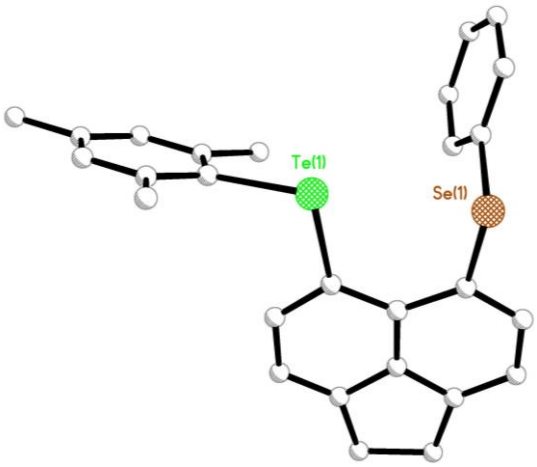
Appendix 2 - Crystal Structures Determined During PhD Studies, Not Discussed in This Thesis

MWS9-FS-3

$P2_1/c$

a = 9.7619(7) Å
b = 30.047(2) Å
c = 8.084(2) Å
β = 113.571(8)°
V = 2173.2(5) $Å^3$

R_1 = 0.0213

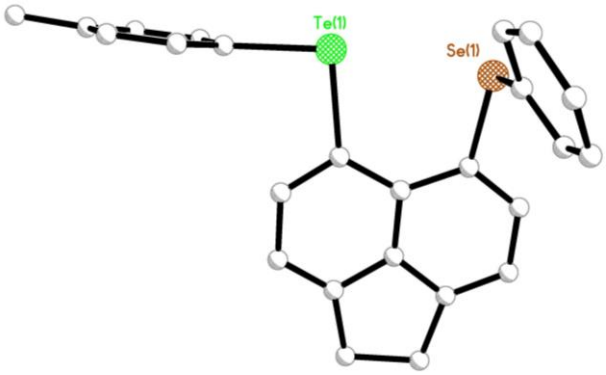


MWS10-FS

P-1

a = 10.854(2) Å
b = 12.244(2) Å
c = 17.599(2) Å
α = 106.370(8)°
β = 92.585(7)°
γ = 114.888(8)°
V = 1999.4(5) $Å^3$

R_1 = 0.0343

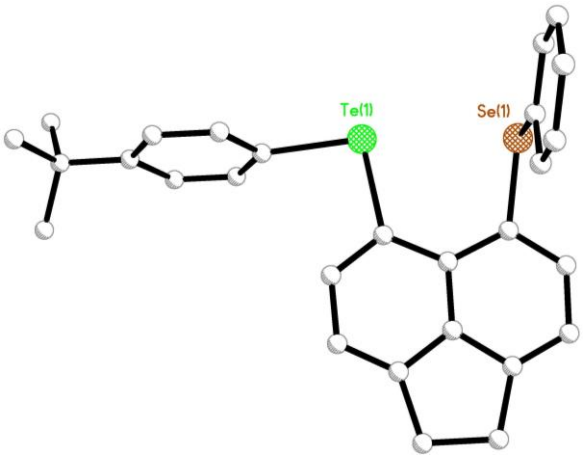


MWS11-FS

P-1

a = 9.656(1) Å
b = 10.492(2) Å
c = 12.795(2) Å
α = 79.476(6)°
β = 73.922(6)°
γ = 70.177(5)°
V = 1166.2(3) $Å^3$

R_1 = 0.0239

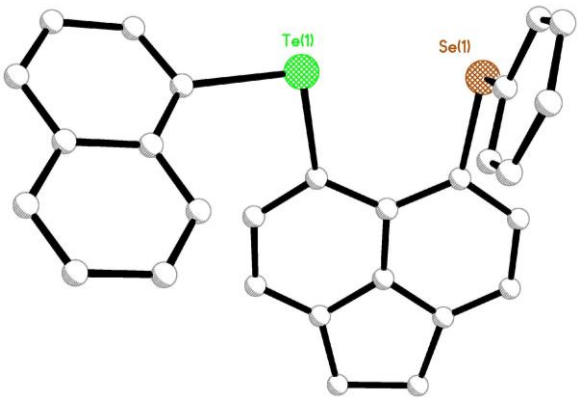


MWS17-2FS

C2/c

a = 29.375(3) Å
b = 7.6824(8) Å
c = 19.044(2) Å
β = 95.737(7)°
V = 4276.1(8) Å^3

R_1 = 0.0248

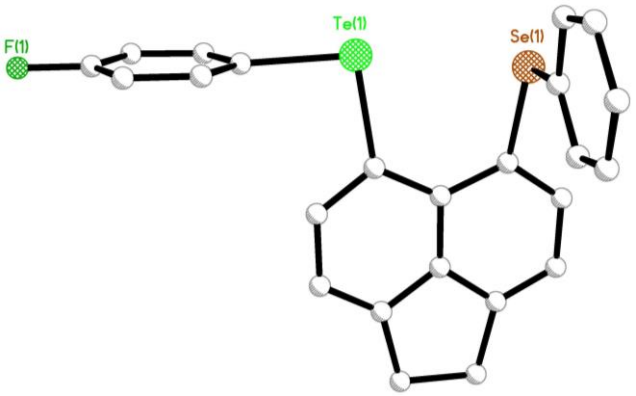


MWS20-B-FS

$P2_1/c$

a = 9.8746(9) Å
b = 22.045(2) Å
c = 9.7763(8) Å
β = 116.385(8)°
V = 1906.4(4) Å^3

R_1 = 0.0178

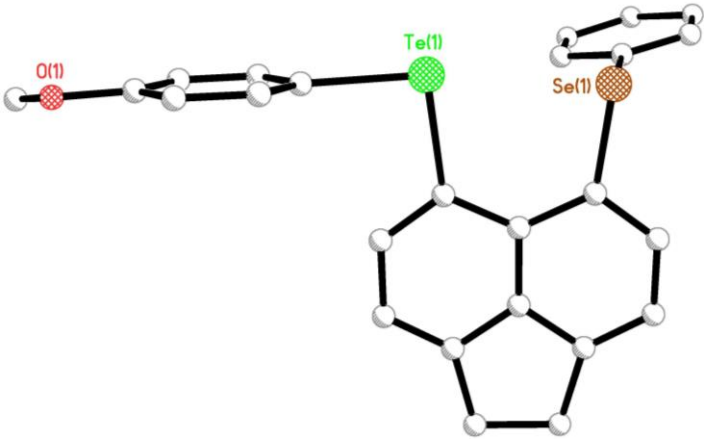


MWS21-FS

$P2_1/n$

a = 8.212(5) Å
b = 11.442(2) Å
c = 22.113(3) Å
β = 99.96(4)°
V = 2046(2) Å^3

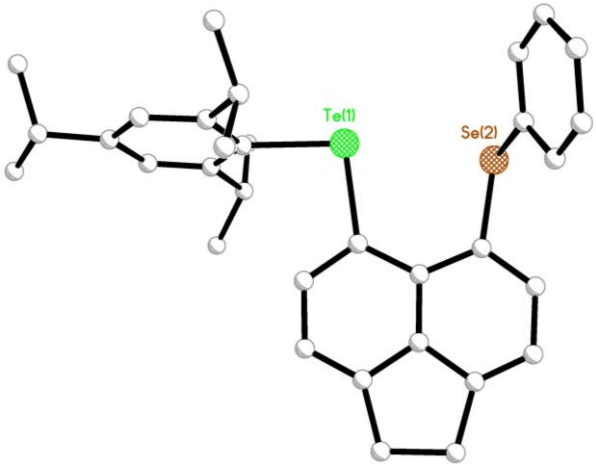
R_1 = 0.0667



MWS23-FS
$P2_1/n$

a = 14.697(2) Å
b = 14.367(2) Å
c = 14.835(2) Å
β = 119.048(9)°
V = 2738.6(5) Å^3

R_1 = 0.0284

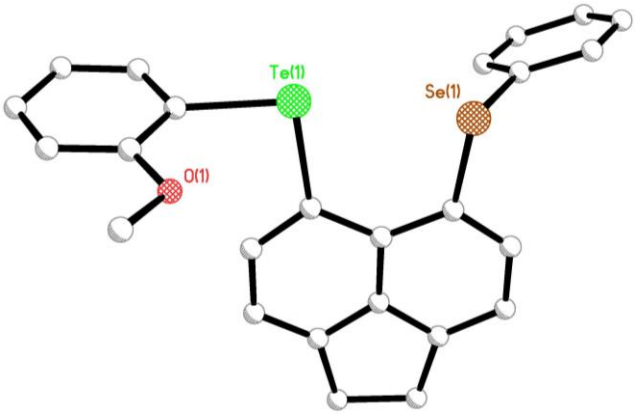


MWS24-2

P-1

a = 8.645(4) Å
b = 14.625(7) Å
c = 17.253(9) Å
α = 109.466(12)°
β = 97.975(10)°
γ = 93.276(6)°
V = 2024(2) Å^3

R_1 = 0.0655

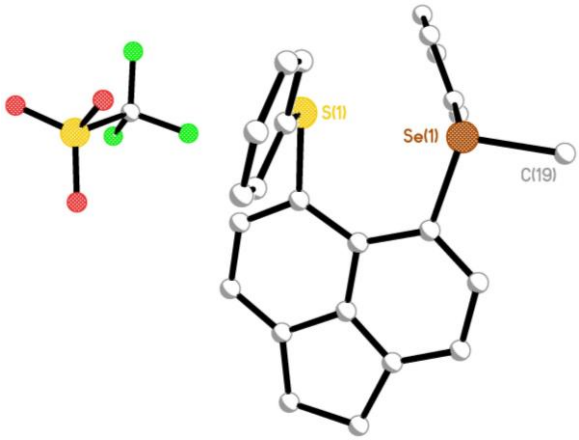


Ferg105-2

P-1

a = 10.549(5) Å
b = 12.528(5) Å
c = 19.099(8) Å
α = 78.09(3)°
β = 88.67(3)°
γ = 79.24(3)°
V = 2426(2) Å^3

R_1 = 0.1001

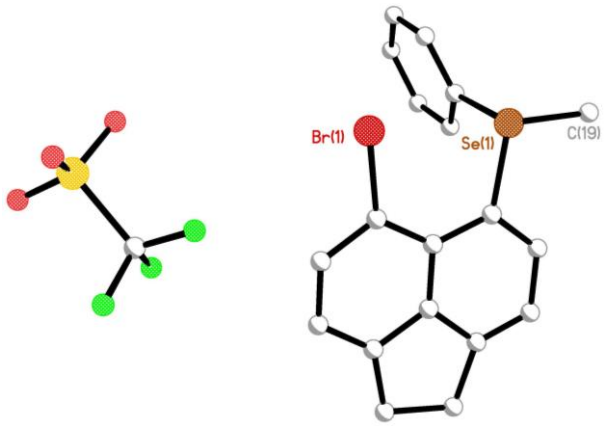


Ferg106-3

P-1

a = 7.898(6) Å
b = 11.451(10) Å
c = 12.050(10) Å
α = 106.39(2)°
β = 93.18(2)°
γ = 96.52(2)°
V = 1034(2) Å^3

R_1 = 0.0871

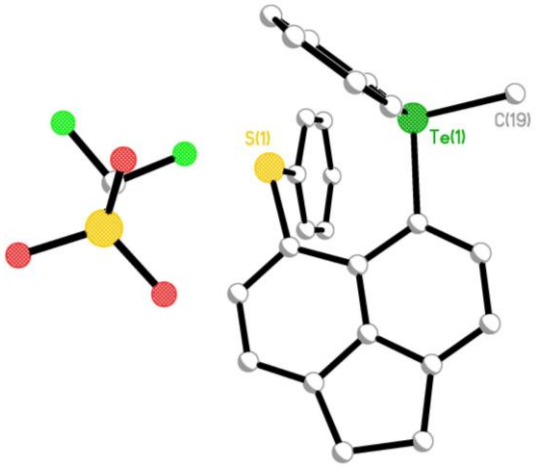


Ferg107_off

P-1

a = 10.117(10) Å
b = 11.322(13) Å
c = 12.210(11) Å
α = 76.31(3)°
β = 67.36(3)°
γ = 84.70(4)°
V = 1254(3) Å^3

