

Supplementary Information

The unexpected case of reactions of halogens and interhalogens with halide substituted Pd(II) σ -butadienyl complexes.

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1. NMR spectra of the complexes studied

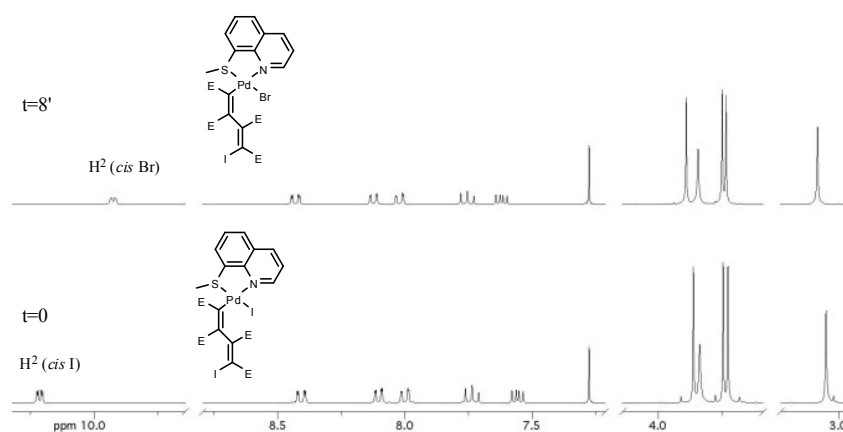


Fig. S1a: ^1H NMR spectrum of complex **1a** and that of **1a** + IBr (**1d**) recorded after 8 min. in CDCl_3 at 298K

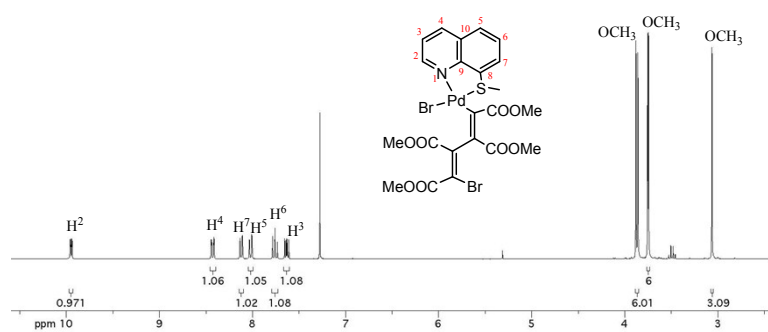


Fig. S1b: ^1H NMR spectrum of the complex **1b** in CDCl_3 at 298 K.

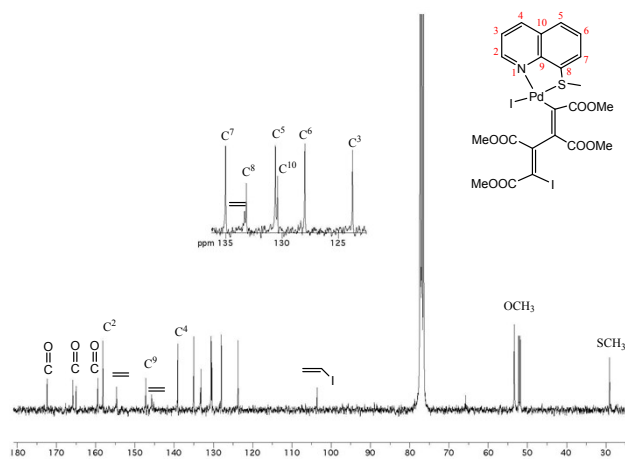


Fig. S1c: ^{13}C NMR spectrum of the complex **1a** in CDCl_3 at 298 K.

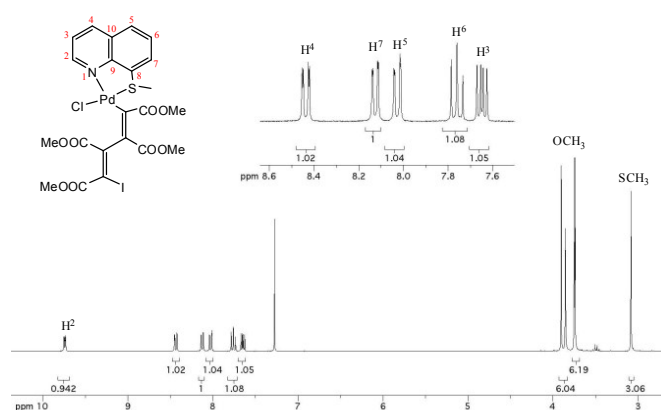


Fig. S1d: ¹H NMR spectrum of the complex **1e** in CDCl₃ at 298 K.

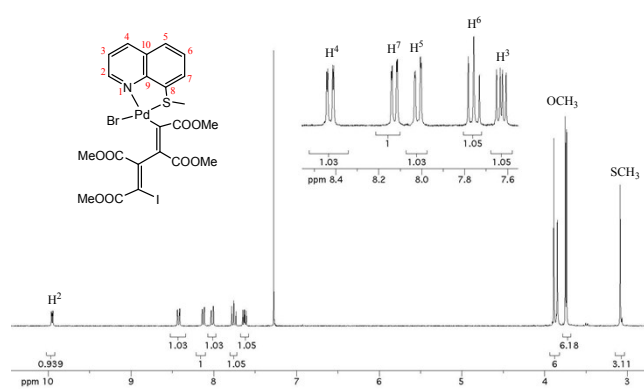


Fig. S1e: ¹H NMR spectrum of the complex **1d** in CDCl₃ at 298 K.

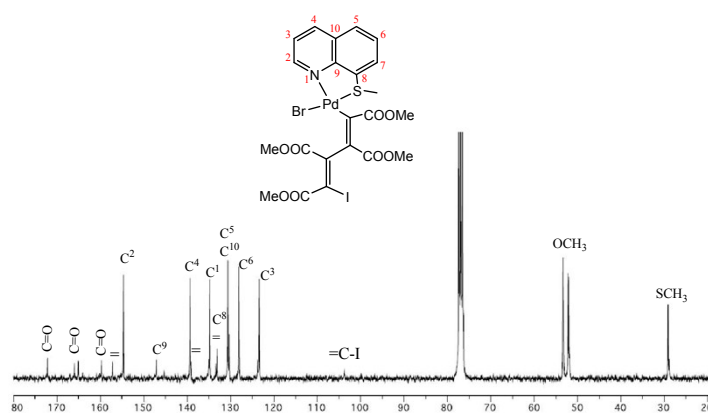


Fig. S1f: ¹³C NMR spectrum of the complex **1d** in CDCl₃ at 298 K.

