)	1.357(4)	C(23)-H(23C)	0.9800
C(5)-C(12)	1.431(4)	C(24)-H(24A)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24B)	0.9800
C(6)-C(7)	1.420(4)	C(24)-H(24C)	0.9800
C(7)-C(8)	1.406(4)	C(24)-H(24D)	0.9800
C(8)-H(8)	0.9500	C(24)-H(24E)	0.9800
C(8)-C(13)	1.385(4)	C(24)-H(24F)	0.9800
C(9)-C(11)	1.405(4)	C(25)-H(25A)	0.9800
C(9)-C(12)	1.421(4)	C(25)-H(25B)	0.9800
C(9)-C(14)	1.505(4)	C(25)-H(25C)	0.9800
C(10)-C(11)	1.436(4)	C(26)-H(26A)	0.9800
C(12)-C(13)	1.429(4)	C(26)-H(26B)	0.9800
C(14)-C(15)	1.397(4)	C(26)-H(26C)	0.9800
C(14)-C(19)	1.410(4)	P(1)-F(1)	1.589(2)
C(15)-C(16)	1.401(4)	P(1)-F(2)	1.593(2)
C(15)-C(24)	1.505(4)	P(1)-F(3)	1.604(2)
C(16)-H(16)	0.9500	P(1)-F(4)	1.606(2)

P(1)-F(5)	1.596(2)	C(1)-C(10)-Te(1)	115.8(2)
P(1)-F(6)	1.597(2)	C(1)-C(10)-C(11)	121.9(2)
C(13)-Te(1)-C(10)	94.63(12)	C(11)-C(10)-Te(1)	122.2(2)
C(2)-N(1)-C(20)	120.5(2)	C(4)-C(11)-C(10)	114.5(2)
C(2)-N(1)-C(21)	122.2(3)	C(9)-C(11)-C(4)	119.5(2)
C(20)-N(1)-C(21)	116.5(2)	C(9)-C(11)-C(10)	126.0(2)
C(7)-N(2)-C(22)	119.7(3)	C(9)-C(12)-C(5)	119.2(2)
C(7)-N(2)-C(23)	120.0(3)	C(9)-C(12)-C(13)	126.4(2)
C(22)-N(2)-C(23)	117.7(3)	C(13)-C(12)-C(5)	114.4(2)
C(2)-C(1)-H(1)	119.0	C(8)-C(13)-Te(1)	115.8(2)
C(10)-C(1)-H(1)	119.0	C(8)-C(13)-C(12)	122.2(2)
C(10)-C(1)-C(2)	122.1(2)	C(12)-C(13)-Te(1)	121.9(2)
N(1)-C(2)-C(1)	121.4(3)	C(15)-C(14)-C(9)	122.7(3)
N(1)-C(2)-C(3)	121.6(3)	C(15)-C(14)-C(19)	120.0(3)
C(1)-C(2)-C(3)	117.0(2)	C(19)-C(14)-C(9)	117.3(3)
C(2)-C(3)-H(3)	119.6	C(14)-C(15)-C(16)	118.9(3)
C(4)-C(3)-C(2)	120.7(3)	C(14)-C(15)-C(24)	121.1(3)
C(4)-C(3)-H(3)	119.6	C(16)-C(15)-C(24)	120.0(3)
C(3)-C(4)-H(4)	118.1	C(15)-C(16)-H(16)	119.0
C(3)-C(4)-C(11)	123.8(3)	C(17)-C(16)-C(15)	122.1(3)
C(11)-C(4)-H(4)	118.1	C(17)-C(16)-H(16)	119.0
C(6)-C(5)-H(5)	118.1	C(16)-C(17)-C(18)	117.7(3)
C(6)-C(5)-C(12)	123.8(3)	C(16)-C(17)-C(25)	121.3(3)
C(12)-C(5)-H(5)	118.1	C(18)-C(17)-C(25)	121.0(3)
C(5)-C(6)-H(6)	119.6	C(17)-C(18)-H(18)	119.0
C(5)-C(6)-C(7)	120.8(3)	C(19)-C(18)-C(17)	122.1(3)
C(7)-C(6)-H(6)	119.6	C(19)-C(18)-H(18)	119.0
N(2)-C(7)-C(6)	120.8(3)	C(14)-C(19)-C(26)	120.0(3)
N(2)-C(7)-C(8)	121.8(3)	C(18)-C(19)-C(14)	119.2(3)
C(8)-C(7)-C(6)	117.4(3)	C(18)-C(19)-C(26)	120.8(3)
C(7)-C(8)-H(8)	119.3	N(1)-C(20)-H(20A)	109.5
C(13)-C(8)-C(7)	121.4(3)	N(1)-C(20)-H(20B)	109.5
C(13)-C(8)-H(8)	119.3	N(1)-C(20)-H(20C)	109.5
C(11)-C(9)-C(12)	127.8(3)	H(20A)-C(20)-H(20B)	109.5
C(11)-C(9)-C(14)	116.7(2)	H(20A)-C(20)-H(20C)	109.5
C(12)-C(9)-C(14)	115.5(2)	H(20B)-C(20)-H(20C)	109.5

N(1)-C(21)-H(21A)	109.5	H(24C)-C(24)-H(24D)	56.3
N(1)-C(21)-H(21B)	109.5	H(24C)-C(24)-H(24E)	56.3
N(1)-C(21)-H(21C)	109.5	H(24C)-C(24)-H(24F)	141.1
H(21A)-C(21)-H(21B)	109.5	H(24D)-C(24)-H(24E)	109.5
H(21A)-C(21)-H(21C)	109.5	H(24D)-C(24)-H(24F)	109.5
H(21B)-C(21)-H(21C)	109.5	H(24E)-C(24)-H(24F)	109.5
N(2)-C(22)-H(22A)	109.5	C(17)-C(25)-H(25A)	109.5
N(2)-C(22)-H(22B)	109.5	C(17)-C(25)-H(25B)	109.5
N(2)-C(22)-H(22C)	109.5	C(17)-C(25)-H(25C)	109.5
H(22A)-C(22)-H(22B)	109.5	H(25A)-C(25)-H(25B)	109.5
H(22A)-C(22)-H(22C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(22B)-C(22)-H(22C)	109.5	H(25B)-C(25)-H(25C)	109.5
N(2)-C(23)-H(23A)	109.5	C(19)-C(26)-H(26A)	109.5
N(2)-C(23)-H(23B)	109.5	C(19)-C(26)-H(26B)	109.5
N(2)-C(23)-H(23C)	109.5	C(19)-C(26)-H(26C)	109.5
H(23A)-C(23)-H(23B)	109.5	H(26A)-C(26)-H(26B)	109.5
H(23A)-C(23)-H(23C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(23B)-C(23)-H(23C)	109.5	H(26B)-C(26)-H(26C)	109.5
C(15)-C(24)-H(24A)	109.5	F(1)-P(1)-F(2)	179.70(17)
C(15)-C(24)-H(24B)	109.5	F(1)-P(1)-F(3)	90.31(14)
C(15)-C(24)-H(24C)	109.5	F(1)-P(1)-F(4)	90.01(14)
C(15)-C(24)-H(24D)	109.5	F(1)-P(1)-F(5)	89.67(15)
C(15)-C(24)-H(24E)	109.5	F(1)-P(1)-F(6)	90.63(14)
C(15)-C(24)-H(24F)	109.5	F(2)-P(1)-F(3)	89.40(14)
H(24A)-C(24)-H(24B)	109.5	F(2)-P(1)-F(4)	89.91(13)
H(24A)-C(24)-H(24C)	109.5	F(2)-P(1)-F(5)	90.62(15)
H(24A)-C(24)-H(24D)	141.1	F(2)-P(1)-F(6)	89.44(13)
H(24A)-C(24)-H(24E)	56.3	F(3)-P(1)-F(4)	89.59(12)
H(24A)-C(24)-H(24F)	56.3	F(5)-P(1)-F(3)	179.80(15)
H(24B)-C(24)-H(24C)	109.5	F(5)-P(1)-F(4)	90.21(13)
H(24B)-C(24)-H(24D)	56.3	F(5)-P(1)-F(6)	90.14(13)
H(24B)-C(24)-H(24E)	141.1	F(6)-P(1)-F(3)	90.06(13)
H(24B)-C(24)-H(24F)	56.3	F(6)-P(1)-F(4)	179.27(13)