R_1 = 0.0651

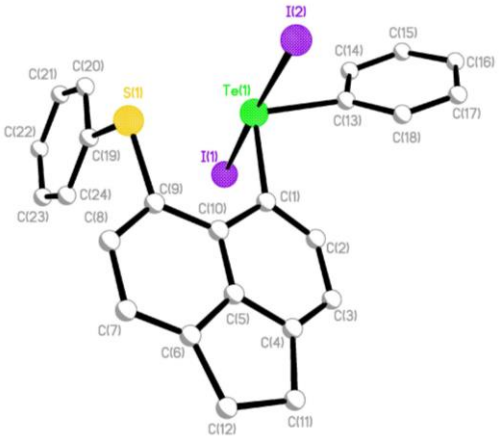


Ferg-108

$P2_1/n$

a = 11.129(6) Å
b = 16.603(9) Å
c = 12.582(7) Å
β = 102.416(10)°
V = 2270(2) Å^3

R_1 = 0.0758

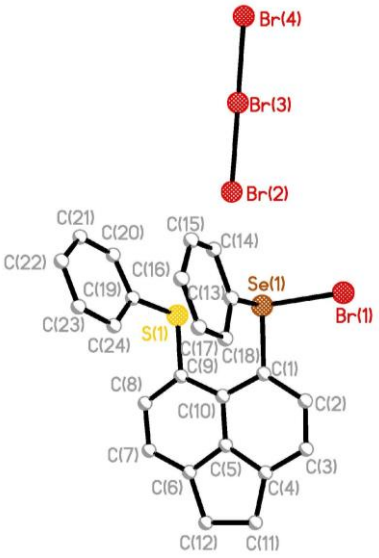


Ferg-109-3_off

P-1

a = 10.822(8) Å
b = 11.568(8) Å
c = 11.940(10) Å
α = 81.42(3)°
β = 73.07(3)°
γ = 71.07(3)°
V = 1350(2) Å^3

R_1 = 0.0866

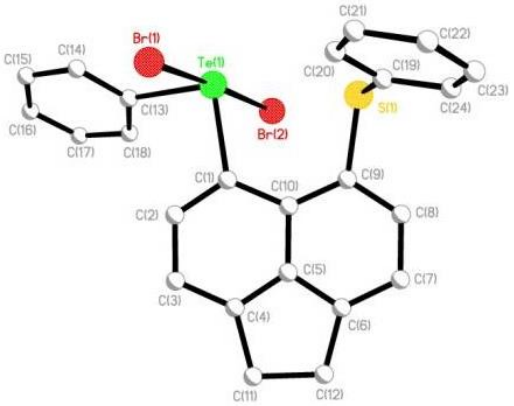


Ferg110-3

$P2_1/n$

a = 12.516(5) Å
b = 12.616(5) Å
c = 14.436(6) Å
β = 112.682(8)°
V = 2103(2) Å^3

R_1 = 0.0950

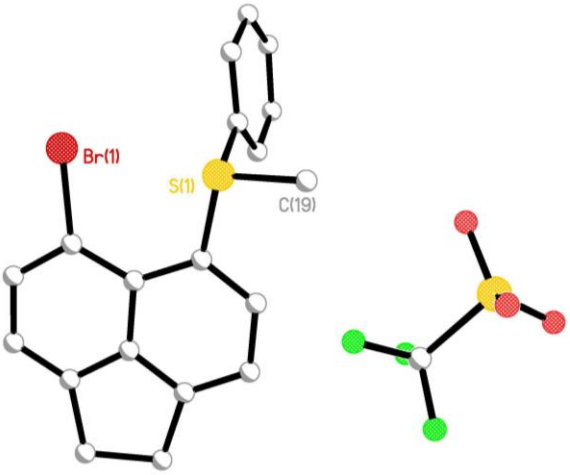


Ferg111-6

P-1

a = 8.046(7) Å
b = 10.746(10) Å
c = 14.582(12) Å
α = 96.49(3)°
β = 90.31(2)°
γ = 94.56(3)°
V = 1248(2) Å^3

R_1 = 0.0688

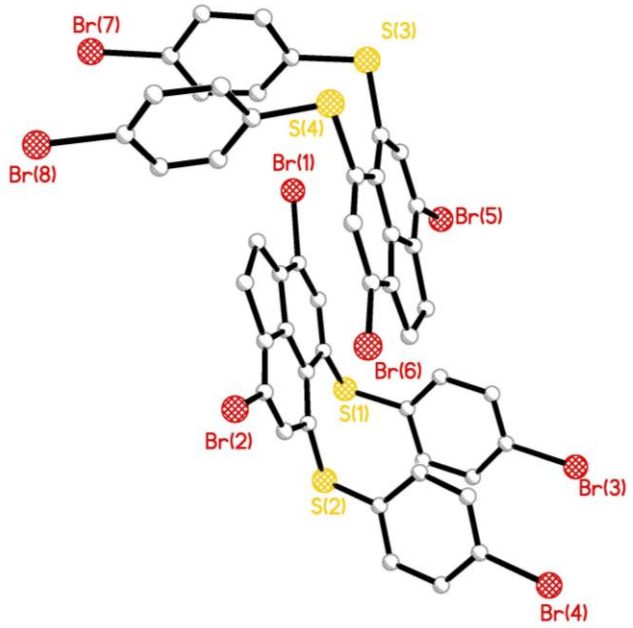


Ferg-114

P-1

a = 7.439(4) Å
b = 17.541(7) Å
c = 17.903(7) Å
α = 74.70(3)°
β = 83.12(3)°
γ = 87.06(3)°
V = 2237(2) Å^3

R_1 = 0.1362

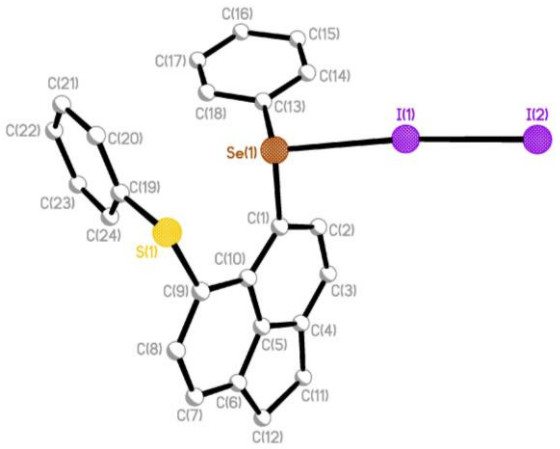


Ferg-115-B_off

P2$_1$/n

a = 9.578(4) Å
b = 8.184(3) Å
c = 28.084(10) Å
β = 96.485(9)°
V = 2187.4(13) Å^3

R_1 = 0.0411

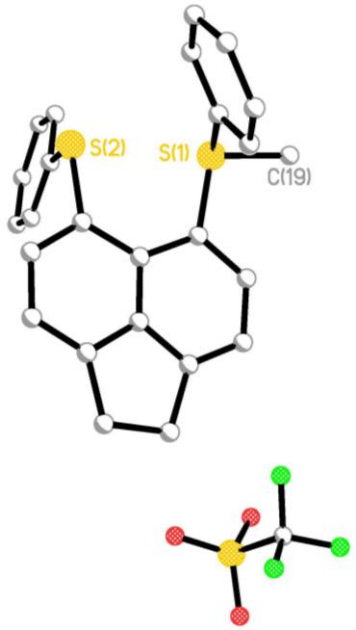


Ferg116-5

P2$_1$/n

a = 10.563(4) Å
b = 12.522(4) Å
c = 18.796(7) Å
α = 78.53(2)°
β = 88.85(3)°
γ = 79.85(3)°
V = 2398(2) Å^3

R_1 = 0.1011

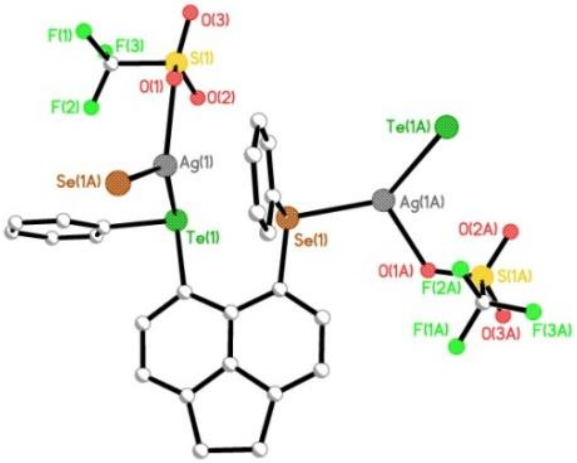


Ferg117

$P2_1/n$

a = 15.135(5) Å
b = 10.141(3) Å
c = 17.970(5) Å
β = 92.633(8)°
V = 2755(2) Å^3

R_1 = 0.0535

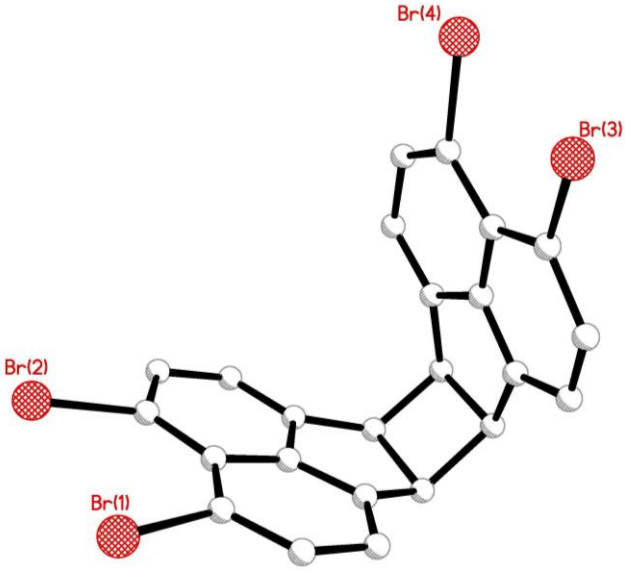


Ferg198-2

P-1

a = 9.263(5) Å
b = 9.747(5) Å
c = 10.895(7) Å
α = 83.86(5)°
β = 86.93(5)°
γ = 69.74(4)°
V = 917.5(9) Å^3

R_1 = 0.1391

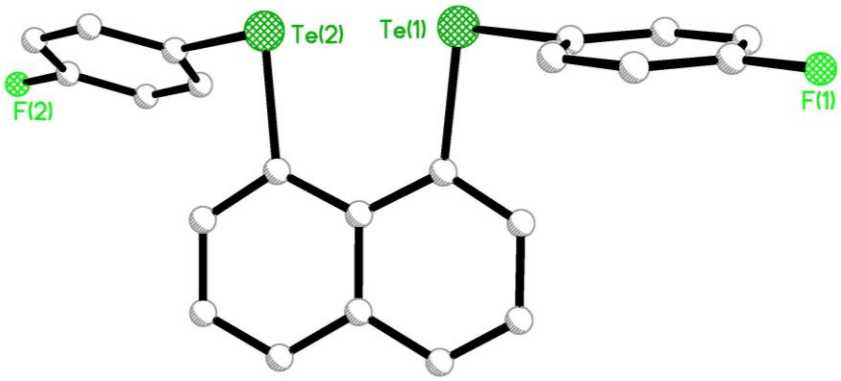


FK478-FS

$P2_1/n$

a = 7.398(2) Å
b = 14.984(3) Å
c = 17.508(3) Å
β = 98.031(7)°
V = 1921.8(6) Å^3

R_1 = 0.0360

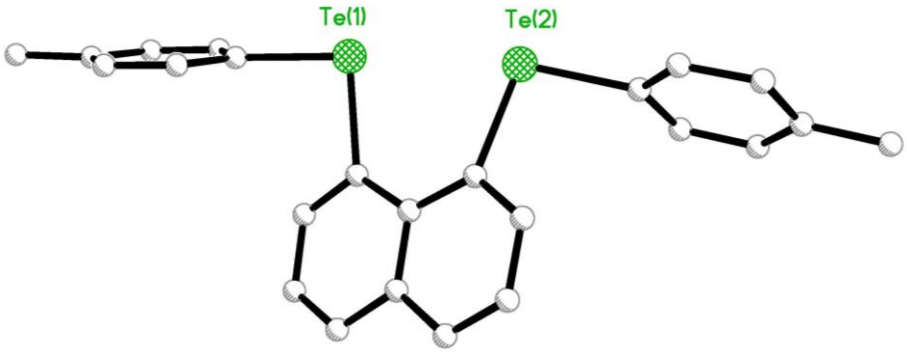


FK-374-A-FS

$P2_1/n$

a = 7.652(2) Å
b = 14.945(4) Å
c = 17.352(4) Å
β = 94.187(8)°
V = 1979.1(8) $Å^3$

