

Table S1. Data for the Competitive Debromination Reactions

ArBr	Ar'Br	[ArBr/Ar'Br] _i	Residual ArBr (mmol)	Residual Ar'Br (mmol)	Total Conversion (%)	k(ArBr)/k(Ar'Br)
13	14	0.5/0.5 = 1	0.11	0.32	57	3.40
15	16	0.5/0.5 = 1	0.26	0.39	45	2.63
13	16	0.5/0.5 = 1	0.19	0.41	40	4.87
13	15	0.35/0.5 = 0.7	0.2	0.39	31	2.3
16	14	0.5/0.5 = 1	0.28	0.27	45	1.0
12	14	0.5/0.5 = 1	0.14	0.31	55	2.7
12	18	0.5/0.5 = 1	0.4	0.4	20	1.0
15	11	1/1 = 1				k ₁₁ >> k ₁₅

Table S2. Experimental Details for Crystallographic Study of 2

Crystal Data	
empirical formula	C ₃₀ H ₄₆ Se ₂
formula wt	566.785
habit	colorless block
size, mm	0.10 × 0.20 × 0.56
crystal system	monoclinic
lattice parameters	
<i>a</i> , Å	15.546(9)
<i>b</i> , Å	17.587(16)
<i>c</i> , Å	22.445(4)
<i>V</i> , Å ³	61372(7)
space group	<i>P</i> _{cab}
<i>Z</i>	8
<i>d</i> _{calc}	1.222 g cm ⁻³
Intensity Measurements	
diffractometer	Enraf-Nonius CAD-4
temp (°C)	22
scan type	ω-2θ
<i>F</i> ₀₀₀	302
μ(Mo Kα), mm ⁻¹	0.89
2θ range (deg)	3.62–50.04°
data collected	+ <i>h</i> , + <i>k</i> , ± <i>l</i>
reflections measured	11628
unique reflections (<i>R</i> _{int})	5987 (0.139)
Structure Solution and Refinement	
observations (<i>I</i> > 2σ(<i>I</i>))	1550
variables	199
residuals	<i>R</i> = 0.090, <i>R</i> _w = 0.060*
residuals (all data)	<i>R</i> = 0.253, <i>R</i> _w = 0.076
<i>GOF</i> (all data)	2.403 (1.557)
final difference map,	
max / min, e Å ⁻³	1.70, -1.53
function minimized	$\sum [w(F_O - F_C)^2]; w = 1 / \sigma(F_O)$

$$^* R = R = \Sigma(|F_O| - |F_C|) / \Sigma|F_O|; R_w = [\Sigma(w||F_O| - |F_C|)^2 / \Sigma(|F_O|)^2]^{1/2}; w = 1 / \sigma(F)$$

Table S3. Positional and Isotopic Thermal Parameters for Non-Hydrogen Atoms for 2

	x/a	y/b	z/c	U
Se(1)	0.0699(2)	0.7890(1)	0.62283(8)	* 0.068(2)
Se(2)	0.0649(2)	0.7125(1)	0.70782(8)	* 0.066(1)
C(11)	0.167(2)	0.751(1)	0.5846(9)	* 0.05(2)
C(12)	0.241(2)	0.793(1)	0.5827(9)	* 0.05(1)
C(13)	0.315(2)	0.770(1)	0.553(1)	* 0.08(2)
C(14)	0.310(2)	0.700(1)	0.521(1)	* 0.09(2)
C(15)	0.236(2)	0.657(1)	0.523(1)	* 0.07(2)
C(16)	0.164(2)	0.680(1)	0.5537(9)	* 0.05(2)
C(121)	0.337(2)	0.873(1)	0.650(1)	0.101(8)
C(122)	0.255(2)	0.865(1)	0.615(1)	0.079(8)
C(123)	0.228(2)	0.933(1)	0.575(1)	0.13(1)
C(141)	0.425(2)	0.598(1)	0.510(1)	0.121(9)
C(142)	0.391(2)	0.673(1)	0.488(1)	0.079(7)
C(143)	0.366(2)	0.668(1)	0.415(1)	0.13(1)
C(161)	0.037(2)	0.629(1)	0.493(1)	0.115(9)
C(162)	0.092(1)	0.628(1)	0.5520(9)	0.074(7)
C(163)	0.112(1)	0.553(1)	0.5764(9)	0.081(7)
C(21)	0.153(2)	0.757(1)	0.753(1)	* 0.06(2)
C(22)	0.143(2)	0.827(1)	0.782(1)	* 0.06(2)
C(23)	0.210(2)	0.855(1)	0.814(1)	* 0.08(2)
C(24)	0.291(2)	0.818(1)	0.8178(9)	* 0.07(2)
C(25)	0.302(2)	0.754(1)	0.789(1)	* 0.07(2)
C(26)	0.237(2)	0.720(1)	0.758(1)	* 0.09(2)
C(221)	0.058(2)	0.951(1)	0.756(1)	0.16(1)
C(222)	0.051(2)	0.866(1)	0.779(1)	0.077(7)
C(223)	0.016(2)	0.866(1)	0.843(1)	0.107(8)
C(241)	0.350(2)	0.836(1)	0.923(1)	0.15(1)
C(242)	0.356(2)	0.847(1)	0.856(1)	0.091(8)
C(243)	0.398(2)	0.915(1)	0.839(1)	0.18(1)
C(261)	0.332(2)	0.640(1)	0.691(1)	0.102(9)
C(262)	0.252(2)	0.640(1)	0.726(1)	0.067(7)
C(263)	0.276(2)	0.578(1)	0.770(1)	0.13(1)