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1B**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te1	17(1)	16(1)	19(1)	0(1)	-4(1)	1(1)
N1	20(1)	16(1)	25(1)	-3(1)	4(1)	-2(1)
N2	25(1)	18(1)	25(1)	2(1)	3(1)	1(1)
C1	12(1)	19(1)	17(1)	-2(1)	1(1)	1(1)
C2	12(1)	17(1)	19(1)	-2(1)	3(1)	-2(1)
C3	18(1)	18(1)	23(1)	2(1)	0(1)	0(1)
C4	16(1)	17(1)	20(1)	2(1)	-3(1)	1(1)
C5	19(1)	17(1)	19(1)	-3(1)	-2(1)	-1(1)
C6	22(1)	18(1)	26(2)	-2(1)	2(1)	-1(1)
C7	18(1)	19(1)	23(1)	3(1)	6(1)	2(1)
C8	16(1)	22(1)	18(1)	3(1)	0(1)	1(1)
C9	11(1)	18(1)	19(1)	0(1)	4(1)	0(1)
C10	14(1)	16(1)	18(1)	4(1)	2(1)	3(1)
C11	11(1)	17(1)	16(1)	2(1)	1(1)	1(1)
C12	12(1)	19(1)	16(1)	-2(1)	0(1)	-1(1)
C13	13(1)	19(1)	16(1)	-4(1)	2(1)	-2(1)
C14	16(1)	15(1)	15(1)	-2(1)	0(1)	0(1)
C15	16(1)	18(1)	18(1)	1(1)	-2(1)	-1(1)
C16	16(1)	19(1)	24(2)	-1(1)	-3(1)	0(1)
C17	27(2)	16(1)	17(1)	1(1)	-2(1)	1(1)
C18	27(2)	22(2)	19(2)	1(1)	6(1)	1(1)
C19	18(1)	23(2)	22(2)	1(1)	3(1)	-1(1)
C20	21(1)	22(1)	27(2)	-5(1)	0(1)	-4(1)
C21	29(2)	16(1)	38(2)	1(1)	2(1)	0(1)
C22	35(2)	19(2)	36(2)	8(1)	-5(1)	4(1)
C23	34(2)	17(1)	34(2)	1(1)	6(1)	2(1)
C24	14(1)	38(2)	26(2)	-4(1)	0(1)	-1(1)
C25	37(2)	33(2)	18(2)	1(1)	-4(1)	1(1)
C26	19(2)	52(2)	29(2)	-1(1)	6(1)	-2(1)
P1	18(1)	41(1)	24(1)	-6(1)	2(1)	-10(1)
F1	50(1)	49(1)	61(2)	-4(1)	12(1)	-26(1)

F2	51(1)	43(1)	52(1)	-7(1)	12(1)	-18(1)
F3	23(1)	68(2)	40(1)	1(1)	2(1)	1(1)
F4	35(1)	76(2)	28(1)	-7(1)	10(1)	-6(1)
F5	25(1)	82(2)	50(1)	3(1)	-1(1)	2(1)
F6	40(1)	70(2)	25(1)	-13(1)	7(1)	-14(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **1B**.

	x	y	z	U(eq)
H1	7862	5866	5245	20
H3	4642	6622	3199	24
H4	4132	5582	2671	22
H5	4246	3271	2637	23
H6	4874	2225	3119	27
H8	7936	2970	5220	23
H16	583	4381	1128	24
H18	5109	4379	406	27
H20A	7653	6817	5827	36
H20B	7943	7557	5526	36
H20C	9051	6964	5258	36
H21A	6753	7664	3678	42
H21B	6117	7952	4500	42
H21C	4893	7501	3830	42
H22A	9307	1927	5124	47
H22B	8382	1266	5346	47
H22C	7934	1962	5730	47
H23A	5249	1293	3707	43
H23B	6785	873	4221	43
H23C	7052	1323	3429	43
H24A	1742	4039	3186	32
H24B	293	4421	2550	32
H24C	1729	4831	3157	32
H24D	767	4821	2743	32
H24E	2217	4440	3378	32
H24F	780	4029	2772	32
H25A	1537	3836	-426	46
H25B	2628	4442	-673	46
H25C	844	4577	-405	46
H26A	7522	4810	2272	50
H26B	7628	4453	1387	50

H26C	7559	4019	2220	50

Table S12. Torsion angles [°] for **1B**.

Te1-C10-C11-C4	-177.57(19)	C12-C9-C11-C4	-172.7(3)
Te1-C10-C11-C9	2.1(4)	C12-C9-C11-C10	7.6(5)
N1-C2-C3-C4	178.8(3)	C12-C9-C14-C15	92.2(3)
N2-C7-C8-C13	178.1(3)	C12-C9-C14-C19	-86.1(3)
C1-C2-C3-C4	-1.5(4)	C14-C9-C11-C4	11.0(4)
C1-C10-C11-C4	-1.3(4)	C14-C9-C11-C10	-168.6(2)
C1-C10-C11-C9	178.4(3)	C14-C9-C12-C5	-11.0(4)
C2-C1-C10-Te1	177.6(2)	C14-C9-C12-C13	169.6(2)
C2-C1-C10-C11	1.0(4)	C14-C15-C16-C17	0.6(4)
C2-C3-C4-C11	1.3(5)	C15-C14-C19-C18	-0.7(4)
C3-C4-C11-C9	-179.6(3)	C15-C14-C19-C26	-180.0(3)
C3-C4-C11-C10	0.1(4)	C15-C16-C17-C18	-1.5(4)
C5-C6-C7-N2	-178.1(3)	C15-C16-C17-C25	177.0(3)
C5-C6-C7-C8	2.0(4)	C16-C17-C18-C19	1.4(4)
C5-C12-C13-Te1	176.86(18)	C17-C18-C19-C14	-0.3(4)
C5-C12-C13-C8	1.2(4)	C17-C18-C19-C26	179.0(3)
C6-C5-C12-C9	179.3(3)	C19-C14-C15-C16	0.6(4)
C6-C5-C12-C13	-1.2(4)	C19-C14-C15-C24	-179.7(2)
C6-C7-C8-C13	-2.1(4)	C20-N1-C2-C1	3.7(4)
C7-C8-C13-Te1	-175.5(2)	C20-N1-C2-C3	-176.6(3)
C7-C8-C13-C12	0.4(4)	C21-N1-C2-C1	173.7(3)
C9-C12-C13-Te1	-3.7(4)	C21-N1-C2-C3	-6.6(4)
C9-C12-C13-C8	-179.4(3)	C22-N2-C7-C6	173.0(3)
C9-C14-C15-C16	-177.7(2)	C22-N2-C7-C8	-7.2(4)
C9-C14-C15-C24	2.0(4)	C23-N2-C7-C6	11.8(4)
C9-C14-C19-C18	177.7(2)	C23-N2-C7-C8	-168.3(3)
C9-C14-C19-C26	-1.6(4)	C24-C15-C16-C17	-179.1(3)
C10-C1-C2-N1	-179.9(2)	C25-C17-C18-C19	-177.1(3)
C10-C1-C2-C3	0.4(4)		
C11-C9-C12-C5	172.7(3)		
C11-C9-C12-C13	-6.7(5)		
C11-C9-C14-C15	-91.0(3)		
C11-C9-C14-C19	90.6(3)		
C12-C5-C6-C7	-0.4(4)		