2. Schematic representation of the energies involved in the reaction between *1b* and ICl

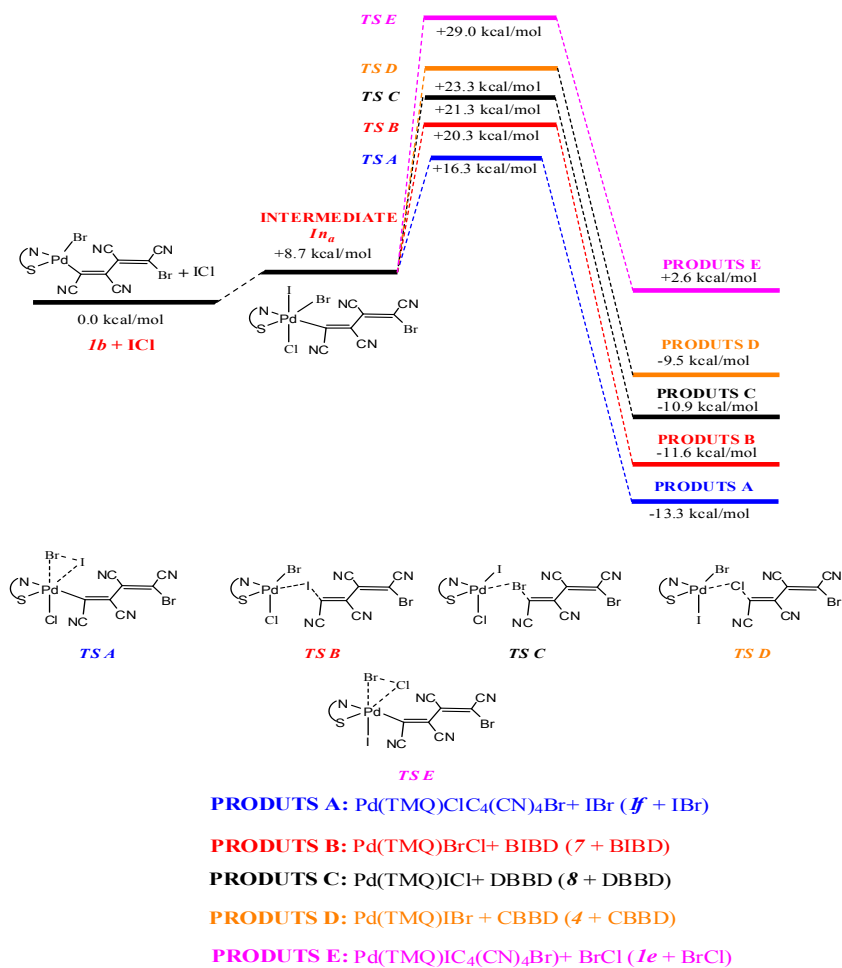


Fig. S2: Computed energies for the reaction between complex *1b* and ICl yielding *If**.

In order to save computer time the simulation was carried out on the complex *1b* instead of *1e*, whereas the crystallographic data are related to the better crystallizing *1f*.

3. ^1H NMR spectra related to Scheme 6 (text)

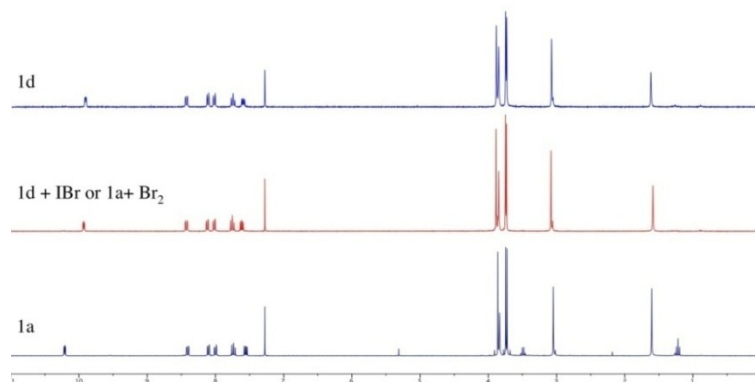


Fig. S3: ^1H NMR spectra in CDCl_3 at RT of the complexes **1a** (lower spectrum) and **1d** (upper spectrum) and the ensuing ^1H NMR spectrum independently recorded soon after the mixing of the reactants Br_2 to **1a** or IBr to **1d** indicating the fast equilibrium between **1a** and **1d** (middle spectrum).

4. Reaction between **1b** and IBr GC-MS spectrum)

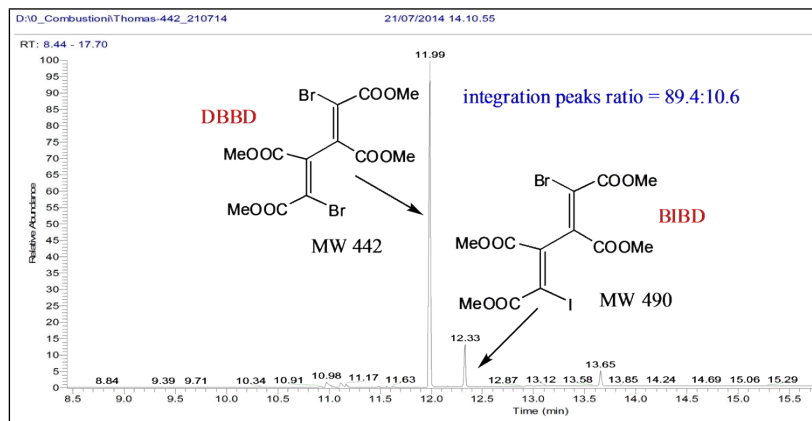


Fig. S4: GC-MS spectrum of the organic fraction of the reaction: **1b** + $\text{IBr}_{(\text{exc})}$ $\rightarrow$ **5** + DBBD + BIBD.

4. ^1H NMR spectra for the reaction of halogen metathesis

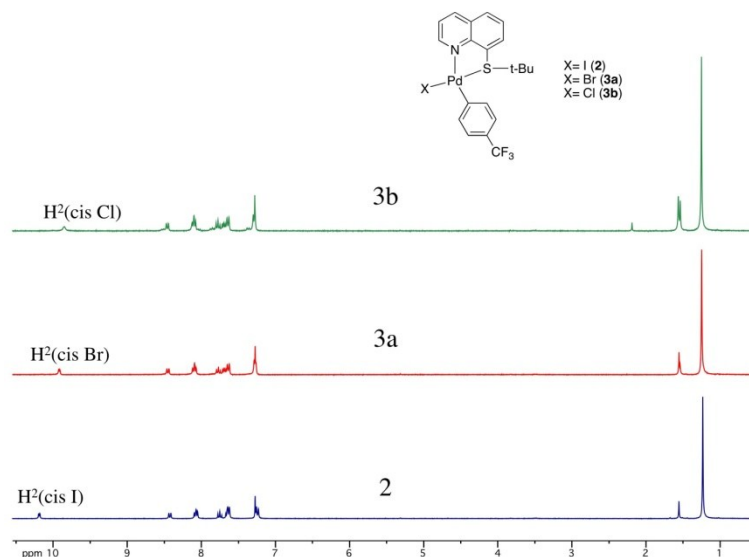


Fig. S5: ^1H NMR spectra in CDCl_3 at RT for the reactions: **2** + IBr $\rightarrow$ **3a** and **2** + ICl $\rightarrow$ **3b**

Table S1. Crystallographic data.