R_1 = 0.0407

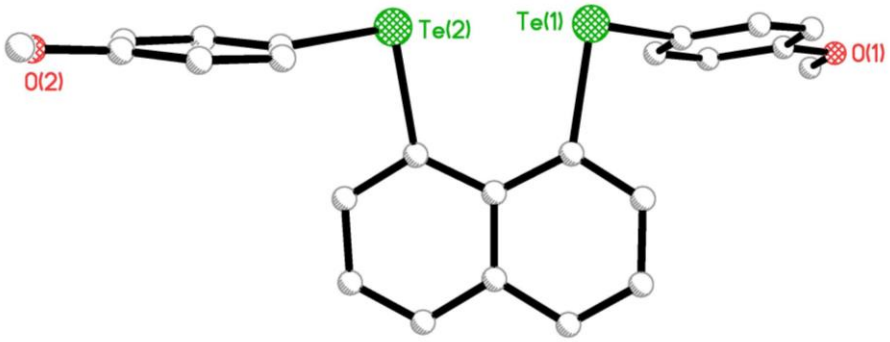


FK378-2

$P2_1/c$

a = 11.005(5) Å
b = 16.412(6) Å
c = 12.017(5) Å
β = 98.480(11)°
V = 2147(2) $Å^3$

R_1 = 0.0610

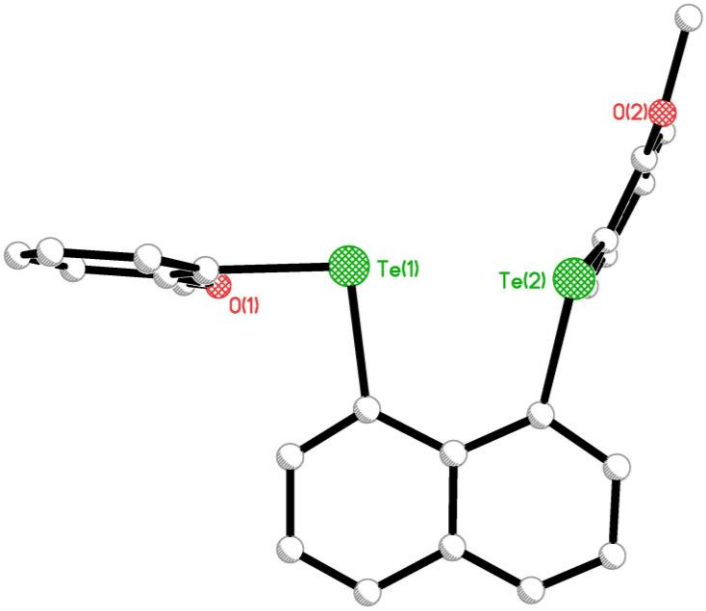


FK388-2FS

$P2_1/n$

a = 12.367(2) Å
b = 8.227(1) Å
c = 22.652(3) Å
β = 93.954(7)°
V = 2299.4(5) $Å^3$

R_1 = 0.0580

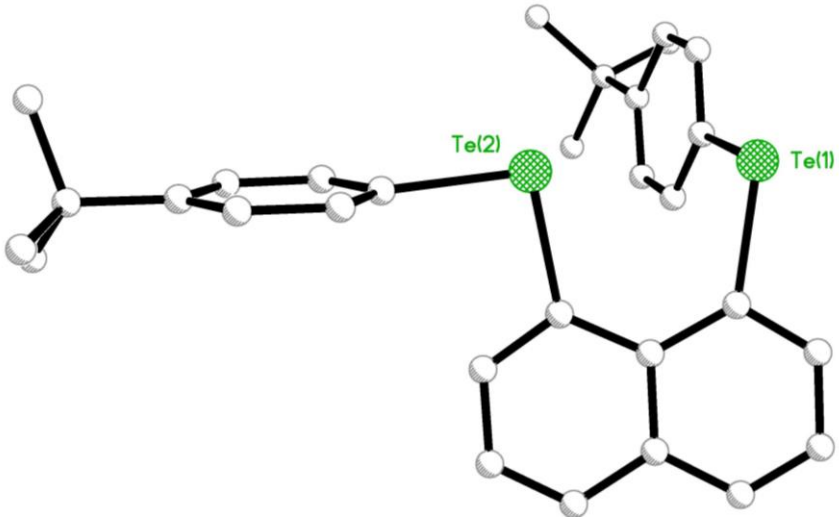


FK469-3-FS

P-1

a = 10.374(2) Å
b = 10.661(2) Å
c = 13.686(2) Å
α = 104.976(8)°
β = 99.039(7)°
γ = 110.342(8)°
V = 1319.1(4) Å^3

R_1 = 0.0222

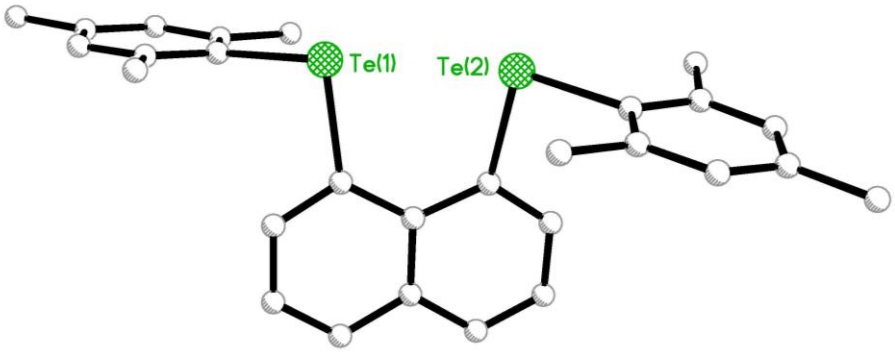


FK-374-FS

P-1

a = 8.110(2) Å
b = 9.991(2) Å
c = 15.133(3) Å
α = 79.880(7)°
β = 78.493(7)°
γ = 88.963(7)°
V = 1182.7(5) Å^3

R_1 = 0.0322

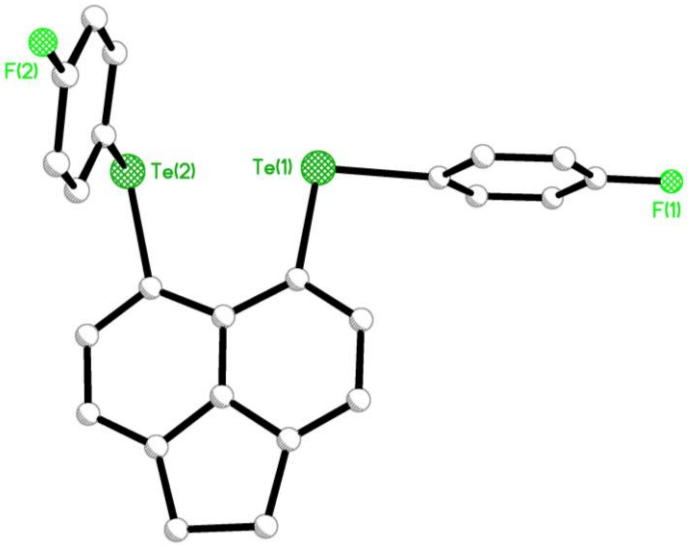


FK-479

P-1

a = 9.972(3) Å
b = 10.057(3) Å
c = 12.196(3) Å
α = 106.468(6)°
β = 97.958(4)°
γ = 115.546(4)°
V = 1009.1(5) Å^3

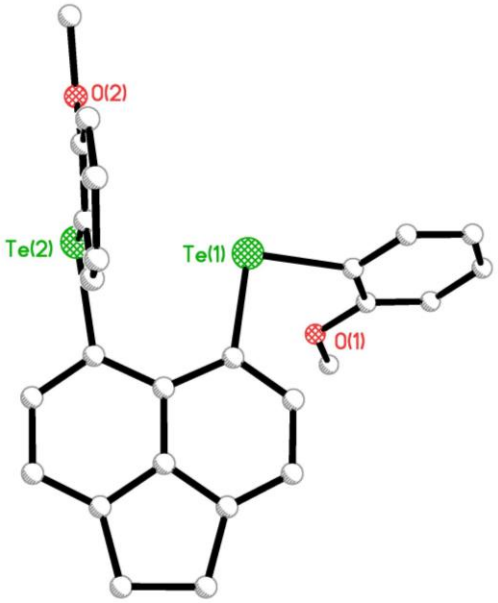
R_1 = 0.0437



FK404A
P-1

a = 8.058(2) Å
b = 12.219(3) Å
c = 13.919(3) Å
α = 109.429(8)°
β = 100.393(7)°
γ = 94.297(7)°
V = 1257.6(4) Å^3

R_1 = 0.0335

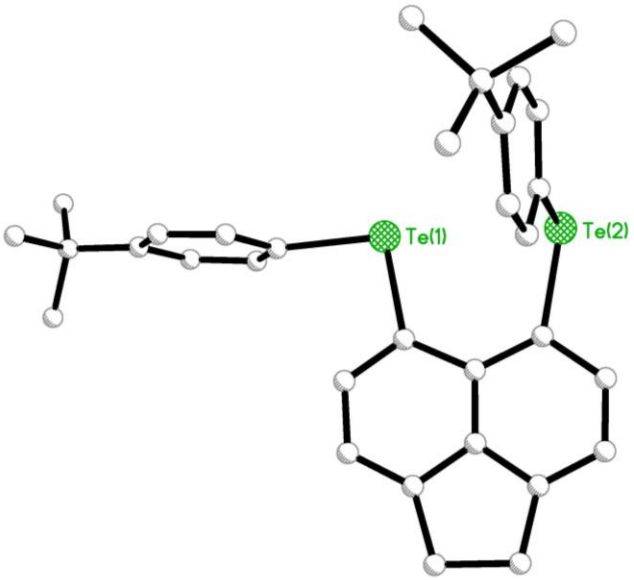


FK-464

P-1

a = 10.486(4) Å
b = 11.219(5) Å
c = 13.456(5) Å
α = 108.590(7)°
β = 101.810(8)°
γ = 100.001(6)°
V = 1419.2(10) Å^3