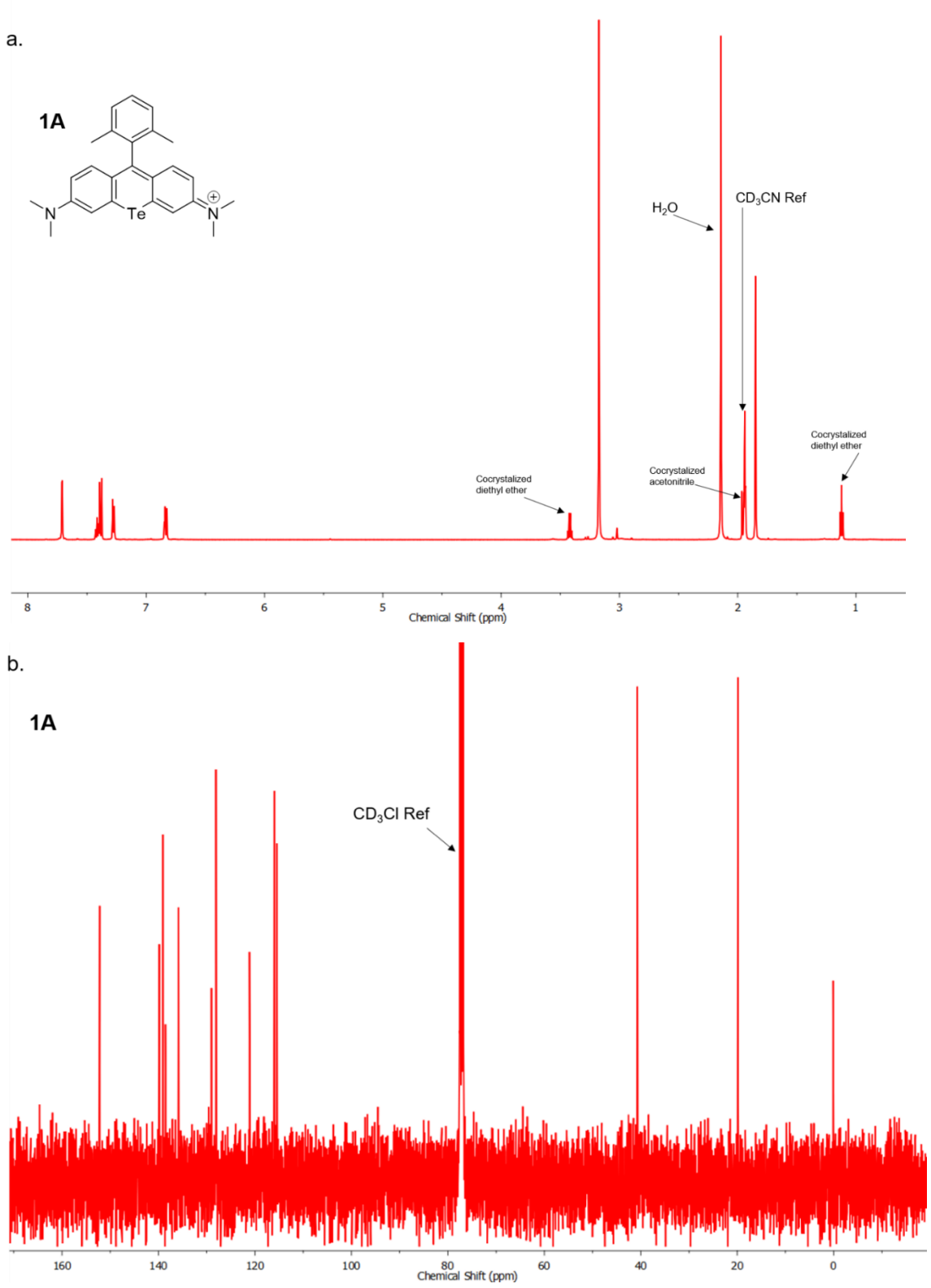


Figure S1. a.) ^{1}H NMR of **1A** in CD_3CN and b.) ^{13}C NMR of **1A** in $CDCl_3$. Residual solvent labeled according to Ref[2].