* = refined anisotropically

Table S4. Positional and Isotopic Thermal Parameters for Non-Hydrogen Atoms for 2

	x/a	y/b	z/c	U
Se(1)	0.0699(2)	0.7890(1)	0.62283(8)	* 0.068(2)
Se(2)	0.0649(2)	0.7125(1)	0.70782(8)	* 0.066(1)
C(11)	0.167(2)	0.751(1)	0.5846(9)	* 0.05(2)
C(12)	0.241(2)	0.793(1)	0.5827(9)	* 0.05(1)
C(13)	0.315(2)	0.770(1)	0.553(1)	* 0.08(2)
C(14)	0.310(2)	0.700(1)	0.521(1)	* 0.09(2)
C(15)	0.236(2)	0.657(1)	0.523(1)	* 0.07(2)
C(16)	0.164(2)	0.680(1)	0.5537(9)	* 0.05(2)
C(121)	0.337(2)	0.873(1)	0.650(1)	0.101(8)
C(122)	0.255(2)	0.865(1)	0.615(1)	0.079(8)
C(123)	0.228(2)	0.933(1)	0.575(1)	0.13(1)
C(141)	0.425(2)	0.598(1)	0.510(1)	0.121(9)
C(142)	0.391(2)	0.673(1)	0.488(1)	0.079(7)
C(143)	0.366(2)	0.668(1)	0.415(1)	0.13(1)
C(161)	0.037(2)	0.629(1)	0.493(1)	0.115(9)
C(162)	0.092(1)	0.628(1)	0.5520(9)	0.074(7)
C(163)	0.112(1)	0.553(1)	0.5764(9)	0.081(7)
C(21)	0.153(2)	0.757(1)	0.753(1)	* 0.06(2)
C(22)	0.143(2)	0.827(1)	0.782(1)	* 0.06(2)
C(23)	0.210(2)	0.855(1)	0.814(1)	* 0.08(2)
C(24)	0.291(2)	0.818(1)	0.8178(9)	* 0.07(2)
C(25)	0.302(2)	0.754(1)	0.789(1)	* 0.07(2)
C(26)	0.237(2)	0.720(1)	0.758(1)	* 0.09(2)
C(221)	0.058(2)	0.951(1)	0.756(1)	0.16(1)
C(222)	0.051(2)	0.866(1)	0.779(1)	0.077(7)
C(223)	0.016(2)	0.866(1)	0.843(1)	0.107(8)
C(241)	0.350(2)	0.836(1)	0.923(1)	0.15(1)
C(242)	0.356(2)	0.847(1)	0.856(1)	0.091(8)
C(243)	0.398(2)	0.915(1)	0.839(1)	0.18(1)
C(261)	0.332(2)	0.640(1)	0.691(1)	0.102(9)
C(262)	0.252(2)	0.640(1)	0.726(1)	0.067(7)
C(263)	0.276(2)	0.578(1)	0.770(1)	0.13(1)

* = refined anisotropically

Table S5. Calculated Positional and Isotopic Thermal Parameters for Hydrogen Atoms