Complex	1f
Formula	$\text{C}_{25}\text{H}_{27}\text{BrClINO}_8\text{PdS}$
M	723.30
Space group	$P2_1/c$
Crystal system	Monoclinic
a/Å	9.8374(2)
b/Å	17.9906(7)
c/Å	17.3653(5)
$\beta/^\circ$	91.846(2)
U/Å ³	3071.7(2)
Z	4
T/K	295
$D_c/\text{g cm}^{-3}$	1.564
F(000)	1448

$\mu(\text{Mo-K}\alpha)/\text{mm}^{-1}$	2.104
Measured Reflections	25898
Unique Reflections	8905
R_{int}	0.0388
Obs. Refl.ns [$I \geq 2\sigma(I)$]	6212
$\theta_{\text{min}} - \theta_{\text{max}}/^\circ$	3.18 – 30.00
hkl ranges	-13,13;-25,25;-24,24
$R(F^2)$ (Obs.Refl.ns)	0.0387
$wR(F^2)$ (All Refl.ns)	0.1017
No. Variables	350
Goodness of fit	1.025
$\Delta\rho_{\text{max}}; \Delta\rho_{\text{min}} / \text{e } \text{\AA}^{-3}$	0.550; -0.800
CCDC Deposition N.	1472780

Cartesian coordinates of the computed species

PdI(TMQ)C₄(CN)₄I (*1a*) + IBr (Fig. 1 Text)