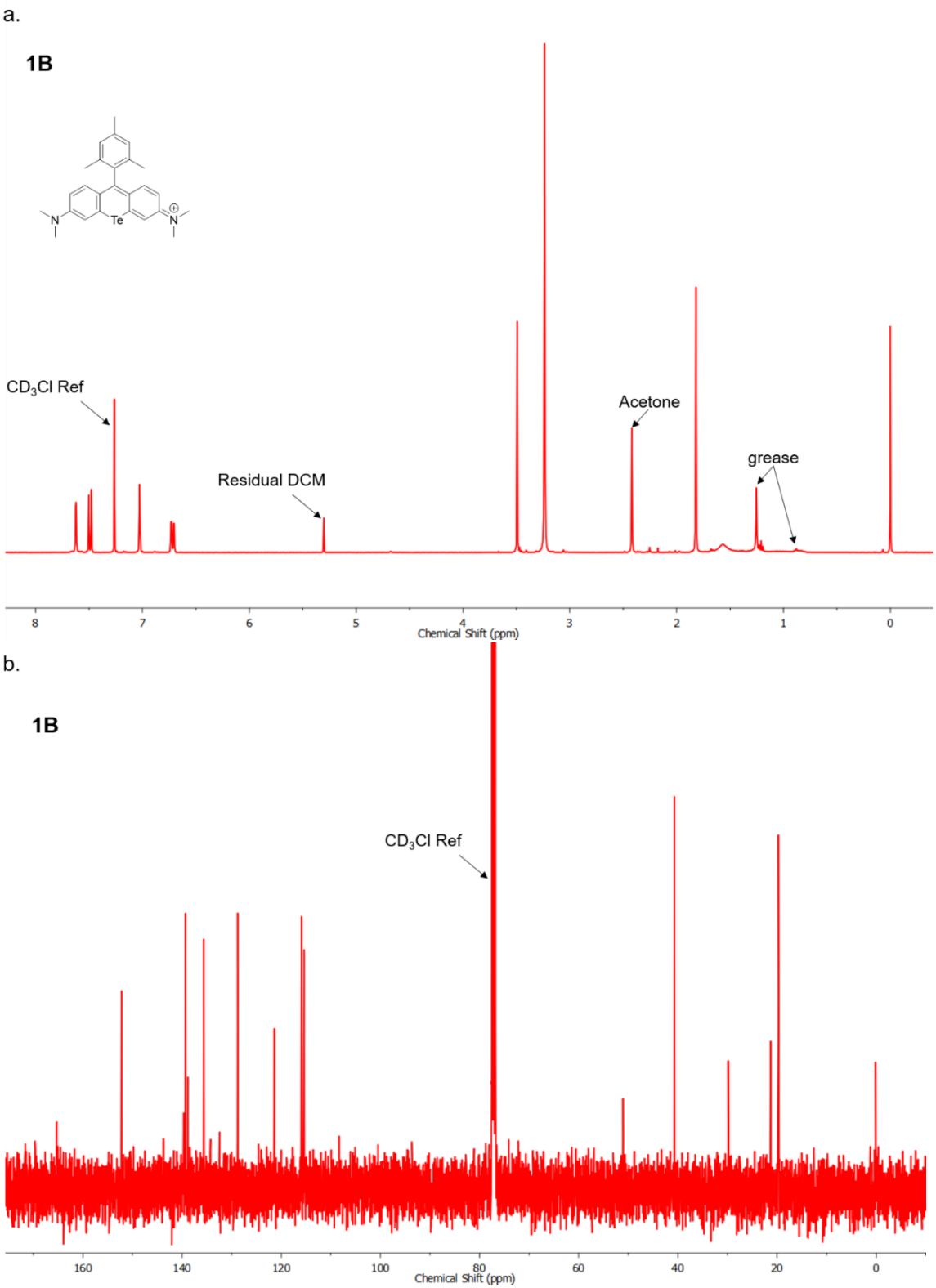


Figure S2. a.) ^{1}H NMR of **1B** in $CDCl_3$ and b.) ^{13}C NMR of **1B** in $CDCl_3$. Residual solvent labeled according to Ref[2].

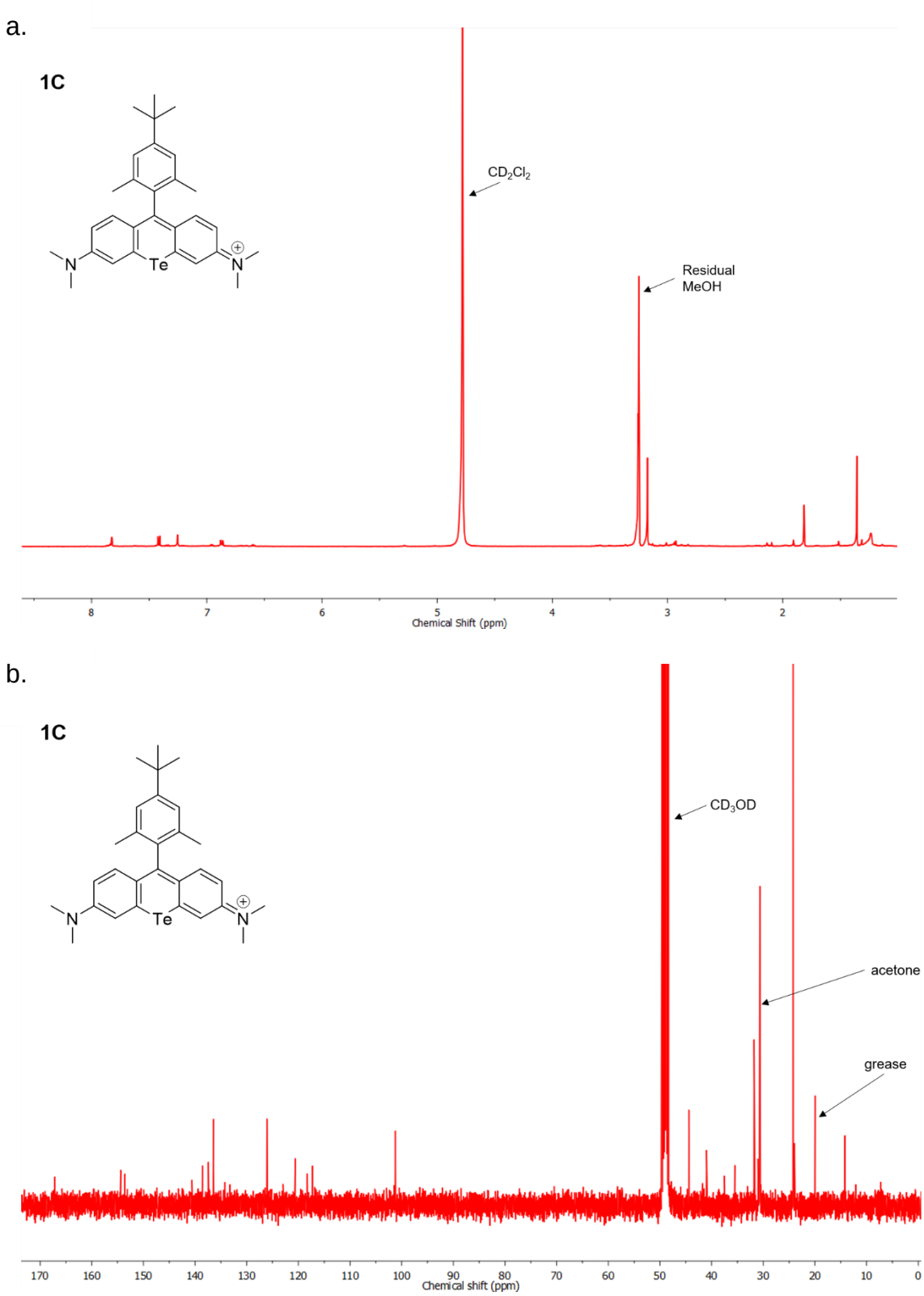


Figure S3. a.) ^{1}H NMR of **1C** in CD_2Cl_2 and b.) ^{13}C NMR of **1C** in CD_3OD. Residual solvent labeled according to Ref[2].