	x/a	y/b	z/c		x/a	y/b	z/c
H(121a)	0.3821	0.8812	0.6220	H(221a)	0.0033	0.9740	0.7569
H(121b)	0.3311	0.9156	0.6749	H(221b)	0.0968	0.9779	0.7808
H(121c)	0.3536	0.8308	0.6741	H(221c)	0.0795	0.9506	0.7162
H(122)	0.2163	0.8646	0.6478	H(222)	0.0140	0.8397	0.7517
H(123a)	0.2217	0.9759	0.6003	H(223a)	0.0549	0.8932	0.8675
H(123b)	0.2726	0.9414	0.5473	H(223b)	-0.0386	0.8893	0.8436
H(123c)	0.1757	0.9279	0.5531	H(223c)	0.0119	0.8149	0.8563
H(13)	0.3657	0.8004	0.5527	H(23)	0.2026	0.9017	0.8342
H(141a)	0.3825	0.5604	0.5037	H(241a)	0.4064	0.8353	0.9393
H(141b)	0.4751	0.5856	0.4874	H(241b)	0.3189	0.8777	0.9397
H(141c)	0.4392	0.6011	0.5506	H(241c)	0.3216	0.7903	0.9349
H(142)	0.4365	0.7077	0.4960	H(242)	0.3946	0.8069	0.8466
H(143a)	0.4164	0.6550	0.3933	H(243a)	0.3672	0.9569	0.8553
H(143b)	0.3237	0.6299	0.4096	H(243b)	0.4547	0.9145	0.8549
H(143c)	0.3448	0.7153	0.4017	H(243c)	0.4019	0.9219	0.7971
H(15)	0.2344	0.6098	0.5030	H(25)	0.3574	0.7314	0.7895
H(161a)	0.0670	0.6015	0.4636	H(261a)	0.3804	0.6543	0.7149
H(161b)	-0.0163	0.6041	0.5016	H(261b)	0.3430	0.5929	0.6726
H(161c)	0.0235	0.6779	0.4775	H(261c)	0.3170	0.6787	0.6634
H(162)	0.0525	0.6497	0.5795	H(262)	0.2005	0.6315	0.7039
H(163a)	0.0595	0.5279	0.5847	H(263a)	0.2870	0.5308	0.7517
H(163b)	0.1428	0.5253	0.5468	H(263b)	0.3244	0.5922	0.7940
H(163c)	0.1459	0.5526	0.6117	H(263c)	0.2243	0.5779	0.7928

Table S6. Atomic Displacement Parameters for Isotropically Refined Atoms

	U11	U22	U33	U12	U13	U23
Se(1)	0.079(2)	0.076(1)	0.048(1)	0.018(2)	-0.005(2)	-0.008(1)
Se(2)	0.069(2)	0.081(1)	0.049(1)	-0.024(2)	-0.003(2)	-0.008(1)
C(11)	0.06(2)	0.04(1)	0.06(1)	-0.01(1)	-0.02(2)	0.01(1)
C(12)	0.06(2)	0.03(1)	0.06(2)	0.01(1)	0.03(1)	-0.02(1)
C(13)	0.11(2)	0.04(2)	0.09(2)	0.04(2)	-0.05(2)	-0.01(1)
C(14)	0.08(2)	0.08(2)	0.10(2)	0.05(2)	0.05(2)	0.03(2)
C(15)	0.06(2)	0.07(2)	0.09(2)	-0.02(2)	0.03(2)	-0.00(1)
C(16)	0.06(2)	0.05(1)	0.03(1)	-0.01(1)	0.01(1)	-0.01(1)
C(21)	0.07(2)	0.05(2)	0.05(1)	-0.00(1)	0.02(2)	0.00(1)
C(22)	0.05(2)	0.07(2)	0.07(2)	-0.00(1)	0.00(2)	0.01(1)
C(23)	0.10(2)	0.06(2)	0.08(2)	-0.03(2)	-0.02(2)	0.00(1)
C(24)	0.12(3)	0.06(2)	0.02(1)	-0.04(2)	-0.03(2)	0.00(1)
C(25)	0.08(2)	0.10(2)	0.05(1)	-0.04(1)	-0.01(2)	-0.02(2)
C(26)	0.17(3)	0.05(2)	0.05(2)	0.01(2)	0.03(2)	0.01(2)

Table S7. Intramolecular Distances (Å) and Angles (degrees) for Non-Hydrogen Atoms

atoms	distance	atoms	distance
Se1-Se2	2.336(3)	Se2-C21	1.87(2)
Se1-C11	1.86(2)	C21-C22	1.40(3)
C11-C12	1.36(3)	C21-C26	1.47(4)
C11-C16	1.43(3)	C22-C23	1.35(4)
C12-C13	1.38(3)	C23-C24	1.42(4)
C13-C14	1.44(3)	C24-C25	1.30(3)
C14-C15	1.37(4)	C25-C26	1.37(4)
C15-C16	1.37(3)	C22-C222	1.60(3)
C12-C122	1.47(3)	C221-C222	1.58(3)
C121-C122	1.51(4)	C222-C223	1.53(3)
C122-C123	1.55(3)	C24-C242	1.42(4)
C14-C142	1.54(4)	C241-C242	1.52(4)
C141-C142	1.49(3)	C242-C243	1.42(4)
C142-C143	1.68(4)	C26-C262	1.60(3)
C16-C162	1.44(3)	C261-C262	1.47(4)
C161-C162	1.58(3)	C262-C263	1.52(3)
C162-C163	1.47(3)		