REACTANT (*1a*)

```

H  7.1071270000  6.1359840000  2.7861950000
C  6.5222130000  5.4773460000  2.1514930000
H  4.8136120000  6.7690540000  2.0803430000
C  5.2541470000  5.8263970000  1.7636500000
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C  4.4860590000  4.9666550000  0.9432380000
C  7.0780740000  4.2573830000  1.7177070000
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C	6.8638830000	-3.0694080000	-0.2380120000
N	7.5634930000	-3.9781970000	-0.4397910000
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INTERMEDIATE In_b

H	5.6660880000	3.9205550000	0.7894490000
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TS C

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H 8.8686210000 1.4045560000 -2.7211930000
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PRODUCT B (4)

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S -0.5120000000 1.9180000000 0.2520000000
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B 1.5570000000 -2.4060000000 -0.0630000000
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PRODUCT C (5)

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 H -1.7411990000 -3.3964510000 1.6439200000
 Pd 0.3515380000 -0.0690430000 -0.0483320000
 I 1.8856170000 2.0953240000 0.0212660000
 I 2.5221750000 -1.5662740000 -0.1186510000

PdI(TMQ)C₄(CN)₄I (*1a*)+ Br₂ (Fig. 3 Text)

INTERMEDIATE *In_a*

H 6.0641110000 3.5693460000 0.3360090000
 C 5.3552670000 2.7984440000 0.0504610000
 H 6.6391780000 1.9041630000 -1.4143940000
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 H 6.0101860000 -0.0465640000 -2.7805450000
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 N 2.5925070000 -0.1771620000 -0.9680130000
 S 1.5312130000 1.8597050000 1.0252050000
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 C -0.8995040000 -0.4647480000 1.4363920000
 C -3.3537110000 1.6188550000 -0.1607940000
 C -2.0126790000 0.3124430000 1.5085380000
 C -2.3472330000 1.5449480000 0.7430160000
 C -3.6683980000 2.8459800000 -0.8060150000
 N -3.9272320000 3.8406590000 -1.3523650000
 C -1.6569920000 2.7374200000 1.1191200000
 N -1.0932910000 3.6957580000 1.4641580000
 C -3.0294700000 -0.0126890000 2.4712290000
 N -3.8762600000 -0.2444280000 3.2354810000
 C -0.8714020000 -1.5516350000 2.3613490000
 N -0.9008080000 -2.4246940000 3.1326580000
 C 1.8576960000 1.7683790000 2.8088650000
 H 2.3312310000 2.7039540000 3.1166480000
 H 2.4847640000 0.9040200000 3.0392600000
 H 0.8825380000 1.6812760000 3.2965610000
 I -0.2172460000 -2.6071960000 -0.8174990000
 Br -0.3280020000 0.9190540000 -1.7238900000

Br 2.2402030000 -1.5976570000 1.8167150000
I -4.4340640000 -0.0308120000 -0.8139110000

TS 1

H -1.6420000000 -5.9580000000 -0.4870000000
C -1.9000000000 -4.9300000000 -0.2590000000
H -3.9930000000 -5.2000000000 -0.6060000000
C -3.2030000000 -4.5100000000 -0.3280000000
C -1.1850000000 -2.7210000000 0.4090000000
C -3.5430000000 -3.1670000000 -0.0420000000
C -0.8830000000 -4.0310000000 0.1230000000
C -2.5160000000 -2.2450000000 0.3050000000
C -4.8680000000 -2.6810000000 -0.0830000000
H 0.1430000000 -4.3750000000 0.1970000000
C -5.1160000000 -1.3660000000 0.2100000000
H -5.6740000000 -3.3590000000 -0.3470000000
H -6.1190000000 -0.9590000000 0.1970000000
C -4.0300000000 -0.5180000000 0.5040000000
H -4.1930000000 0.5390000000 0.6850000000
N -2.7790000000 -0.9320000000 0.5390000000
S 0.1040000000 -1.6370000000 1.0040000000
P -0.8390000000 0.5370000000 0.1790000000
C 0.8980000000 1.9270000000 0.4310000000
C 3.4880000000 -0.7280000000 0.5590000000
C 2.1890000000 1.4270000000 0.3780000000
C 2.7460000000 0.2790000000 1.1120000000
C 4.0720000000 -1.7370000000 1.3620000000
N 4.5380000000 -2.5940000000 1.9950000000
C 2.6190000000 0.2740000000 2.5350000000
N 2.5270000000 0.2610000000 3.6940000000
C 3.1300000000 2.1360000000 -0.4200000000
N 3.9370000000 2.6970000000 -1.0430000000
C 0.6850000000 3.1980000000 -0.1710000000
N 0.5760000000 4.2610000000 -0.6280000000
C -0.2760000000 -1.7080000000 2.7930000000
H -0.1820000000 -2.7460000000 3.1150000000
H -1.2820000000 -1.3350000000 2.9770000000
H 0.4580000000 -1.0940000000 3.3120000000
I -2.4480000000 2.3570000000 -0.9100000000
B -0.5070000000 -0.3430000000 -2.1220000000
B -0.2620000000 1.9000000000 2.2700000000
I 3.7860000000 -0.9940000000 -1.4850000000

INTERMEDIATE In_b

H 5.4265190000 3.9048420000 1.0595360000
C 4.7760450000 3.1618280000 0.6089760000
H 6.1108540000 2.7075970000 -1.0060240000
C 5.1543500000 2.5016150000 -0.5316680000
C 2.6844250000 1.9469840000 0.6497600000
C 4.3075670000 1.5340610000 -1.1188270000

C 3.5245770000 2.8939340000 1.1942820000
 C 3.0557240000 1.2325140000 -0.5145790000
 C 4.6677390000 0.8370230000 -2.2932230000
 H 3.2189790000 3.4537730000 2.0749280000
 C 3.8166210000 -0.0998250000 -2.8163400000
 H 5.6220160000 1.0566480000 -2.7663910000
 H 4.0542470000 -0.6535260000 -3.7180090000
 C 2.6096270000 -0.3634120000 -2.1502630000
 H 1.9245420000 -1.1197740000 -2.5304230000
 N 2.2456470000 0.2646580000 -1.0458600000
 S 1.0539670000 1.7236760000 1.3430050000
 Pd 0.4295200000 -0.2455920000 0.0312830000
 C -1.2284560000 -0.7363140000 1.1863770000
 C -3.7074240000 1.5010580000 -0.0054480000
 C -2.3622110000 -0.0280440000 1.4342200000
 C -2.7485890000 1.3191580000 0.9315980000
 C -4.0925610000 2.7973910000 -0.4465790000
 N -4.4000810000 3.8533370000 -0.8253460000
 C -2.1707410000 2.4528960000 1.5770930000
 N -1.6934280000 3.3545680000 2.1374950000
 C -3.3716100000 -0.5835150000 2.2928450000
 N -4.2171890000 -0.9973530000 2.9773930000
 C -1.1754620000 -2.0058190000 1.8378150000
 N -1.1860980000 -3.0359410000 2.3827040000
 C 1.4199980000 1.2809050000 3.0673390000
 H 1.7013140000 2.1928300000 3.5998300000
 H 2.2114720000 0.5293510000 3.1114780000
 H 0.4910120000 0.8872930000 3.4904490000
 I -0.4241280000 -2.2823900000 -1.4989420000
 Br -4.5269740000 0.0630640000 -0.8963490000
 Br -0.6832700000 1.4000240000 -1.6178640000
 I 2.0991560000 -1.9134250000 1.3659240000

TS 2

H 3.4810170000 5.4764130000 1.2924920000
 C 3.2499110000 4.4982570000 0.8822370000
 H 4.4833710000 4.7350350000 -0.8538480000
 C 3.8016850000 4.0901620000 -0.3042940000
 C 2.0700210000 2.3964820000 1.0826880000
 C 3.4887770000 2.8228170000 -0.8514040000
 C 2.3803140000 3.6392950000 1.5847930000
 C 2.5907070000 1.9636750000 -0.1618260000
 C 4.0274030000 2.3783720000 -2.0786410000
 H 1.9529660000 3.9539670000 2.5345770000
 C 3.6737620000 1.1495390000 -2.5721110000