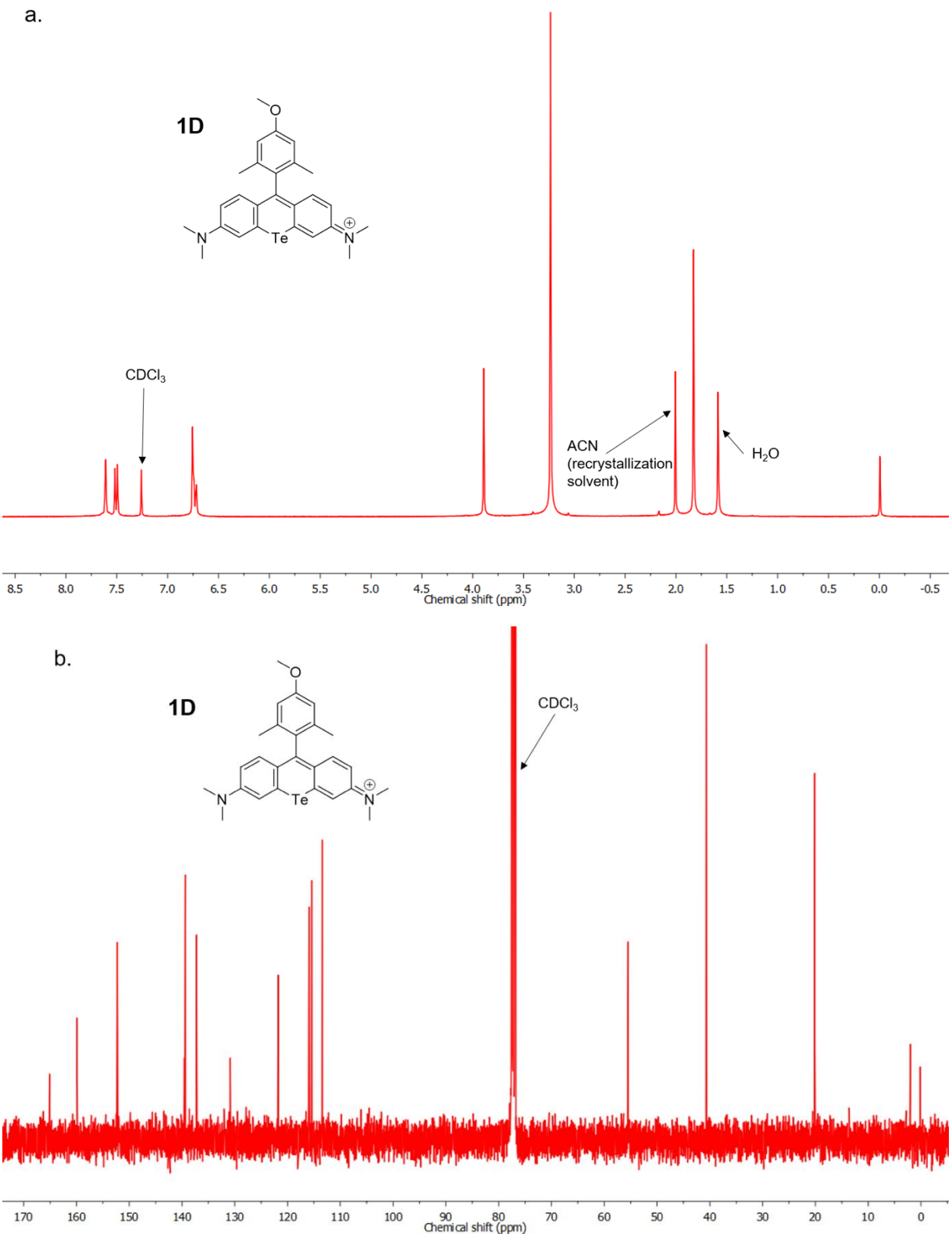


Figure S4. a.) ^{1}H NMR of **1D** in $CDCl_3$ and b.) ^{13}C NMR of **1D** in $CDCl_3$. Residual solvent labeled according to Ref[2].

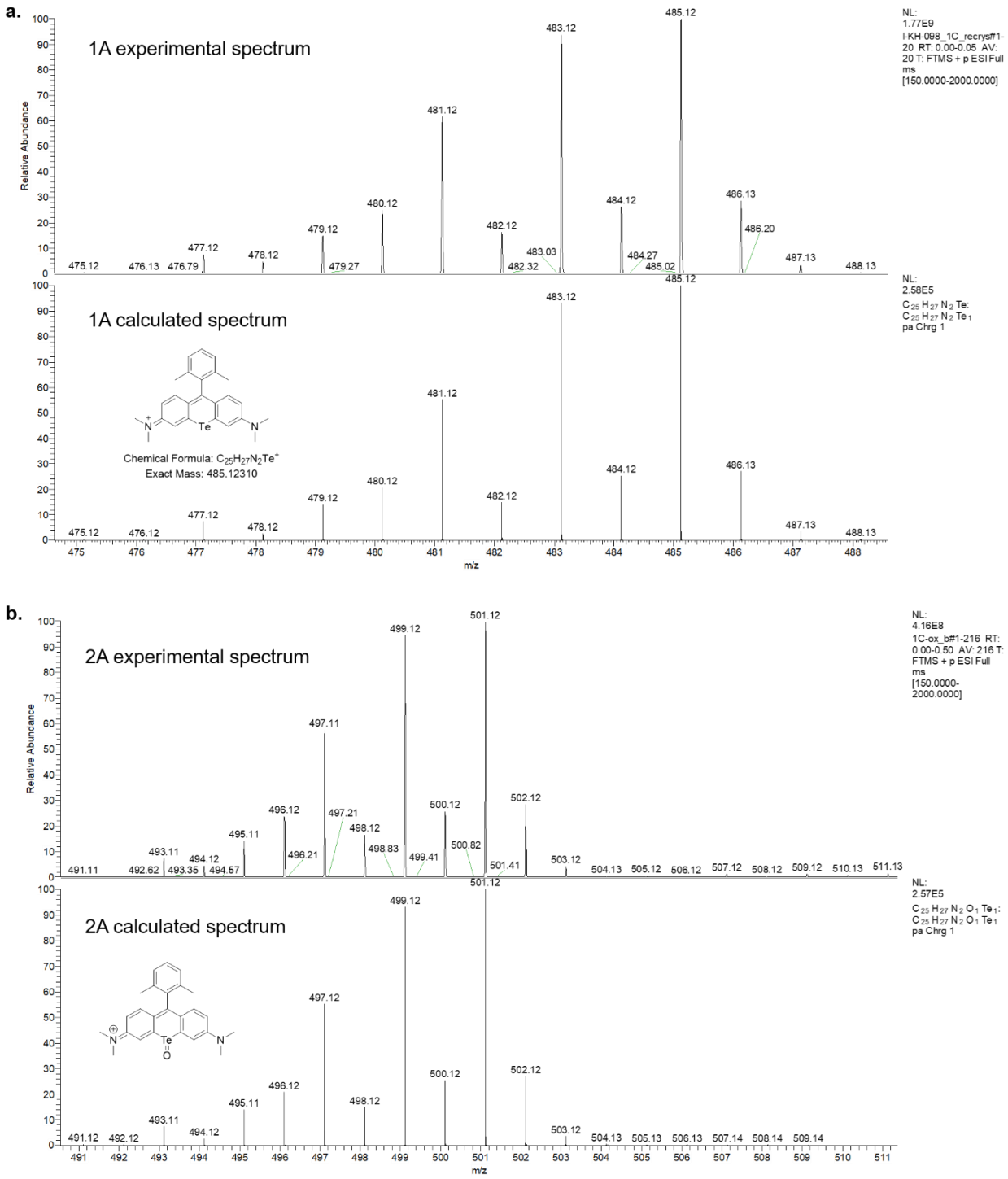
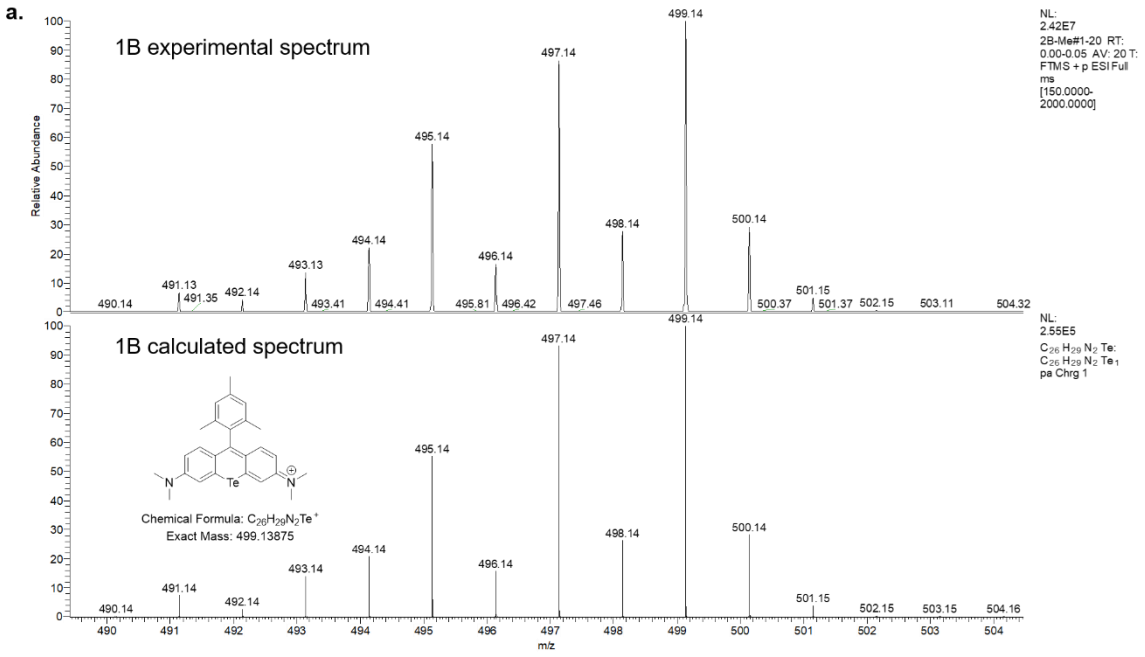