R_1 = 0.0650

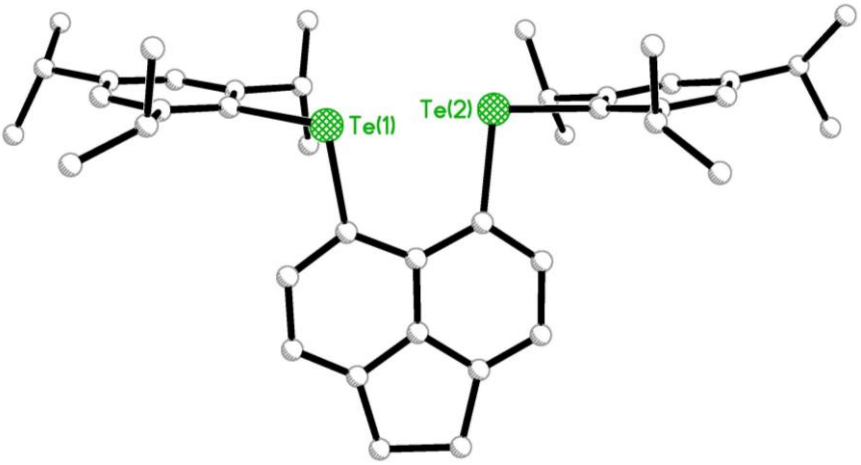


FK-391-FS_off

P-1

a = 9.9521(9) Å
b = 12.658(1) Å
c = 16.291(2) Å
α = 108.862(8)°
β = 95.632(7)°
γ = 102.253(8)°
V = 1866.6(3) Å^3

R_1 = 0.0338

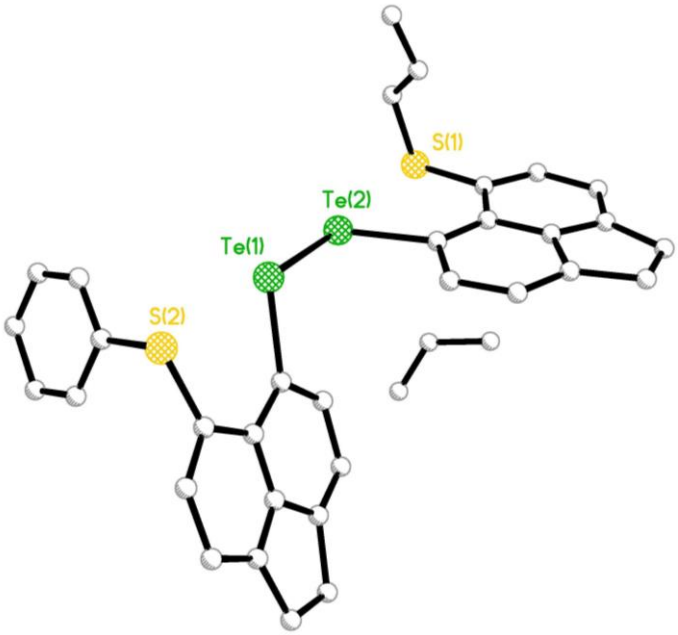


FK-448

$P2_1/c$

a = 13.052(5) Å
b = 17.927(6) Å
c = 12.823(5) Å
β = 91.692(9)°
V = 2999(2) Å^3

R_1 = 0.0883

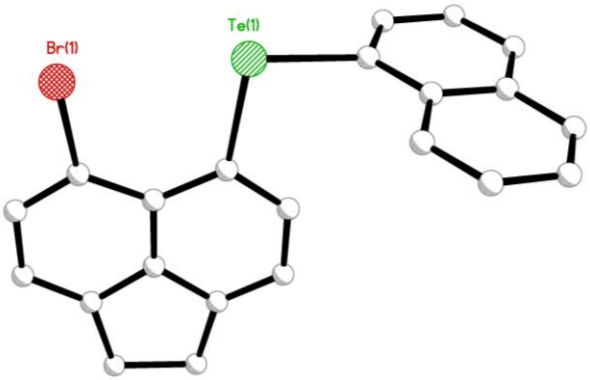


FK490-FS

P-1

a = 8.062(2) Å
b = 8.248(2) Å
c = 13.987(3) Å
α = 88.973(7)°
β = 81.374(6)°
γ = 66.026(5)°
V = 839.3(3) Å^3

R_1 = 0.0235

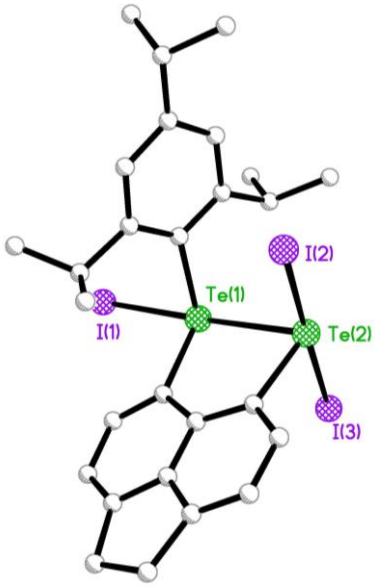


FK457A

I2/a

a = 19.886(3) Å
b = 9.4518(8) Å
c = 31.219(6) Å
β = 100.12(2)°
V = 5776(2) Å^3

R_1 = 0.0278

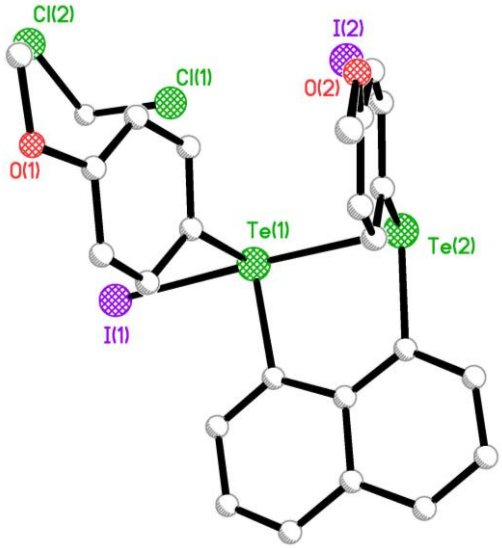


FK-409-A-2

$P2_1/c$

a = 12.850(6) Å
b = 18.425(7) Å
c = 12.324(6) Å
β = 104.895(11)°
V = 2820(2) Å^3

R_1 = 0.0917

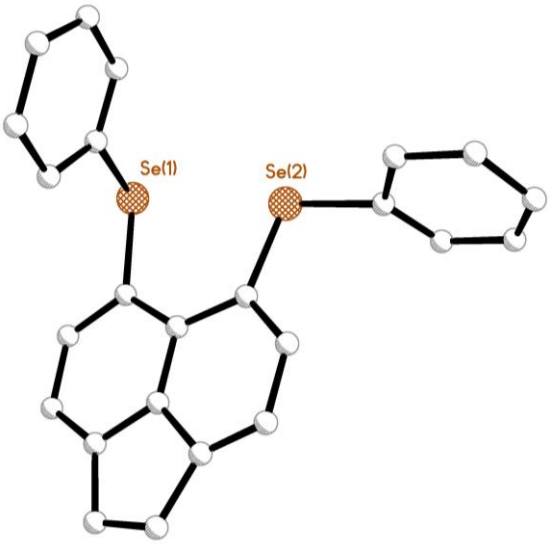


LMDO11_Off

$P2_1/c$

a = 9.292(6) Å
b = 25.932(12) Å
c = 8.688(5) Å
β = 114.183(13)°
V = 1910(2) Å^3

R_1 = 0.0795

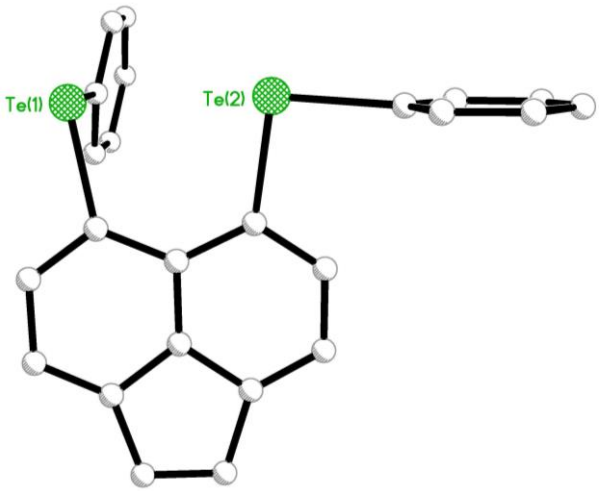


LMDO15

P-1

a = 9.968(5) Å
b = 10.048(6) Å
c = 11.903(7) Å
α = 108.391(6)°
β = 97.753(6)°
γ = 116.885(6)°
V = 953.3(9) Å^3

R_1 = 0.0546

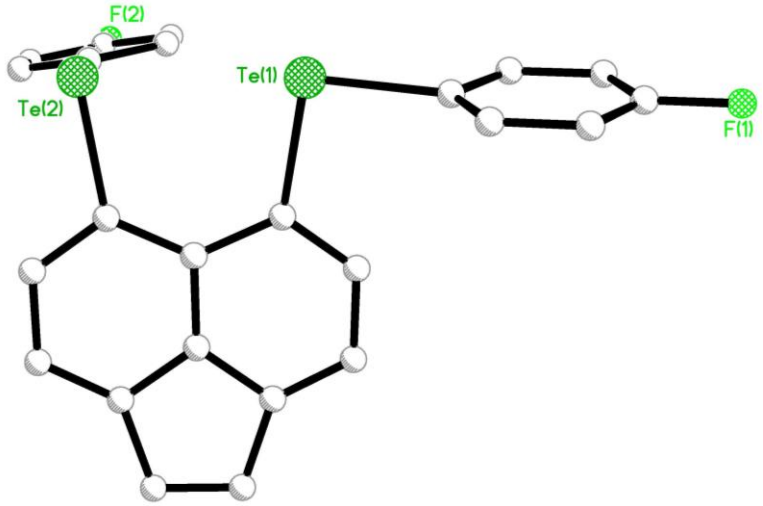


LMD122-FS

P-1

a = 9.6123(9) Å
b = 10.507(1) Å
c = 11.381(2) Å
α = 94.508(7)°
β = 107.709(8)°
γ = 113.654(8)°
V = 976.1(2) Å^3

R_1 = 0.0238

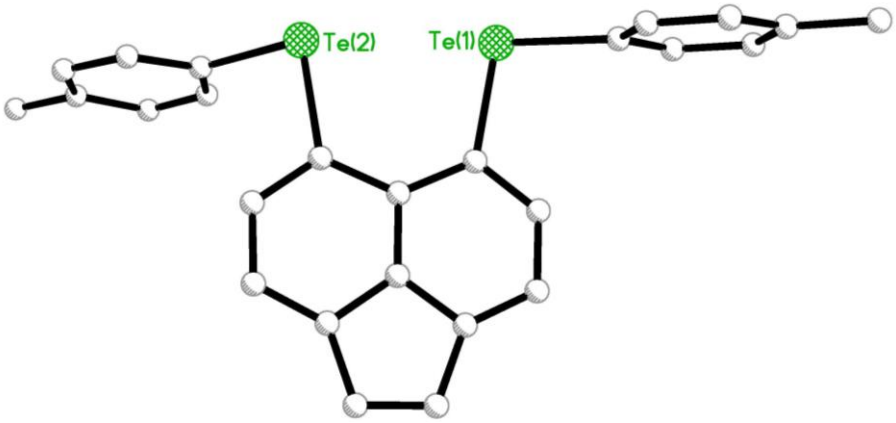


LMDO-60-1-FS

$P2_1/c$

a = 14.277(4) Å
b = 13.026(4) Å
c = 11.898(3) Å
β = 99.403(8)°
V = 2183(1) Å^3

R_1 = 0.0812

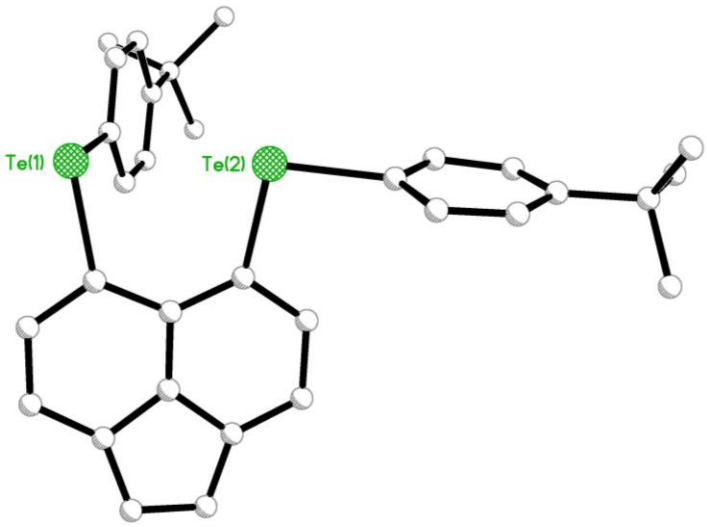


LMD118-FS

$P2_1/c$

a = 10.769(6) Å
b = 10.835(5) Å
c = 14.3250(7) Å
α = 83.380(1)°
β = 69.84(2)°
γ = 60.792(2)°
V = 1367(1) Å^3