atoms	angle	atoms	angle
Se2-Se1-C11	101.5(6)	Se1-Se2-C21	100.1(7)
Se1-C11-C12	121(2)	Se2-C21-C22	123(2)
Se1-C11-C16	120(2)	Se2-C21-C26	121(2)
C12-C11-C16	119(2)	C22-C21-C26	116(2)
C11-C12-C13	124(2)	C21-C22-C23	119(2)
C11-C12-C122	124(2)	C21-C22-C222	116(2)
C13-C12-C122	111(2)	C23-C22-C222	124(2)
C12-C13-C14	116(2)	C22-C23-C24	123(2)
C13-C14-C15	120(2)	C23-C24-C25	119(3)
C13-C14-C142	117(2)	C23-C24-C242	120(2)
C15-C14-C142	123(2)	C25-C24-C242	121(3)
C14-C15-C16	123(2)	C24-C25-C26	122(3)
C11-C16-C15	118(2)	C21-C26-C25	120(2)
C11-C16-C162	126(2)	C21-C26-C262	119(2)
C15-C16-C162	115(2)	C25-C26-C262	121(3)
C12-C122-C121	117(2)	C22-C222-C221	111(2)
C12-C122-C123	110(2)	C22-C222-C223	105(2)
C12-C122-H122	107(2)	C221-C222-C223	109(2)
C121-C122-C123	117(2)	C24-C242-C241	121(2)
C14-C142-C141	114(2)	C24-C242-C243	118(2)
C14-C142-C143	107(2)	C241-C242-C243	114(2)
C141-C142-C143	111(2)	C26-C262-C261	111(2)
C16-C162-C161	116(2)	C26-C262-C263	111(2)
C16-C162-C163	113(2)	C26-C262-H262	104(2)
C161-C162-C163	116(2)	C261-C262-C263	98(2)

Table S8. Torsional Angles (degrees) for Non-Hydrogen Atoms

atoms	angle	atoms	angle
C11-Se1-Se2-C21	76(1)	Se1-Se2-C21-C22	75(2)
Se1-C11-C12-C122	6(3)	Se1-Se2-C21-C26	-104(2)
Se1-C11-C12-C13	-176(2)	Se2-C21-C22-C222	3(3)
Se1-C11-C16-C15	176(2)	Se2-C21-C22-C23	-180(2)
Se1-C11-C16-C162	-5(3)	Se2-C21-C26-C25	177(2)
Se2-Se1-C11-C12	-108(2)	Se2-C21-C26-C262	0(3)
Se2-Se1-C11-C16	76(2)	C21-C22-C222-C221	-127(2)
C11-C12-C122-C121	132(2)	C21-C22-C222-C223	115(2)
C11-C12-C122-C123	-90(3)	C21-C22-C23-C24	0(4)
C11-C12-C13-C14	0(3)	C21-C26-C262-C261	131(2)
C11-C16-C162-C161	103(2)	C21-C26-C262-C263	-121(2)
C11-C16-C162-C163	-120(2)	C222-C22-C23-C24	178(2)
C122-C12-C13-C14	179(2)	C22-C21-C26-C25	-3(3)
C12-C11-C16-C15	0(3)	C22-C21-C26-C262	180(2)
C12-C11-C16-C162	178(2)	C22-C23-C24-C242	-174(2)
C12-C13-C14-C142	-178(2)	C22-C23-C24-C25	1(4)
C12-C13-C14-C15	-2(3)	C23-C22-C222-C221	56(3)
C13-C12-C122-C121	-45(3)	C23-C22-C222-C223	-63(3)
C13-C12-C122-C123	92(2)	C23-C24-C242-C241	75(3)
C13-C14-C142-C141	119(2)	C23-C24-C242-C243	-73(3)
C13-C14-C142-C143	-119(2)	C23-C24-C25-C26	-4(4)
C13-C14-C15-C16	2(4)	C242-C24-C25-C26	171(2)
C142-C14-C15-C16	178(2)	C24-C25-C26-C21	5(4)
C14-C15-C16-C11	0(3)	C24-C25-C26-C262	-177(2)
C14-C15-C16-C162	-179(2)	C25-C24-C242-C241	-100(3)
C15-C14-C142-C141	-57(3)	C25-C24-C242-C243	113(3)
C15-C14-C142-C143	65(3)	C25-C26-C262-C261	-47(3)
C15-C16-C162-C161	-79(2)	C25-C26-C262-C263	61(3)
C15-C16-C162-C163	59(3)	C26-C21-C22-C222	-178(2)
C16-C11-C12-C122	-177(2)	C26-C21-C22-C23	0(3)
C16-C11-C12-C13	0(3)		