Figure S5. Experimental and calculated mass spectra of a.) **1A** and b.) **2A**.



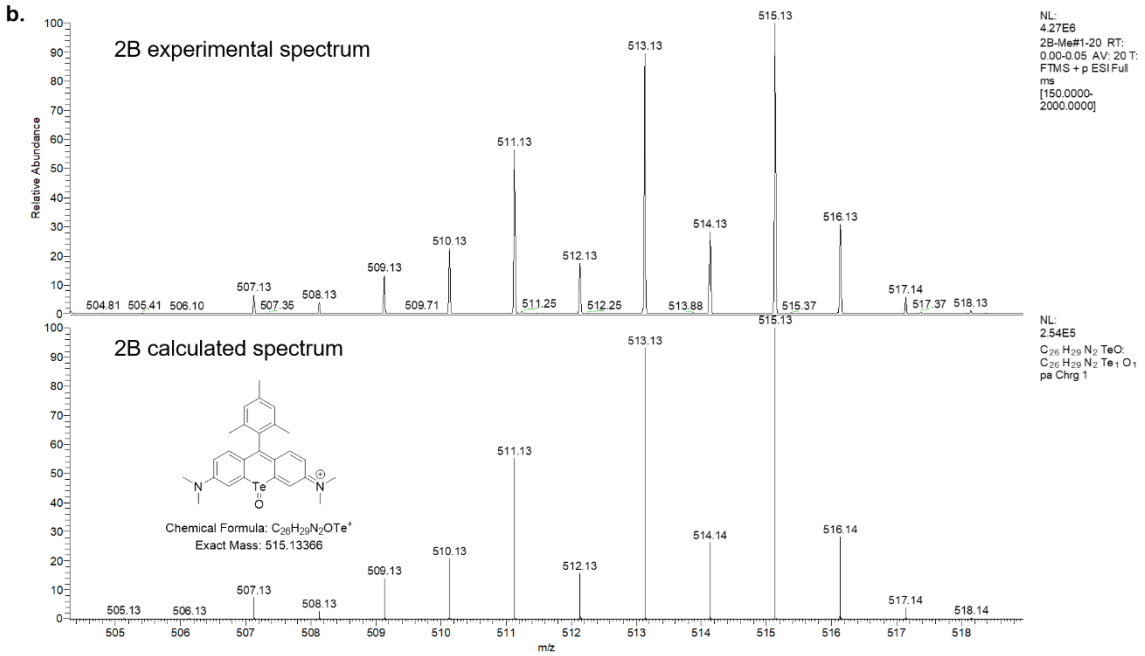


Figure S6. Experimental and calculated mass spectra of a.) **1B** and b.) **2B**.

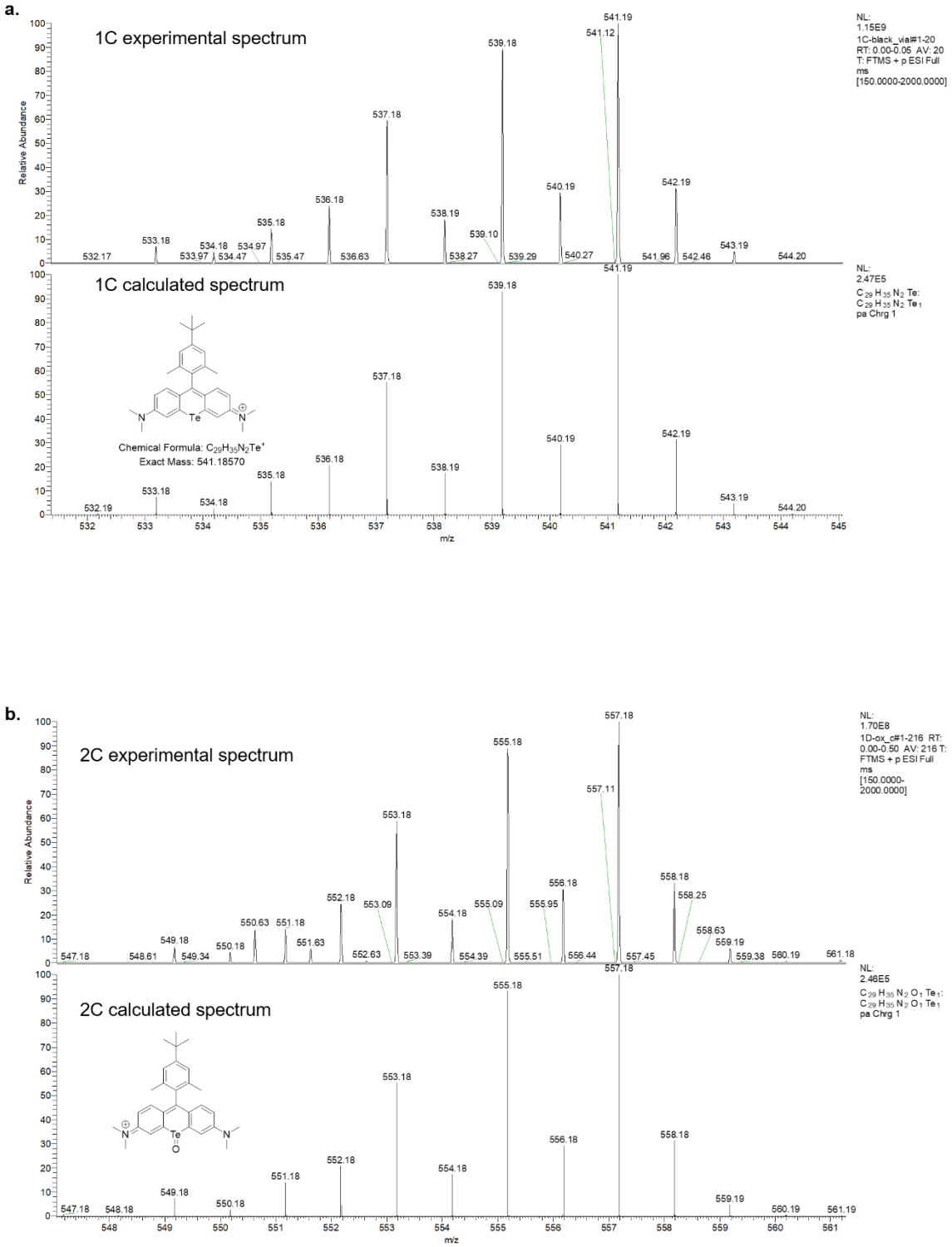


Figure S7. Experimental and calculated mass spectra of a.) **1C** and b.) **2C**.