 H 4.7163470000 3.0237220000 -2.6187680000
 H 4.0670980000 0.7718430000 -3.5095500000
 C 2.7517880000 0.3739180000 -1.8530080000
 H 2.4132410000 -0.5823740000 -2.2484330000
 N 2.2278550000 0.7572460000 -0.7005830000
 S 1.0401000000 1.3084310000 2.0629660000

Pd 0.5075200000 -0.1917840000 0.1721800000
C -1.1685410000 -0.8028020000 1.1593230000
C -3.8513550000 1.3516020000 0.0268710000
C -2.3618490000 -0.1706160000 1.3321480000
C -2.7629640000 1.1596040000 0.8112010000
C -4.2381290000 2.6461650000 -0.4151970000
N -4.5537880000 3.7004700000 -0.7927400000
C -2.0281670000 2.3117820000 1.2316710000
N -1.4467070000 3.2565120000 1.5834060000
C -3.3740890000 -0.7978990000 2.1353990000
N -4.1992340000 -1.2881840000 2.7939120000
C -1.0302140000 -2.0519580000 1.8318300000
N -0.9091650000 -3.0696220000 2.3880960000
C 2.3267840000 0.4462720000 3.0125130000
H 2.7798270000 1.1700470000 3.6953230000
H 3.0817760000 0.0187830000 2.3448780000
H 1.8302960000 -0.3461730000 3.5796890000
I 0.2448060000 -2.5029360000 -1.4944920000
Br -4.8448390000 -0.0706740000 -0.7010130000
Br -0.7673800000 1.2554870000 -1.6719840000
I 2.2556930000 -2.3975450000 0.7375300000

PRODUCT (Ib)

H -7.1444100000 6.3251990000 -2.2379460000
C -7.2821750000 5.4921530000 -1.5554820000
H -7.0973540000 6.6827390000 0.2172670000
C -7.2541910000 5.6901520000 -0.1987360000
C -7.6731110000 3.1295790000 -1.2263610000
C -7.4256750000 4.6061610000 0.6941650000
C -7.4953760000 4.1989380000 -2.0738150000
C -7.6269370000 3.2977130000 0.1785790000
C -7.4044450000 4.7711460000 2.0972230000
H -7.5267010000 4.0430730000 -3.1499260000
C -7.5738500000 3.6817930000 2.9101480000
H -7.2538040000 5.7655060000 2.5114630000
H -7.5664850000 3.7677870000 3.9913520000
C -7.7496850000 2.4171790000 2.3238070000
H -7.8634110000 1.5274060000 2.9407540000
N -7.7734560000 2.2210890000 1.0152700000
S -8.0105200000 1.5140450000 -1.9202770000
Pd -7.8567830000 0.2761590000 0.0899400000
C -7.8624020000 -1.4589670000 -0.8988820000
C -4.5350810000 -2.6318810000 -0.0696590000
C -6.7764950000 -2.2372350000 -1.1495520000
C -5.4248780000 -1.8327570000 -0.7119140000
C -3.2328140000 -2.1785710000 0.2804370000
N -2.1657790000 -1.8201000000 0.5744400000
C -5.0302900000 -0.4829920000 -0.9865050000
N -4.7008030000 0.6086070000 -1.2217310000
C -6.9070560000 -3.4598440000 -1.8819950000
N -7.0338780000 -4.4379220000 -2.5006540000

C	-9.1532960000	-1.8453420000	-1.3420910000
N	-10.2430030000	-2.0726820000	-1.6936780000
C	-9.8221430000	1.6484150000	-2.1364250000
H	-10.0200680000	2.3685040000	-2.9341510000
H	-10.2843570000	1.9635140000	-1.1982640000
H	-10.1855670000	0.6585080000	-2.4251910000
Br	-7.7062740000	-1.0762940000	2.1841750000
Br	-4.9348980000	-4.3855010000	0.4890200000

PdBr(TMQ)C₄(CN)₄Br (*Ib*) + IBr (Fig. 4 Text)

INTERMEDIATE *In_a*

H	9.7186620000	4.5799950000	1.8689410000
C	8.8056560000	4.1693920000	1.4487860000
H	7.6312820000	5.9214380000	1.8301990000
C	7.6519690000	4.9105910000	1.4293910000
C	7.6668900000	2.3254370000	0.3782960000
C	6.4580990000	4.3765810000	0.8897410000
C	8.8128920000	2.8644150000	0.9163270000
C	6.4547310000	3.0566890000	0.3641510000
C	5.2510740000	5.1099520000	0.8510030000
H	9.7301060000	2.2796410000	0.9233200000
C	4.1269570000	4.5369350000	0.3178540000
H	5.2338210000	6.1230170000	1.2465260000
H	3.1825690000	5.0680350000	0.2677030000
C	4.1997020000	3.2197710000	-0.1656230000
H	3.3194150000	2.7262300000	-0.5739900000
N	5.3098110000	2.4996810000	-0.1452990000
S	7.7310800000	0.6917620000	-0.3512910000
Pd	5.4080600000	0.4213780000	-0.7082750000
C	5.6303540000	-1.5174540000	-1.1325120000
C	3.8068470000	-2.9527590000	1.6512130000
C	5.3528690000	-2.5532530000	-0.2971350000
C	4.8621090000	-2.3210160000	1.0766260000
C	3.4232430000	-2.7034920000	2.9983100000
N	3.0974640000	-2.5075910000	4.0978520000
C	5.5589150000	-1.3431360000	1.8584040000
N	6.1323900000	-0.5602180000	2.5015580000
C	5.5653540000	-3.9056810000	-0.7143610000
N	5.7690510000	-4.9963580000	-1.0670520000
C	6.1218230000	-1.7499910000	-2.4426680000
N	6.5545890000	-1.8500770000	-3.5222310000
C	8.3162340000	1.1305290000	-2.0281420000
H	9.3522190000	1.4697100000	-1.9522370000
H	7.6772950000	1.9089450000	-2.4511080000
H	8.2616060000	0.2228770000	-2.6352340000
Br	2.9654280000	0.0867860000	-1.1072750000
Br	2.6981660000	-4.1634910000	0.7281110000

TS B

H	2.9045080000	5.4494080000	-0.1756760000
C	2.8448820000	4.3726000000	-0.0521230000
H	4.9661550000	4.0772810000	-0.0841630000
C	3.9859240000	3.6126100000	-0.0082370000
C	1.4921250000	2.3985040000	0.2285700000
C	3.9160140000	2.2061240000	0.1425380000
C	1.5806030000	3.7631960000	0.0949120000
C	2.6438750000	1.5814550000	0.2082790000
C	5.0587350000	1.3828710000	0.2524750000
H	0.6790430000	4.3709380000	0.1171840000
C	4.9039770000	0.0310700000	0.4236250000
H	6.0466250000	1.8357850000	0.2109640000
H	5.7535530000	-0.6329240000	0.5392930000
C	3.6103920000	-0.5156580000	0.4030950000
H	3.4712350000	-1.5925930000	0.4639590000
N	2.5198220000	0.2211510000	0.2678730000
S	-0.0869750000	1.6504370000	0.6137840000
Pd	0.5213510000	-0.5870770000	-0.2384320000
C	-1.3299380000	-1.3356870000	-0.7073120000
C	-3.2192200000	1.2986440000	0.5523550000
C	-2.5324730000	-0.9798880000	-0.1866340000
C	-2.8173070000	0.0409150000	0.8658860000
C	-3.5606910000	2.2473090000	1.5605520000
N	-3.8162910000	3.0386950000	2.3733360000
C	-2.8302630000	-0.3623290000	2.2365700000
N	-2.8653080000	-0.6721160000	3.3579330000
C	-3.7421040000	-1.5761050000	-0.6797240000
N	-4.7577430000	-2.0135010000	-1.0429270000
C	-1.4137140000	-2.3089320000	-1.7540250000
N	-1.6412880000	-3.1707420000	-2.5054460000
C	0.0313420000	1.7179900000	2.4298700000
H	-0.0150540000	2.7759630000	2.7052550000
H	0.9642750000	1.2628810000	2.7710920000
H	-0.8198070000	1.1949950000	2.8764230000
Br	0.4198330000	0.5694800000	-2.5270220000
I	0.4146570000	-1.8976680000	2.1004990000
Br	1.5958550000	-2.6278900000	-1.1980820000
Br	-3.3392660000	1.9201440000	-1.2126910000

TSC

H	1.7590490000	5.8556960000	0.0912550000
C	1.9848010000	4.7939610000	0.0679280000
H	3.9535680000	5.0556240000	-0.7348810000
C	3.1985940000	4.3509160000	-0.3936000000
C	1.2951780000	2.5264900000	0.5101490000
C	3.4965760000	2.9673670000	-0.4347220000
C	1.0261780000	3.8740210000	0.5447600000
C	2.5139300000	2.0337140000	-0.0157110000
C	4.7401540000	2.4544280000	-0.8690770000
H	0.0842700000	4.2299210000	0.9561530000

C 4.9516400000 1.0998020000 -0.8680910000
H 5.5159810000 3.1449960000 -1.1924740000