R_1 = 0.1280

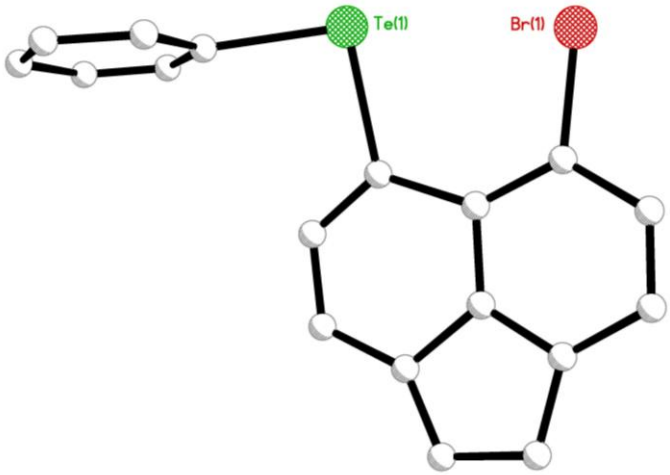


LMDO-26-2

$Pca2_1$

a = 23.46(3) Å
b = 10.579(13) Å
c = 5.796(7) Å
V = 1439(3) $Å^3$

R_1 = 0.0695

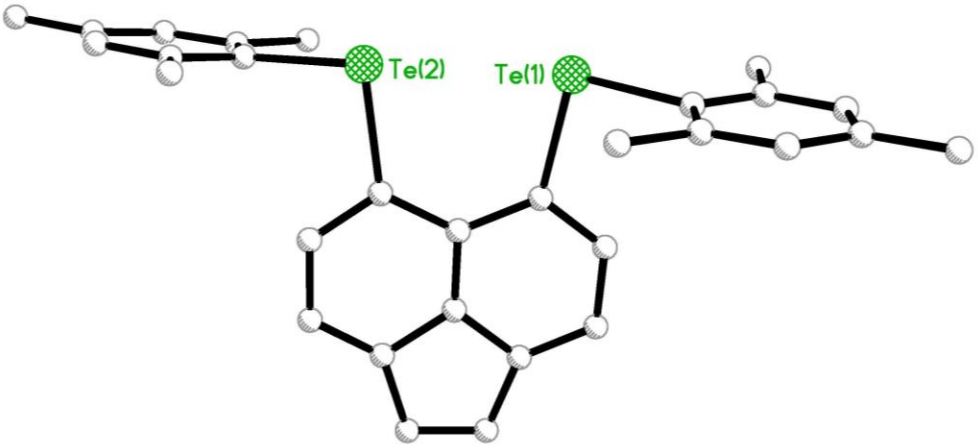


LMDO-27

$P2_1/n$

a = 10.785(3) Å
b = 21.422(6) Å
c = 10.873(3) Å
β = 94.503(9)°
V = 2504.1(11) $Å^3$

R_1 = 0.0564

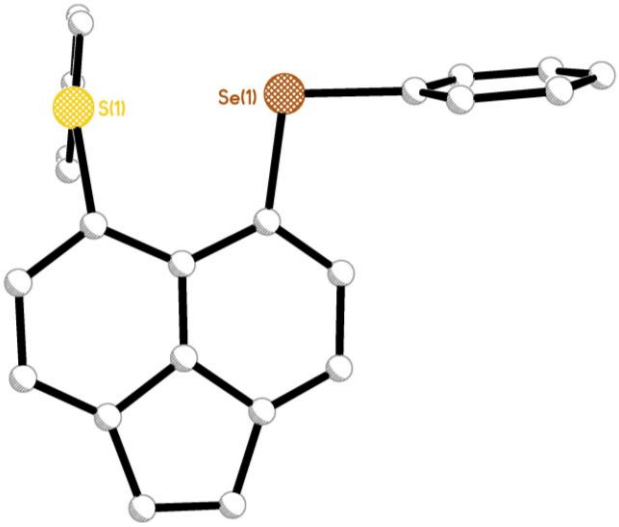


LMDO-53-2

$P2_1/c$

a = 9.680(5) Å
b = 17.417(8) Å
c = 11.528(5) Å
β = 106.228(11)°
V = 1866(2) $Å^3$

R_1 = 0.0736

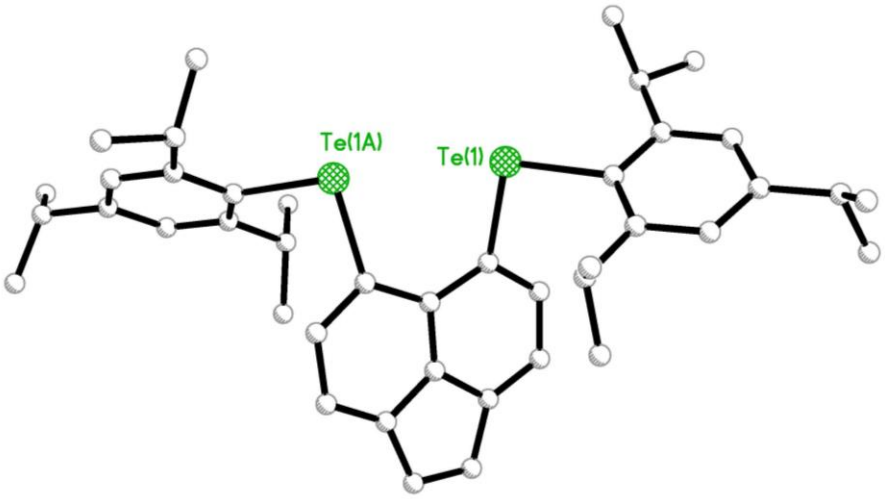


LMDO-85-FS

Pbcn

a = 30.706(3) Å
b = 10.5034(9) Å
c = 11.386(1) Å
V = 3672.1(6) $Å^3$

R_1 = 0.0276

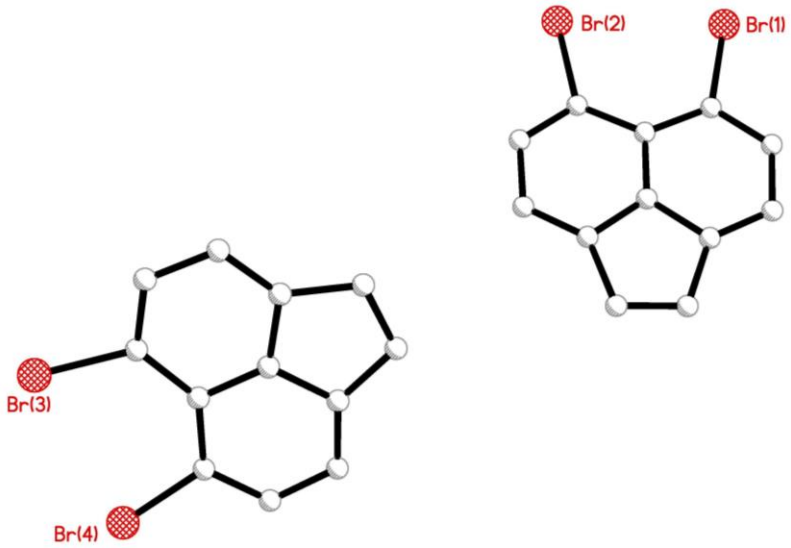


LouD09-3

$P2_1/c$

a = 16.980(2) Å
b = 15.482(2) Å
c = 7.6280(8) Å
β = 101.784(7)°
V = 1963.0(4) $Å^3$

R_1 = 0.0601

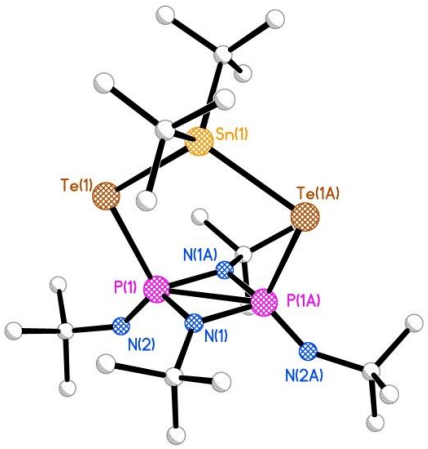


ANDW-45

Fd22

a = 20.116(2) Å
b = 30.241(2) Å
c = 11.5584(7) Å
V = 7031.2(8) $Å^3$

R_1 = 0.0373

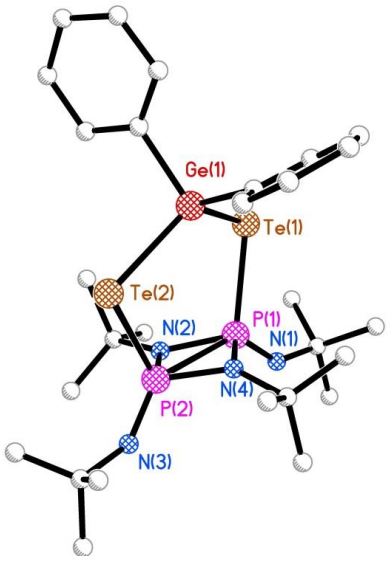


ANDW-52-1

P-1

a = 9.338(2) Å
b = 11.603(2) Å
c = 15.879(3) Å
α = 87.895(6)°
β = 80.914(6)°
γ = 89.309(6)°
V = 1697.6(6) Å^3