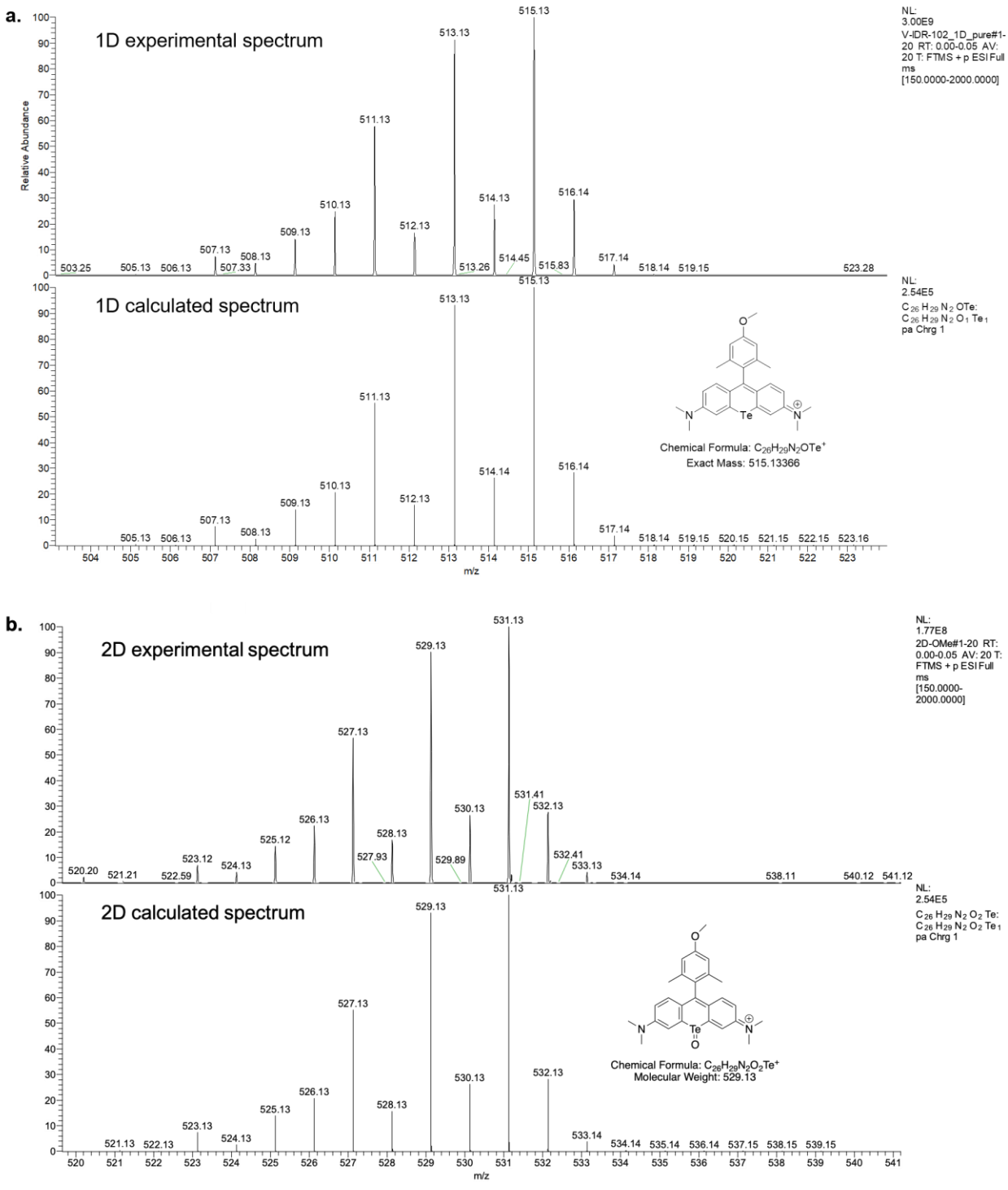


Figure S8. Experimental and calculated mass spectra of a.) **1D** and b.) **2D**.

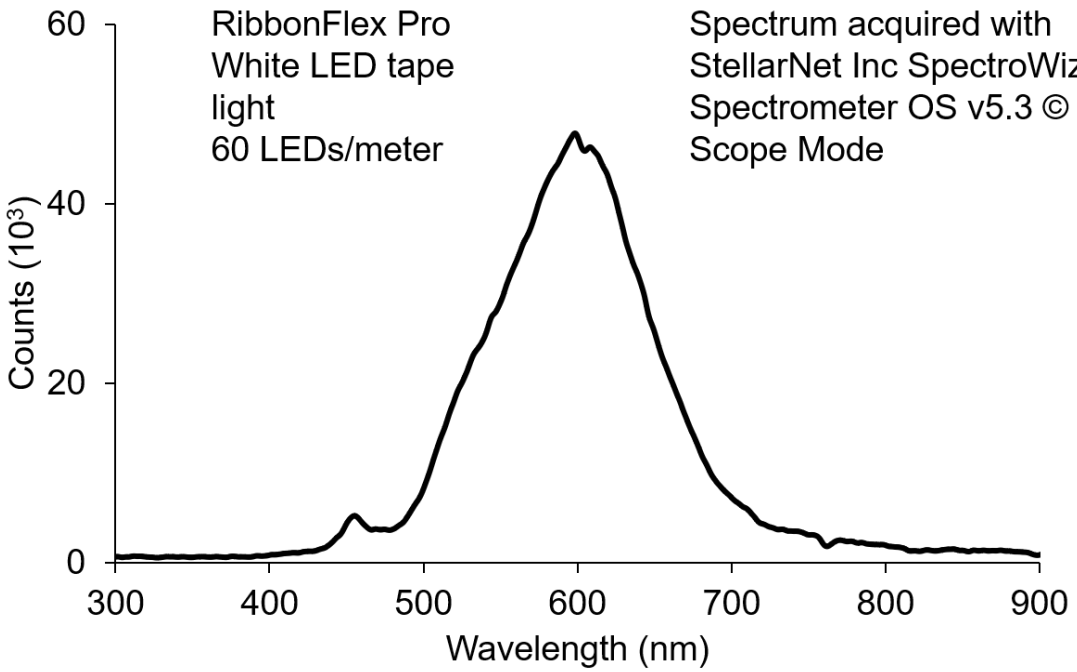


Figure S9. Spectrum of 24 W white LED tape.

Table S13. Hirshfeld charges of Te and O atoms of **1A-2D** and **2A**-**2D**, with experimental rates and ΔG's.