H 5.8987670000 0.6708230000 -1.1778000000
C 3.8973060000 0.2463440000 -0.4908700000
H 4.0178050000 -0.8349290000 -0.5379120000
N 2.7175120000 0.6891390000 -0.0973890000
S 0.1614860000 1.3825490000 1.2870840000
Pd 0.7240940000 -0.5531360000 -0.1380570000
C -1.2871550000 -1.1890510000 -0.7284170000
C -3.4539400000 1.1568180000 0.5594560000
C -2.4012170000 -1.0570600000 0.0711350000
C -2.7227820000 0.0884910000 0.9574240000
C -3.7295090000 2.2475470000 1.4335390000
N -3.9364570000 3.1502460000 2.1369780000
C -2.3337560000 -0.0182090000 2.3291730000
N -2.0121730000 -0.1353110000 3.4421130000
C -3.3825640000 -2.0876180000 0.0946200000
N -4.2152670000 -2.9029550000 0.1445180000
C -1.3028560000 -2.3378420000 -1.5842860000
N -1.4157850000 -3.2714460000 -2.2697700000
C 1.0096430000 1.2013560000 2.8886900000
H 0.9915450000 2.1857860000 3.3639210000
H 2.0336170000 0.8535500000 2.7377500000
H 0.4373560000 0.4833900000 3.4793820000
Br -0.6577410000 0.5276940000 -2.0182010000
I 1.1698920000 -2.2686180000 1.8608780000
Br 1.8250430000 -2.2495600000 -1.6068240000
Br -4.1831440000 1.2961180000 -1.1687580000

PRODUCT B (5)

H -2.5405510000 3.9963880000 0.2957960000
C -2.5052390000 2.9174340000 0.1908360000
H -4.6294940000 2.6229530000 0.1112750000
C -3.6436860000 2.1637520000 0.0901410000
N -1.1143850000 0.9661430000 0.0260820000
C -3.5400240000 0.7613510000 -0.0439030000
C -1.2553440000 2.2766490000 0.1522830000
C -2.2410910000 0.1835750000 -0.0677840000
C -4.6759240000 -0.0745280000 -0.1536420000
H -0.3339980000 2.8513360000 0.2210060000
C -4.5383620000 -1.4328260000 -0.2875780000
H -5.6608650000 0.3862420000 -0.1335890000
H -5.4125690000 -2.0703440000 -0.3768560000
C -3.2536670000 -2.0097580000 -0.3133720000
H -3.1447590000 -3.0864150000 -0.4272310000
C -2.1331630000 -1.2197440000 -0.1938910000
S -0.5082650000 -1.9709730000 -0.2148820000
C -0.4400750000 -2.6145810000 1.4940020000
H -0.6225290000 -1.8059850000 2.2048580000
H 0.5633220000 -3.0249670000 1.6304380000
H -1.1879910000 -3.4047700000 1.5961310000

Pd 0.7586970000 -0.0126740000 -0.0700330000
Br 2.1432620000 2.0591340000 0.0596260000
Br 2.8099320000 -1.3967570000 -0.1695510000

PdBr(TMQ)C₄(CN)₄Br (*Ib*) + ICl (Fig. S2 ESI)

INTERMEDIATE *In_a*

H -5.9328960000 -2.9024690000 1.5733370000
C -5.2392760000 -2.2249060000 1.0855560000
H -6.6475150000 -1.5533790000 -0.3839910000
C -5.6342510000 -1.4806160000 0.0034900000
C -3.0231400000 -1.2663710000 0.9714320000
C -4.7298660000 -0.6021740000 -0.6359470000
C -3.9192210000 -2.1277870000 1.5648590000
C -3.4018760000 -0.4816980000 -0.1432800000
C -5.0978370000 0.1776640000 -1.7551330000
H -3.6111540000 -2.7470070000 2.4040330000
C -4.1829180000 1.0186960000 -2.3313970000
H -6.1101270000 0.0974360000 -2.1444370000
H -4.4286300000 1.6313990000 -3.1916830000
C -2.8921120000 1.0927320000 -1.7837830000
H -2.1435730000 1.7602880000 -2.2080350000
N -2.5205300000 0.3778270000 -0.7372690000
S -1.3296160000 -1.2363530000 1.5520560000
Pd -0.6051990000 0.6468750000 0.2187280000
C 1.1390940000 0.9970940000 1.2823000000
C 3.4838350000 -1.3183550000 -0.0439020000
C 2.2556620000 0.2459070000 1.4572900000
C 2.5516650000 -1.1073120000 0.9153360000
C 3.7881850000 -2.6229500000 -0.5225210000
N 4.0249560000 -3.6850850000 -0.9333410000
C 1.9025500000 -2.2232350000 1.5227460000
N 1.3660000000 -3.1162380000 2.0418270000
C 3.3301190000 0.7550900000 2.2644080000
N 4.2228610000 1.1331250000 2.9081680000
C 1.1592350000 2.2693180000 1.9283920000
N 1.2426650000 3.2985540000 2.4680330000
C -1.5236000000 -0.6730610000 3.2691000000
H -2.0258120000 -1.4702920000 3.8230700000
H -2.0863300000 0.2618910000 3.2982710000
H -0.5148840000 -0.5373350000 3.6692900000
Br 0.2898770000 2.4528250000 -1.2798790000
Br 4.3537990000 0.0944510000 -0.9261710000
Cl -1.8546450000 2.2318230000 1.5832570000
I 0.2540590000 -1.1365330000 -1.6219520000

TS A

H -4.3270000000 -4.3470000000 -1.6350000000
C -4.0000000000 -3.4150000000 -1.1890000000

H -5.8350000000 -2.3840000000 -1.5770000000
C -4.8340000000 -2.3270000000 -1.1620000000
C -2.2680000000 -2.1710000000 -0.0340000000
C -4.4050000000 -1.1080000000 -0.5890000000
C -2.7190000000 -3.3390000000 -0.6070000000
C -3.0850000000 -1.0120000000 -0.0600000000
C -5.2360000000 0.0300000000 -0.5030000000
H -2.0830000000 -4.2170000000 -0.5890000000
C -4.7640000000 1.1740000000 0.0870000000
H -6.2450000000 -0.0210000000 -0.8990000000
H -5.3800000000 2.0580000000 0.1910000000
C -3.4320000000 1.2060000000 0.5330000000
H -3.0080000000 2.1040000000 0.9660000000
N -2.6190000000 0.1710000000 0.4300000000
S -0.7070000000 -2.1660000000 0.8350000000
P -0.5010000000 0.5500000000 0.7800000000
C 1.3860000000 1.1080000000 1.2370000000
C 3.2650000000 -1.5440000000 -0.2250000000
C 2.5480000000 0.4100000000 1.1940000000
C 2.6740000000 -1.0420000000 0.8880000000
C 3.4110000000 -2.9350000000 -0.4560000000
N 3.5250000000 -4.0700000000 -0.6760000000
C 2.2670000000 -1.9450000000 1.9100000000
N 1.9570000000 -2.6560000000 2.7770000000
C 3.7940000000 1.0370000000 1.5060000000
N 4.8330000000 1.4980000000 1.7490000000
C 1.4320000000 2.4760000000 1.6000000000
N 1.4480000000 3.6080000000 1.8750000000
C -1.2860000000 -2.5770000000 2.5180000000
H -1.8620000000 -3.5010000000 2.4790000000
H -1.8670000000 -1.7490000000 2.9210000000
H -0.3840000000 -2.7210000000 3.1130000000
Br -0.8330000000 2.9310000000 -0.8810000000
Br 3.9620000000 -0.4430000000 -1.5840000000
Cl -1.0090000000 0.9620000000 3.0610000000
I 0.0090000000 0.5030000000 -1.9420000000

TS B

H -3.0180000000 -5.2980000000 -0.6250000000
C -3.0420000000 -4.2250000000 -0.4740000000
H -4.9810000000 -3.9760000000 -1.3420000000
C -4.1300000000 -3.4920000000 -0.8760000000
C -1.9540000000 -2.2300000000 0.3520000000
C -4.1610000000 -2.0910000000 -0.6910000000
C -1.9490000000 -3.5920000000 0.1500000000
C -3.0450000000 -1.4400000000 -0.0910000000
C -5.2570000000 -1.2830000000 -1.0740000000
H -1.1020000000 -4.1810000000 0.4840000000
C -5.2070000000 0.0690000000 -0.8630000000
H -6.1250000000 -1.7490000000 -1.5290000000
H -6.0310000000 0.7170000000 -1.1360000000

C -4.0430000000 0.6320000000 -0.3020000000
H -3.9420000000 1.7040000000 -0.1710000000
N -3.0030000000 -0.0910000000 0.0600000000
S -0.5970000000 -1.4830000000 1.2490000000
P -0.8120000000 0.8390000000 0.4660000000
C 1.4340000000 1.3380000000 0.0240000000
C 3.3100000000 -1.5310000000 0.1600000000
C 2.4480000000 0.7580000000 0.7520000000