R_1 = 0.1284

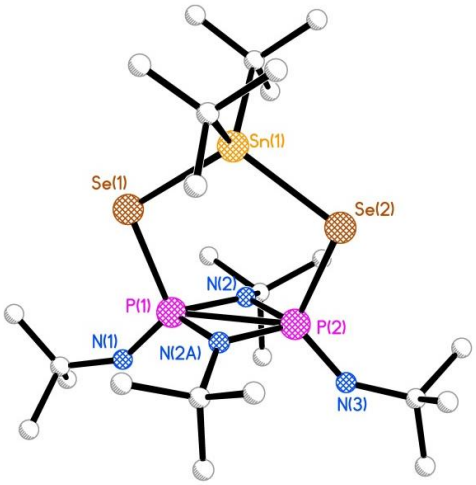


ANDW-64-4_Off

lm

a = 11.33(2) Å
b = 15.20(3) Å
c = 11.43(2) Å
β = 118.57(12)°
V = 1730(5) Å^3

R_1 = 0.0758

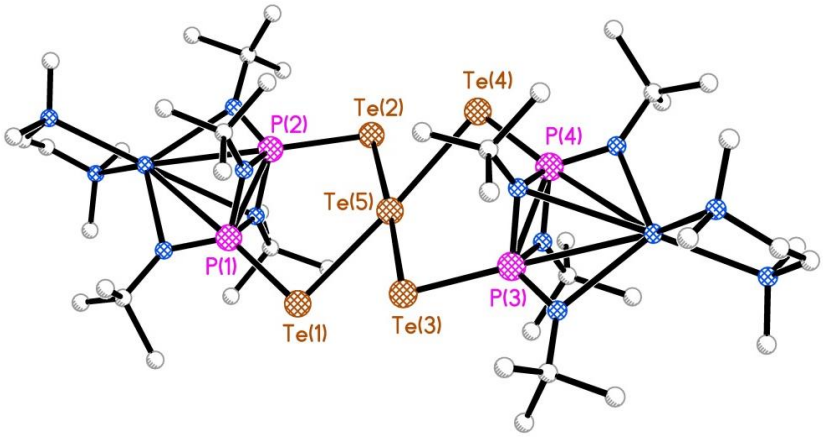


ANDW66-off

Fdd2

a = 32.355(3) Å
b = 34.276(3) Å
c = 25.584(2) Å
V = 28373(4) Å^3

R_1 = 0.0508

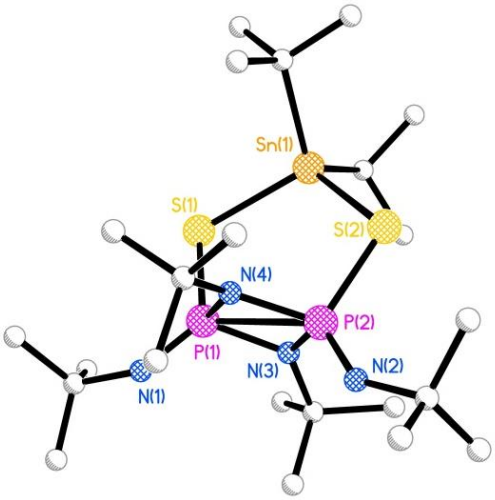


ANDW-67-Off

$P2_1/c$

a = 11.243(3) Å
b = 30.770(7) Å
c = 11.193(3) Å
β = 119.83(2)°
V = 3359(2) Å^3

R_1 = 0.0840

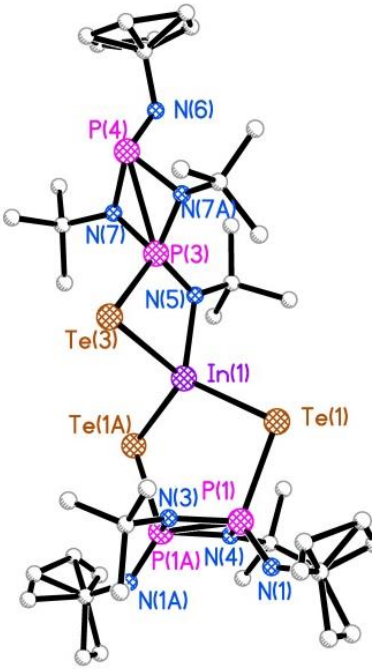


Kas69

$P2_1/m$

a = 10.4809(6) Å
b = 13.7747(8) Å
c = 17.1821(12) Å
β = 98.643(7)°
V = 2452.4(3) Å^3

R_1 = 0.0609

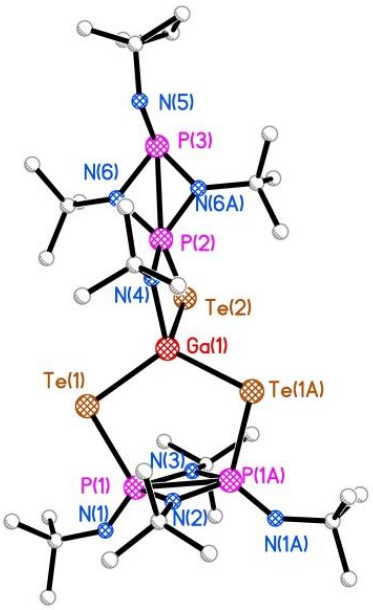


ANDW-72_Off

$P2_1/m$

a = 10.4461(18) Å
b = 13.727(2) Å
c = 16.790(3) Å
β = 98.864(5)°
V = 2378.8(7) Å^3

R_1 = 0.0858

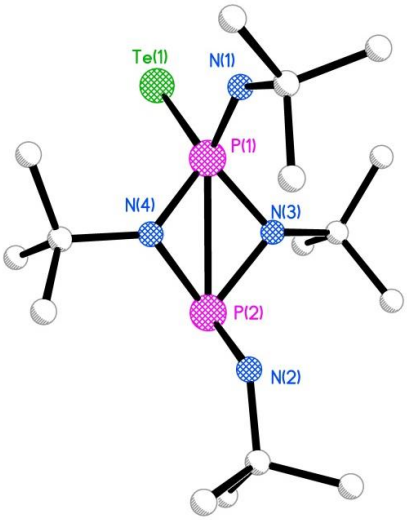


ANDW-74_Off

$P2_1/c$

a = 9.460(2) Å
b = 15.495(4) Å
c = 15.864(4) Å
β = 91.221(6)°
V = 2324.8(9) Å^3

R_1 = 0.0449

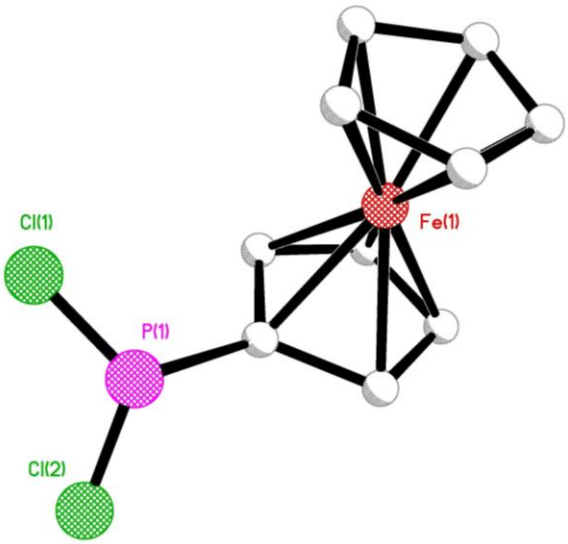


ANDW-100-FS

$P2_1/c$

a = 12.865(4) Å
b = 10.391(3) Å
c = 7.739(3) Å
β = 98.430(8)°
V = 1023.4(6) Å^3

R_1 = 0.0926

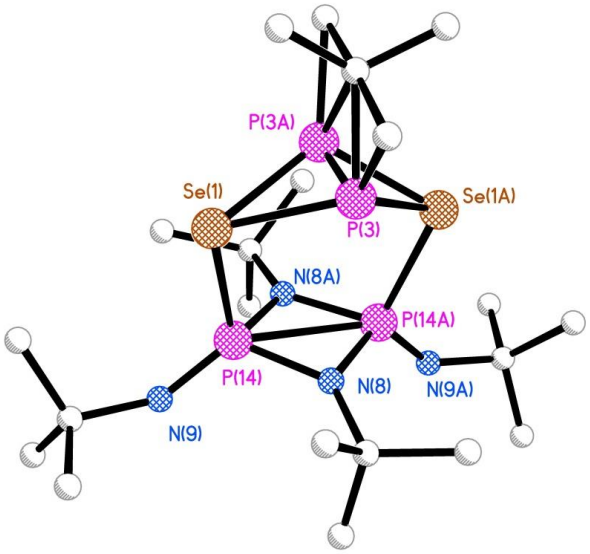


ANDW-114-1

$P2_1/c$

a = 9.445(3) Å
b = 15.473(5) Å
c = 15.817(6) Å
β = 90.797(8)°
V = 2311.2(13) Å^3

R_1 = 0.0590

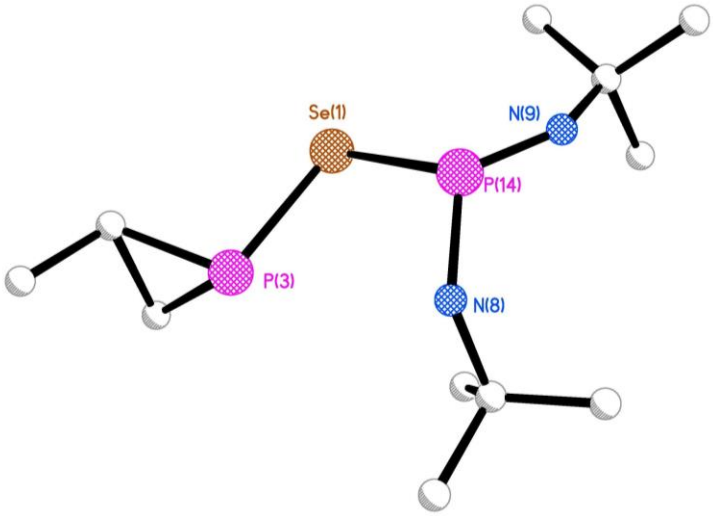


ANDW-116-FS

Pbcn

a = 16.403(4) Å
b = 10.200(2) Å
c = 16.820(4) Å
V = 2814.1(11) $Å^3$

R_1 = 0.0819

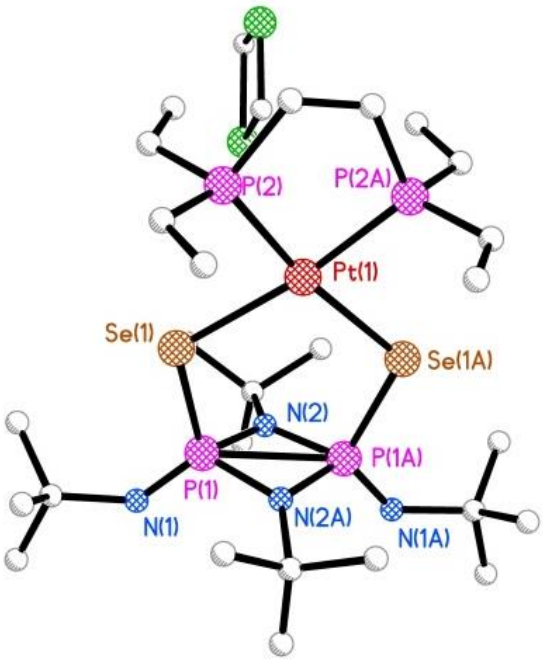


ANDW117-fs

Pmmn

a = 12.930(4) Å
b = 14.656(5) Å
c = 11.169(3) Å
V = 2116.5(11) $Å^3$

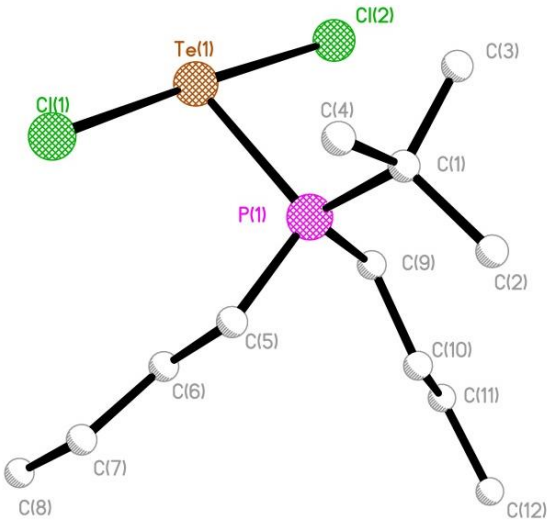
R_1 = 0.1263



ANDW-119-FS
$P2_1/c$

a = 15.963(4) Å
b = 11.788(3) Å
c = 9.033(2) Å
β = 91.467(7)°
V = 1699.2(7) $Å^3$