Dye	Te $Charge_{cal}$	dye	Hammett constant (σ_p)	Te $charge_{cal}$	O $charge_{cal}$
1A	0.0831	**2A**	0.00	0.3218	-0.4494
1B	0.0814	**2B**	-0.17	0.3214	-0.4502
1C	0.0817	**2C**	-0.20	0.3207	-0.4498
1D	0.0812	**2D**	-0.27	0.3212	-0.4504

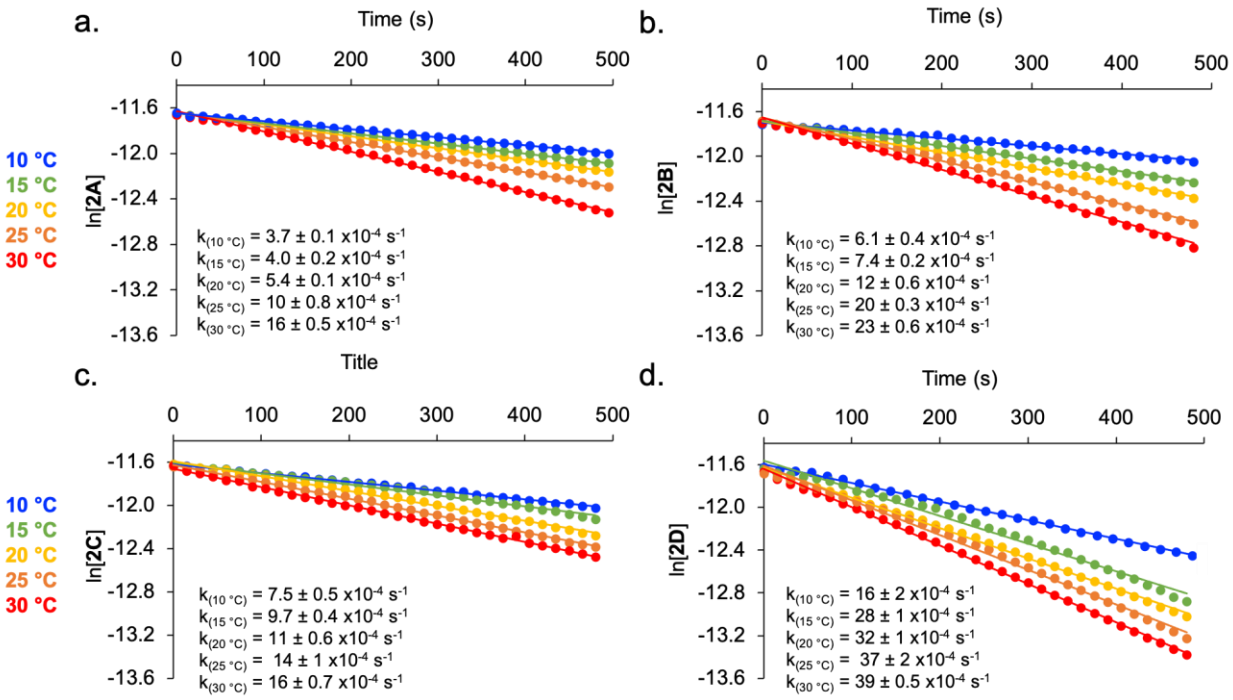


Figure S10. Pseudo-first order rates of reduction of **2A** (top left), **2B** (top right), **2C** (bottom left), and **2D** (bottom right) at a concentration of 8.4 X 10^{-6} M with 100 eq methyldiphenyl silane in 1:1 MeOH/H_2O. Rates were collected at 5 ºC increments over a temperature range of 10-30 ºC.

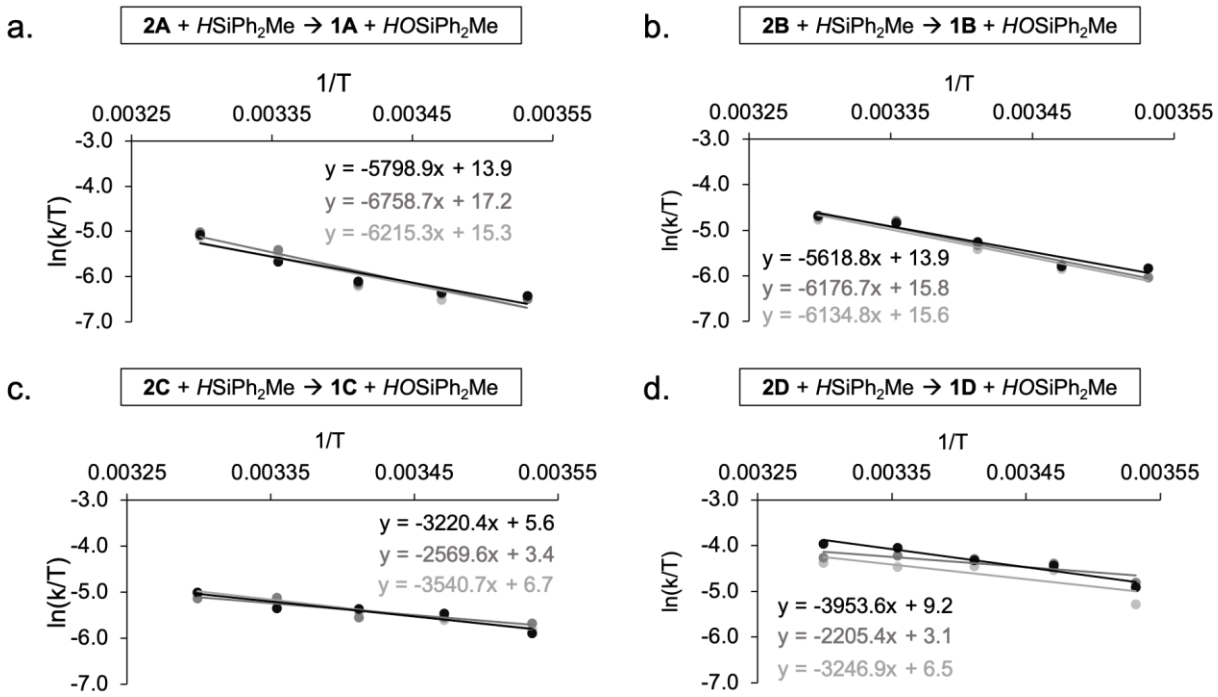


Figure S11. Triplicate Eyring plots of 1/T vs. ln(k/T) for **2A** (top left), **2B** (top right), **2C** (bottom left), and **2D** (bottom right) derived from pseudo-first order rates at 10, 15, 20, 25 and 30 ºC used to calculated experimental values for $\Delta H^{\ddagger}$, $\Delta S^{\ddagger}$, and $\Delta G^{\ddagger}$.

Table S14. Relative energy of optimized structures **1A**-**1D** and **2A**-**2D**. Energies were calculated in kcal/mol from Hartree (627.5 kcal·mol^{-1} /H). The energy values were taken from the free energy corrected values obtained from frequency calculations.

	Functional group on xylene	Energy (Hartree)	Energy (kcal·mol^{-1})
1A	H	-1125.2218	-706076.68
2A	H	-1200.3888	-753243.97
1B	Me	-1125.2218	-706076.68
2B	Me	-1200.3888	-753243.97
1C	tBu	-1243.0779	-780031.38
2C	tBu	-1318.2446	-827198.49
1D	OMe	-1200.4265	-753267.63
2D	OMe	-1275.5931	-800434.67