C 2.6690000000 -0.6890000000 1.0090000000
C 3.4920000000 -2.9090000000 0.4410000000
N 3.6290000000 -4.0450000000 0.6410000000
C 2.3180000000 -1.1660000000 2.3070000000
N 2.0310000000 -1.5070000000 3.3810000000
C 3.4030000000 1.5820000000 1.4060000000
N 4.2260000000 2.1880000000 1.9640000000
C 1.5660000000 2.7270000000 -0.2450000000
N 1.7700000000 3.8440000000 -0.4910000000
C -1.2500000000 -1.5680000000 2.9500000000
H -1.4750000000 -2.6150000000 3.1550000000
H -2.1260000000 -0.9300000000 3.0440000000
H -0.4550000000 -1.2160000000 3.6050000000
Br -1.5850000000 3.0310000000 -0.3530000000
Br 4.0670000000 -0.9530000000 -1.4650000000
Cl -1.0480000000 1.6590000000 2.6670000000
I 0.5080000000 0.2580000000 -1.8320000000

TS C

H -6.5720000000 -0.6250000000 2.4680000000
C -5.7780000000 -0.5430000000 1.7350000000
H -7.0090000000 -1.1160000000 0.0810000000
C -6.0210000000 -0.8150000000 0.4130000000
C -3.4540000000 -0.0450000000 1.2540000000
C -4.9830000000 -0.7180000000 -0.5390000000
C -4.4890000000 -0.1690000000 2.1550000000
C -3.6750000000 -0.3260000000 -0.1250000000
C -5.1830000000 -1.0030000000 -1.9080000000
H -4.3090000000 0.0170000000 3.2080000000
C -4.1380000000 -0.8960000000 -2.7880000000
H -6.1690000000 -1.3070000000 -2.2440000000
H -4.2570000000 -1.1080000000 -3.8440000000
C -2.8830000000 -0.4970000000 -2.2970000000
H -2.0330000000 -0.3940000000 -2.9630000000
N -2.6680000000 -0.2290000000 -1.0280000000
S -1.8310000000 0.4010000000 1.8620000000
P -0.6450000000 0.5520000000 -0.2880000000
C 1.3840000000 1.4940000000 0.1030000000
C 3.6930000000 -1.0080000000 0.4120000000
C 2.2450000000 0.9540000000 1.0430000000
C 2.7280000000 -0.4410000000 1.1800000000
C 4.1240000000 -2.3440000000 0.5960000000
N 4.4860000000 -3.4410000000 0.7200000000

C 2.2700000000 -1.1370000000 2.3410000000
N 1.9080000000 -1.6260000000 3.3310000000
C 2.6760000000 1.7950000000 2.1050000000
N 3.0450000000 2.4300000000 3.0090000000
C 1.2600000000 2.9140000000 0.1130000000
N 1.2510000000 4.0750000000 0.1480000000
C -2.1160000000 2.1030000000 2.4600000000
H -2.8730000000 2.0700000000 3.2440000000
H -2.4080000000 2.7500000000 1.6350000000
H -1.1670000000 2.4350000000 2.8820000000
Br 1.2980000000 0.8230000000 -1.9050000000
Br 4.6090000000 -0.0720000000 -0.9440000000
Cl -1.6070000000 2.6570000000 -0.8280000000
I -0.1100000000 -2.0820000000 -0.0010000000

TSD

H -2.9370000000 -5.2050000000 -0.7560000000
C -2.9310000000 -4.1650000000 -0.4520000000
H -5.0240000000 -3.8800000000 -0.7820000000
C -4.0880000000 -3.4290000000 -0.4690000000
C -1.6900000000 -2.2580000000 0.3550000000
C -4.0830000000 -2.0680000000 -0.0860000000
C -1.7210000000 -3.5790000000 -0.0260000000
C -2.8590000000 -1.4610000000 0.3080000000
C -5.2420000000 -1.2600000000 -0.0780000000
H -0.8130000000 -4.1710000000 0.0060000000
C -5.1470000000 0.0540000000 0.3010000000
H -6.1920000000 -1.6910000000 -0.3750000000
H -6.0150000000 0.7020000000 0.3240000000
C -3.8850000000 0.5800000000 0.6350000000
H -3.7680000000 1.6300000000 0.8790000000
N -2.7820000000 -0.1420000000 0.6310000000
S -0.1840000000 -1.5660000000 1.0230000000
P -0.5850000000 0.8110000000 0.4490000000
C 1.3840000000 1.6860000000 0.6900000000
C 3.3780000000 -1.4060000000 0.2490000000
C 2.5470000000 0.9570000000 0.5130000000
C 2.8440000000 -0.3990000000 0.9990000000
C 3.7290000000 -2.6580000000 0.8090000000
N 3.9970000000 -3.7050000000 1.2380000000
C 2.6930000000 -0.6600000000 2.3950000000
N 2.5790000000 -0.8820000000 3.5300000000
C 3.6260000000 1.5940000000 -0.1630000000
N 4.5400000000 2.0750000000 -0.6980000000
C 1.4410000000 3.0620000000 0.3360000000
N 1.5780000000 4.1850000000 0.0730000000
C -0.6190000000 -1.6610000000 2.8010000000
H -0.8110000000 -2.7090000000 3.0310000000
H -1.4970000000 -1.0490000000 3.0040000000
H 0.2390000000 -1.3050000000 3.3680000000
Br -1.6190000000 2.9550000000 -0.2070000000

Br 3.6560000000 -1.2940000000 -1.6070000000
Cl 0.3840000000 1.6550000000 2.5700000000
I -0.5060000000 0.2050000000 -2.1510000000

TSE

H -5.5490000000 -4.0310000000 0.7070000000
C -4.9080000000 -3.2240000000 0.3710000000
H -6.3360000000 -2.4210000000 -1.0060000000
C -5.3440000000 -2.3340000000 -0.5770000000
C -2.7640000000 -2.0950000000 0.4990000000
C -4.5030000000 -1.2910000000 -1.0200000000
C -3.6060000000 -3.1150000000 0.8910000000
C -3.2000000000 -1.1430000000 -0.4570000000
C -4.9060000000 -0.3740000000 -2.0160000000
H -3.2530000000 -3.8590000000 1.5960000000
C -4.0460000000 0.6110000000 -2.4170000000
H -5.8940000000 -0.4700000000 -2.4540000000
H -4.3110000000 1.3250000000 -3.1860000000
C -2.7890000000 0.7080000000 -1.7970000000
H -2.0930000000 1.4860000000 -2.0800000000
N -2.3870000000 -0.1150000000 -0.8450000000
S -1.0700000000 -2.0880000000 1.0680000000
P -0.5460000000 0.3370000000 0.2360000000
C 1.1730000000 0.8020000000 1.2230000000
C 3.7160000000 -1.3430000000 -0.1780000000
C 2.3690000000 0.1590000000 1.3340000000
C 2.7370000000 -1.1590000000 0.7430000000
C 4.0920000000 -2.6280000000 -0.6430000000
N 4.4100000000 -3.6710000000 -1.0440000000
C 2.1450000000 -2.3030000000 1.3460000000
N 1.6690000000 -3.2010000000 1.9130000000
C 3.4140000000 0.7120000000 2.1390000000
N 4.2910000000 1.1100000000 2.7900000000
C 1.0760000000 2.0410000000 1.9080000000
N 0.9930000000 3.0530000000 2.4780000000
C -1.2850000000 -1.9020000000 2.8560000000
H -2.0140000000 -2.6230000000 3.2250000000
H -1.6160000000 -0.8830000000 3.0910000000
H -0.3100000000 -2.1050000000 3.2970000000
Br -1.7490000000 3.1230000000 0.3390000000
Br 4.6860000000 0.0790000000 -0.9340000000
Cl -2.0710000000 1.3140000000 2.0720000000
I 0.8100000000 0.4550000000 -2.0350000000

PRODUCT A (*If*)

H -6.1161520000 -0.0140620000 2.7210110000
C -5.3557540000 -0.1581320000 1.9594800000
H -6.3945480000 -1.7539930000 0.9774390000
C -5.5092970000 -1.1224610000 0.9958070000
C -3.2323880000 0.4917080000 1.0092800000

C -4.5170520000 -1.3205550000 0.0068120000
C -4.2075920000 0.6595310000 1.9649950000
C -3.3489180000 -0.5127770000 0.0197870000
C -4.6333220000 -2.2997080000 -1.0051840000
H -4.0925590000 1.4303880000 2.7241740000
C -3.6314410000 -2.4433660000 -1.9291350000
H -5.5212320000 -2.9274370000 -1.0345160000
H -3.6882570000 -3.1809080000 -2.7223830000
C -2.4949150000 -1.6222110000 -1.8333290000
H -1.6654870000 -1.7276540000 -2.5303930000
N -2.3501850000 -0.6973890000 -0.8985690000
S -1.8169260000 1.5931530000 0.9923550000
Pd -0.5530760000 0.4389250000 -0.6236070000