R_1 = 0.0459

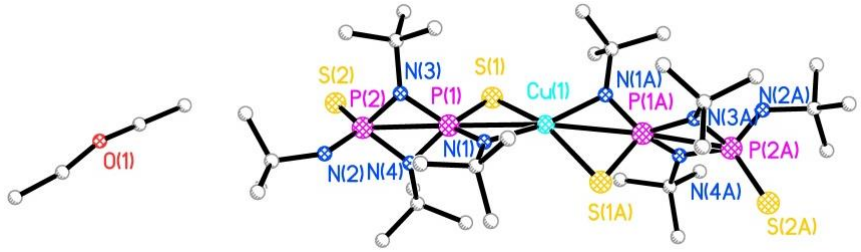


ANDW-124-1-off

C2/c

a = 26.047(8) Å
b = 16.860(5) Å
c = 12.809(5) Å
β = 96.255(8)°
V = 5592(3) Å^3

R_1 = 0.0741

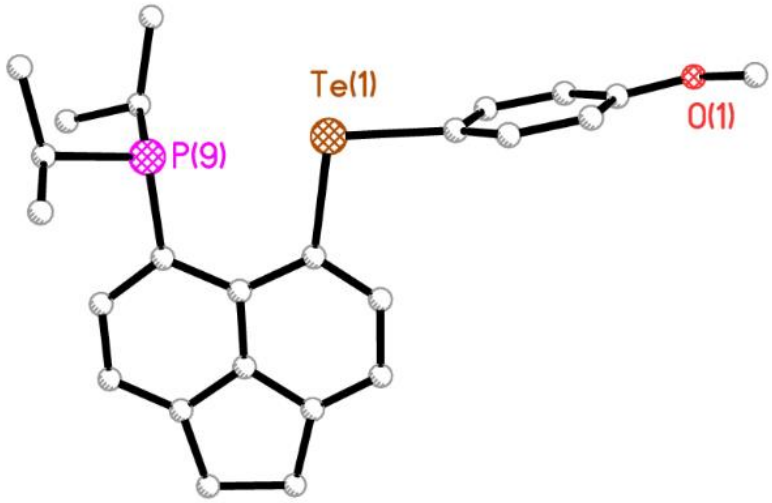


ANDW-132-fs

C2/c

a = 25.365(3) Å
b = 11.5214(13) Å
c = 17.6915(19) Å
β = 93.517(8)°
V = 5160.4(10) Å^3

R_1 = 0.0382

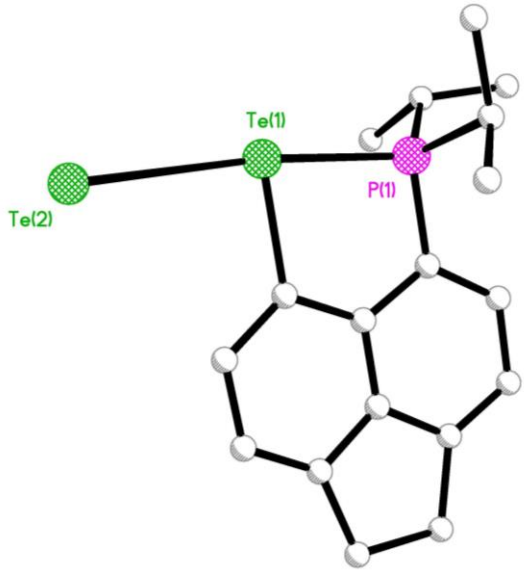


ANDW135-2fs

$P2_1/n$

a = 11.666(2) Å
b = 11.579(2) Å
c = 13.892(2) Å
β = 99.824(7)°
V = 1849.0(5) Å^3

R_1 = 0.0739

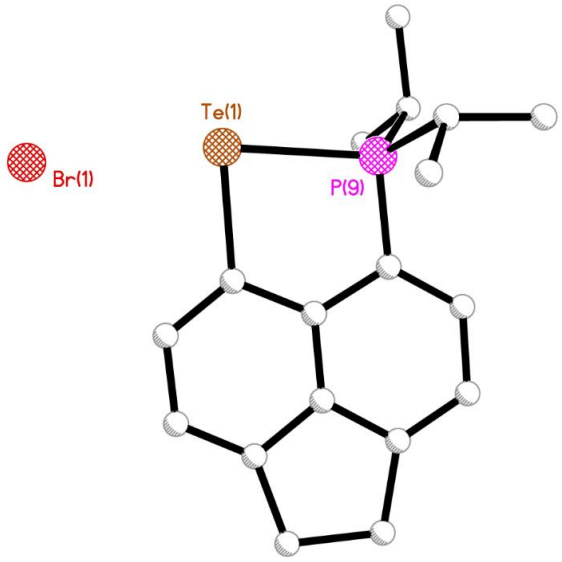


ANDW142-FS

$P2_1/n$

a = 7.7860(8) Å
b = 13.9267(14) Å
c = 16.4054(18) Å
β = 97.078(7)°
V = 1765.3(3) Å^3

R_1 = 0.0230

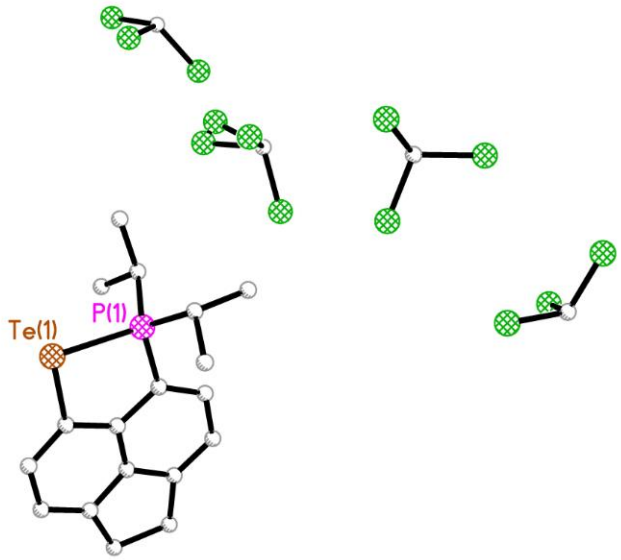


ANDW148-1-fs

$P2_1/c$

a = 11.6588(15) Å
b = 25.620(3) Å
c = 12.0967(16) Å
β = 101.628(7)°
V = 3539.1(8) Å^3

R_1 = 0.0517

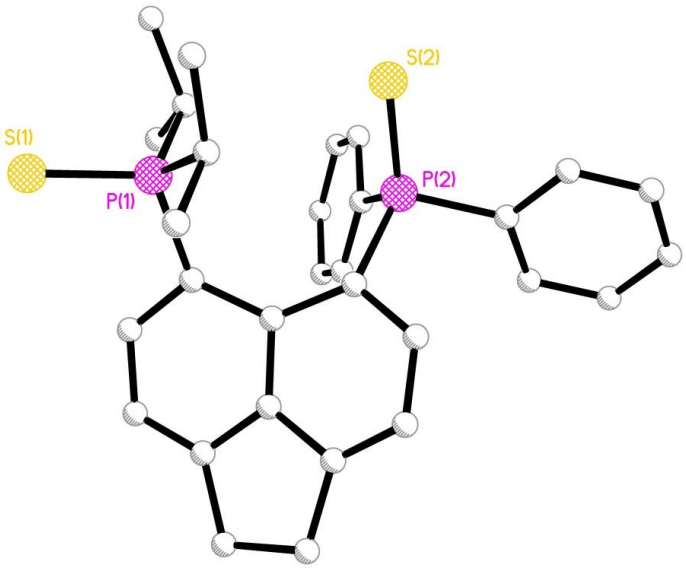


APPK1-FS

Pn

a = 8.950(2) Å
b = 11.086(3) Å
c = 14.038(4) Å
β = 97.158(7)°
V = 1382.1(6) Å^3

R_1 = 0.0517

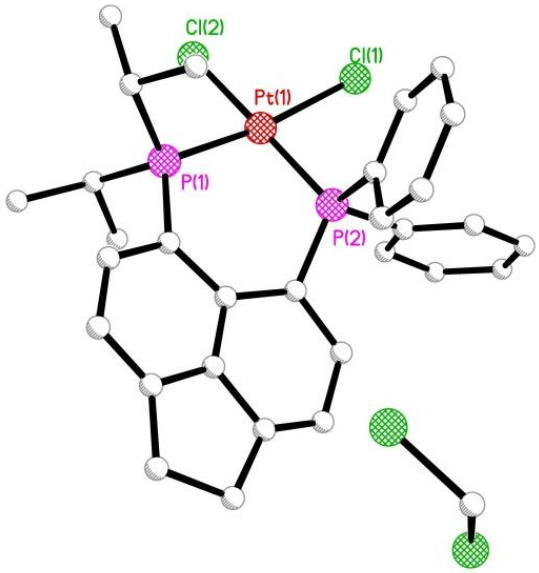


APPK2-FS

$Pna2_1$

a = 14.753(2) Å
b = 17.857(3) Å
c = 11.238(2) Å
V = 2960.5(7) $Å^3$

R_1 = 0.0578

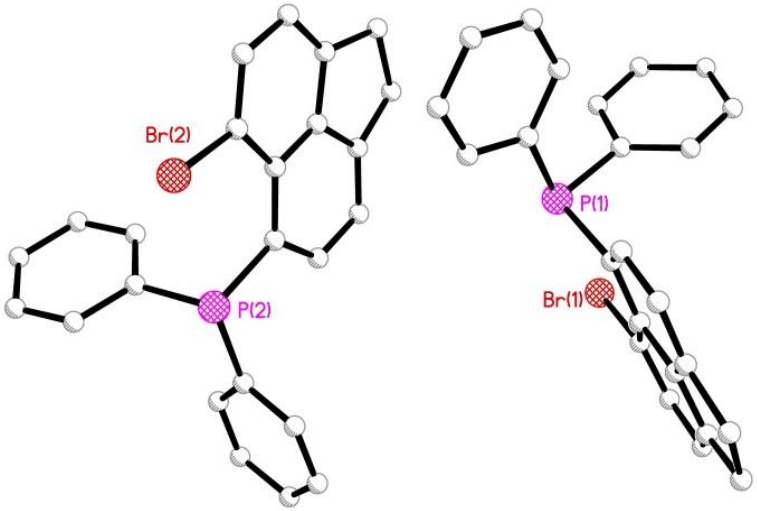


APPK5-FS

P-1

a = 9.613(3) Å
b = 12.077(3) Å
c = 17.219(4) Å
α = 80.753(6)°
β = 83.264(8)°
γ = 70.831(7)°
V = 1859.2(8) $Å^3$

R_1 = 0.0526

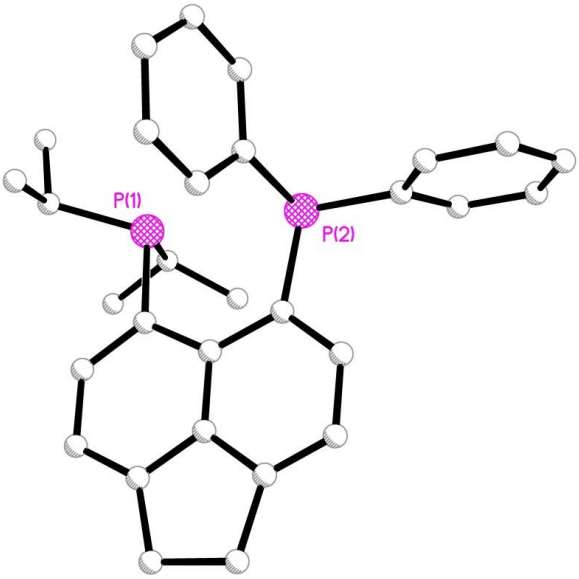


APPK6-FS

P-1

a = 9.837(5) Å
b = 11.404(5) Å
c = 11.644(5) Å
α = 91.10(2)°
β = 107.30(2)°
γ = 92.75(2)°
V = 1245(1) $Å^3$

R_1 = 0.0754

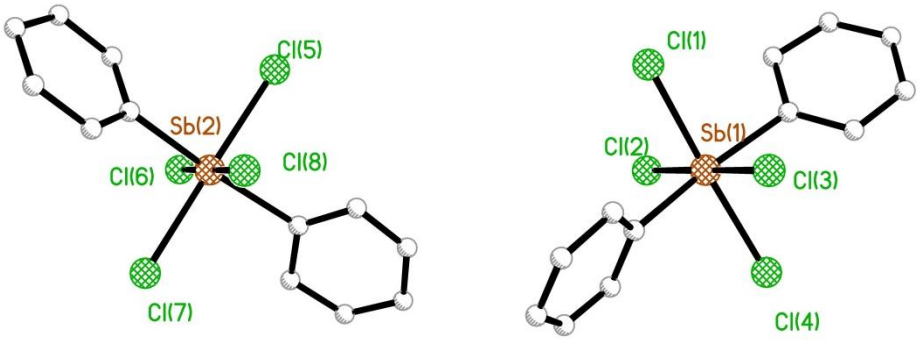


BCPK-27

P-1

a = 8.451(3) Å
b = 9.636(3) Å
c = 17.604(5) Å
α = 90°
β = 90°
γ = 90°
V = 1433.6(8) Å^3