C 1.0845250000 1.5223560000 -0.2585520000
C 3.2554910000 -1.1446610000 0.8833030000
C 2.1893100000 1.0863640000 0.4001860000
C 2.2356080000 -0.2581610000 1.0097360000
C 3.2428810000 -2.4065880000 1.5400770000
N 3.2455160000 -3.4430070000 2.0686530000
C 1.1021660000 -0.6494290000 1.7942360000
N 0.1854020000 -0.9615230000 2.4404450000
C 3.3300610000 1.9356890000 0.5612160000
N 4.2373600000 2.6517420000 0.7002860000
C 1.0309810000 2.8244800000 -0.8171880000
N 0.8915020000 3.8849060000 -1.2850140000
C -2.5172890000 2.9727280000 0.0159740000
H -3.2800020000 3.4682910000 0.6213970000
H -2.9404690000 2.5900550000 -0.9154920000
H -1.6980260000 3.6651640000 -0.1953260000
Br 4.7452290000 -0.8503240000 -0.2306820000
Cl 0.7188550000 -0.7553810000 -2.2264370000

PRODUCT B (7)

H -5.4436680000 -1.3093010000 -0.2106070000
C -4.4710360000 -0.8286530000 -0.1681330000
H -5.2625040000 1.1552570000 0.0091070000
C -4.3715070000 0.5341870000 -0.0466030000
C -2.0629430000 -1.0241210000 -0.1898210000
C -3.1069970000 1.1665010000 0.0025300000
C -3.3050140000 -1.6138870000 -0.2493900000
C -1.9271130000 0.3768260000 -0.0671250000
C -2.9677240000 2.5671940000 0.1207760000
H -3.3852960000 -2.6932150000 -0.3606810000
C -1.7155200000 3.1186740000 0.1632500000
H -3.8601010000 3.1865410000 0.1746790000
H -1.5635040000 4.1888350000 0.2526400000
C -0.5941140000 2.2763840000 0.0891910000
H 0.4124680000 2.6868350000 0.1217890000
N -0.6804860000 0.9589190000 -0.0208120000
S -0.5884820000 -2.0297610000 -0.3078970000
Pd 0.9829530000 -0.3122950000 -0.1217760000

C -0.5577240000 -2.7621770000 1.3649250000
H -1.3788630000 -3.4784330000 1.4466400000
H -0.6432040000 -1.9749520000 2.1167410000
H 0.4028240000 -3.2750240000 1.4544610000
Br 2.7094980000 1.4793340000 0.0889610000
Cl 2.6665190000 -1.9411450000 -0.2095460000

PRODUCT C (8)

H -5.8711140000 -0.6631550000 -0.1644560000
C -4.8418470000 -0.3188940000 -0.1363090000
H -5.3506630000 1.7575250000 0.0284620000
C -4.5552520000 1.0181780000 -0.0304300000
C -2.4806850000 -0.8395380000 -0.1763830000
C -3.2164540000 1.4719770000 0.0006430000
C -3.7929450000 -1.2540770000 -0.2208410000
C -2.1522210000 0.5310220000 -0.0671790000
C -2.8949940000 2.8436830000 0.0966880000
H -4.0190160000 -2.3134430000 -0.3246080000
C -1.5812400000 3.2258580000 0.1194160000
H -3.6985510000 3.5748060000 0.1493730000
H -1.2868000000 4.2675100000 0.1882070000
C -0.5826720000 2.2406580000 0.0527730000
H 0.4672330000 2.5223400000 0.0722230000
N -0.8376670000 0.9425660000 -0.0332140000
S -1.1673720000 -2.0452110000 -0.2997150000
Pd 0.6475770000 -0.5516560000 -0.1338370000
C -1.2346330000 -2.7603300000 1.3798100000
H -2.1802240000 -3.2967370000 1.4908100000
H -1.1405370000 -1.9687910000 2.1262160000
H -0.3960250000 -3.4566400000 1.4529960000
Cl 2.0881000000 -2.4012110000 -0.2466620000
I 2.7684670000 1.0367460000 0.0801760000

PRODUCT E (1e')

H -6.1559480000 2.0912450000 2.2855920000
C -5.4242000000 1.4657480000 1.7835720000
H -6.5277060000 -0.3512990000 2.0528010000
C -5.6290090000 0.1158400000 1.6563830000
C -3.3164060000 1.2776790000 0.6133930000
C -4.6747800000 -0.7032220000 1.0080620000
C -4.2575360000 2.0514300000 1.2533400000
C -3.4859860000 -0.1227090000 0.4875710000
C -4.8595940000 -2.0949360000 0.8535060000
H -4.0994170000 3.1241380000 1.3419250000
C -3.9022540000 -2.8368150000 0.2144050000
H -5.7639990000 -2.5554440000 1.2451460000
H -4.0078740000 -3.9067610000 0.0711040000
C -2.7446290000 -2.1925920000 -0.2532190000
H -1.9579040000 -2.7640480000 -0.7424200000
N -2.5282200000 -0.8928570000 -0.1229810000

S -1.8858130000 2.0764660000 -0.1057170000
 Pd -0.6729070000 0.0945080000 -0.6500170000
 C 0.9739660000 1.1478700000 -1.0417130000
 C 3.1534290000 0.1267020000 1.6809840000
 C 2.0275870000 1.3571830000 -0.2067730000
 C 2.0760830000 0.7498920000 1.1366480000
 C 3.1324250000 -0.3892200000 3.0068360000
 N 3.1288040000 -0.8169480000 4.0888510000
 C 0.8849730000 0.8178390000 1.9312070000
 N -0.0708610000 0.8819250000 2.5930010000
 C 3.1104510000 2.2037970000 -0.6039940000
 N 3.9632400000 2.9203660000 -0.9429580000
 C 0.9418230000 1.7417120000 -2.3307150000
 N 0.8233970000 2.2115550000 -3.3927500000
 C -2.5796680000 2.5486740000 -1.7313920000
 H -3.3208800000 3.3366580000 -1.5777980000
 H -3.0278830000 1.6754510000 -2.2110610000
 H -1.7496830000 2.9257460000 -2.3350880000
 I 0.7839200000 -2.0402910000 -1.2595880000
 Br 4.7547340000 -0.1922450000 0.7402710000

DIHALOBUTADIENES:

DIBD

C	1.521000	1.171000	0.000000
C	0.227000	0.695000	0.000000
C	-0.227000	-0.695000	0.000000
C	-1.521000	-1.171000	0.000000
C	-1.753000	-2.570000	0.000000
N	-2.003000	-3.706000	0.000000
C	0.739000	-1.753000	0.000000
N	1.423000	-2.691000	0.000000
C	-0.739000	1.753000	0.000000
N	-1.423000	2.691000	0.000000
C	1.753000	2.570000	0.000000
N	2.003000	3.706000	0.000000
I	-3.348000	-0.158000	0.000000
I	3.348000	0.158000	0.000000

DBBD

C	1.764000	0.736000	0.000000
C	0.393000	0.616000	0.000000
C	-0.393000	-0.616000	0.000000
C	-1.764000	-0.736000	0.000000
C	-2.381000	-2.012000	0.000000
N	-2.937000	-3.032000	0.000000
C	0.265000	-1.888000	0.000000
N	0.676000	-2.973000	0.000000

C	-0.265000	1.888000	0.000000
N	-0.676000	2.973000	0.000000
C	2.381000	2.012000	0.000000
N	2.937000	3.032000	0.000000
Br	-3.049000	0.644000	0.000000
Br	3.049000	-0.644000	0.000000

BIBD

C	2.160772	-0.634159	0.000000
C	0.792888	-0.518664	0.000000
C	0.000000	0.708422	0.000000
C	-1.369171	0.827124	0.000000
C	-1.951177	2.127636	0.000000
N	-2.468606	3.170542	0.000000
C	0.662466	1.982779	0.000000
N	1.076096	3.069422	0.000000
C	0.144070	-1.798661	0.000000
N	-0.254312	-2.890888	0.000000
C	2.768971	-1.923455	0.000000
N	3.304575	-2.956293	0.000000
Br	3.454922	0.727149	0.000000
I	-2.863763	-0.619356	0.000000

CBBD

C	1.484000	0.529000	0.000000
C	0.120000	0.711000	0.000000
C	-0.916000	-0.322000	0.000000
C	-2.278000	-0.125000	0.000000
C	-3.174000	-1.227000	0.000000
N	-3.958000	-2.085000	0.000000
C	-0.562000	-1.709000	0.000000
N	-0.395000	-2.858000	0.000000
C	-0.251000	2.094000	0.000000
N	-0.445000	3.239000	0.000000
C	2.364000	1.641000	0.000000
N	3.133000	2.512000	0.000000
Br	2.431000	-1.093000	0.000000
Cl	-3.097000	1.385000	0.000000

HALOGENS AND INTERHALOGENS:

Br₂

Br	0.000	0.000	1.156
Br	0.000	0.000	-1.156

I₂

I	0.000	0.000	1.356
I	0.000	0.000	-1.356

ICI

Cl	0.000	0.000	-1.782
I	0.000	0.000	0.572

IBr

I	0.000	0.000	0.996
Br	0.000	0.000	-1.508

BrCl

Cl	0.000	0.000	-1.457
Br	0.000	0.000	0.708