R_1 = 0.0986

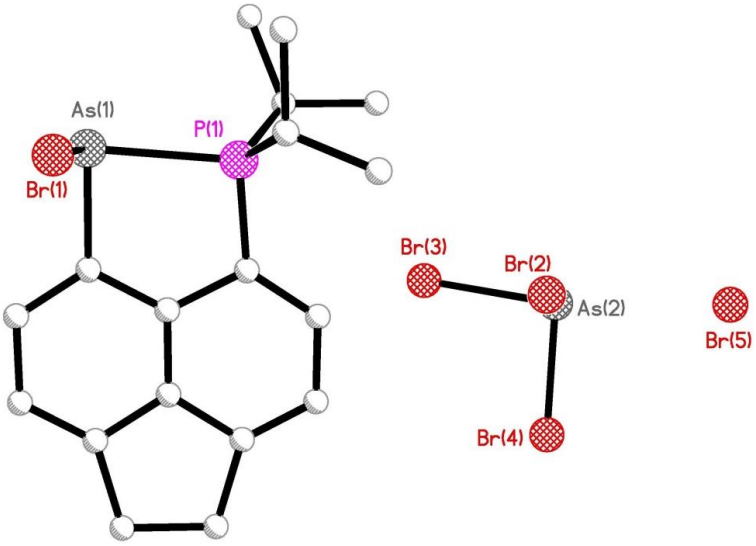


BCPK35

P-1

a = 10.5185(11) Å
b = 11.1333(10) Å
c = 11.3740(11) Å
α = 76.955(12)°
β = 79.891(12)°
γ = 66.596(8)°
V = 1185.3(3) Å^3

R_1 = 0.0475

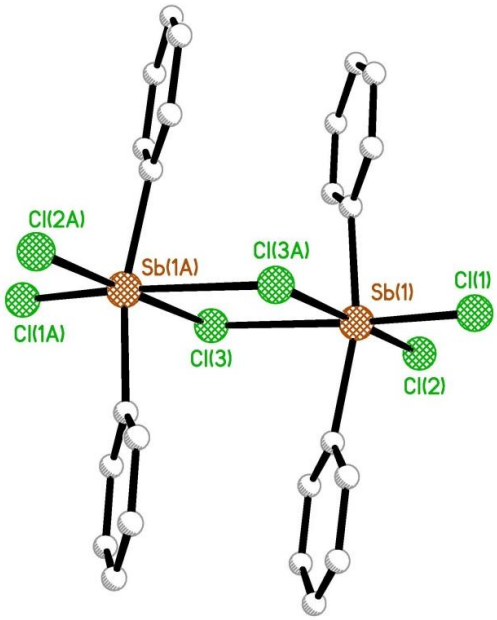


BCPK-37-1

Pnnm

a = 8.462(2) Å
b = 10.390(3) Å
c = 14.781(4) Å
V = 1299.5(5) Å^3

R_1 = 0.0280

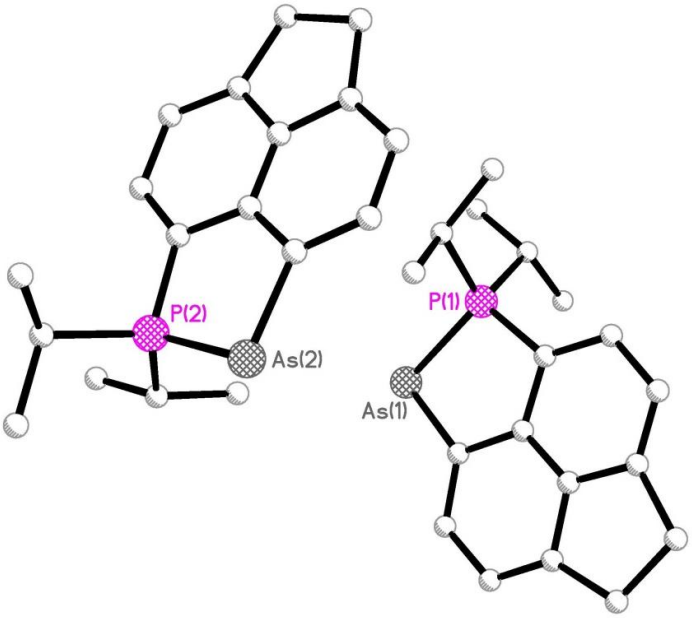


BCPK39

$P2_1/n$

a = 16.485(4) Å
b = 11.922(3) Å
c = 18.093(5) Å
β = 113.769(6)°
V = 3254(2) Å^3

R_1 = 0.0765

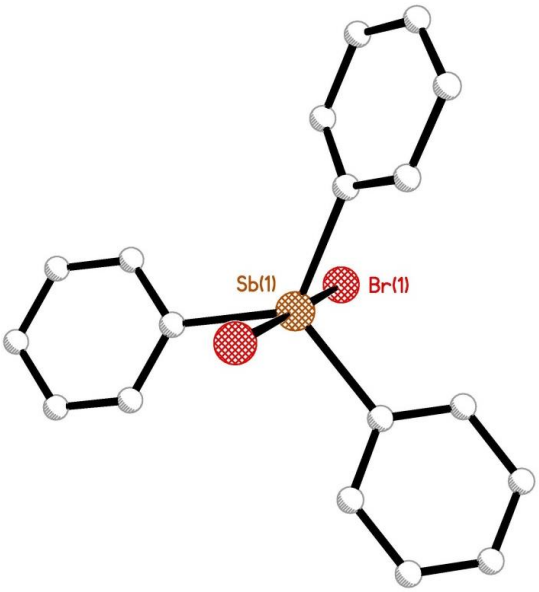


BCPK-41-4-_FS

Fdd2

a = 24.256(7) Å
b = 10.342(3) Å
c = 14.247(3) Å
V = 3574(2) Å^3

R_1 = 0.0400

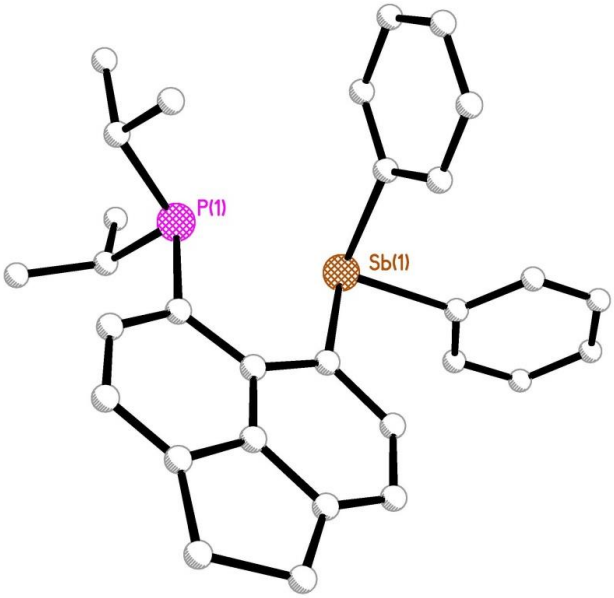


BCPK-47

P-1

a = 10.558(8) Å
b = 10.576(7) Å
c = 11.463(9) Å
α = 89.65(4)°
β = 89.63(3)°
γ = 79.35(3)°
V = 1258(2) Å^3

R_1 = 0.1398

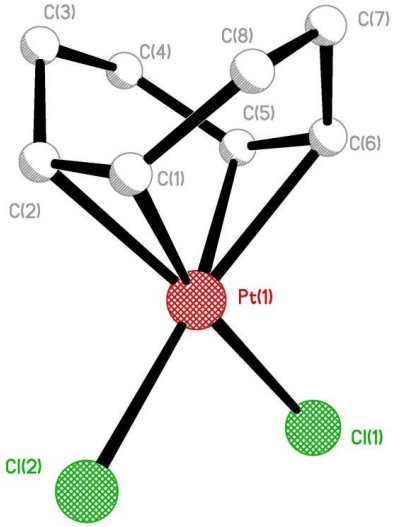


BCPK52

$P2_12_12_1$

a = 6.834(2) Å
b = 10.679(3) Å
c = 12.427(4) Å
V = 907.0(5) $Å^3$

R_1 = 0.0281

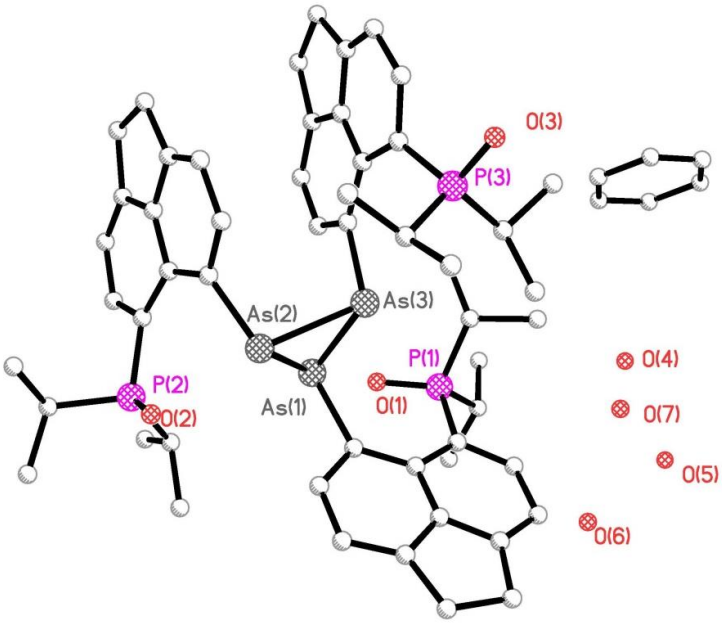


BCPK-58

P-1

a = 14.244(2) Å
b = 14.748(2) Å
c = 16.041(3) Å
α = 82.916(6)°
β = 73.841(6)°
γ = 64.684(5)°
V = 2925.7(8) $Å^3$

R_1 = 0.0622

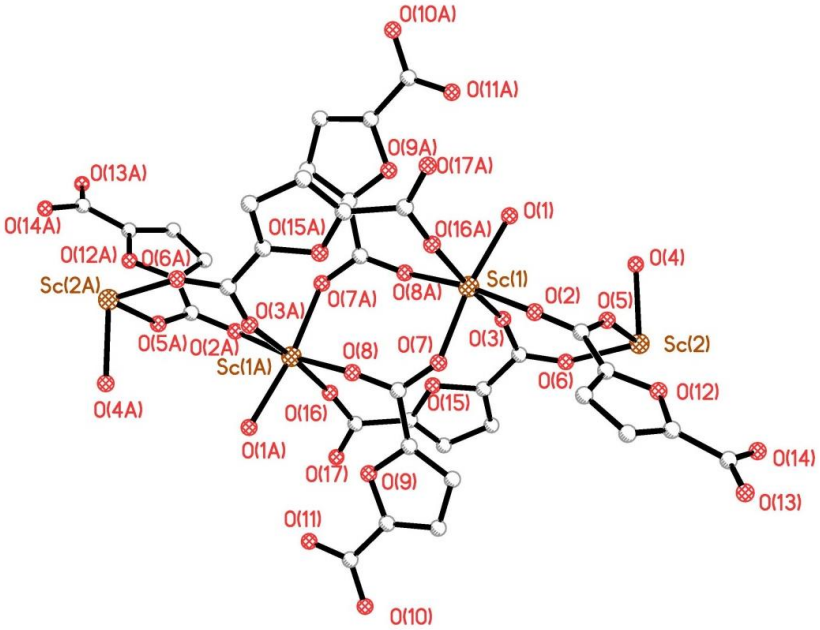


BGPW3_Off

P-1

a = 8.775(4) Å
b = 10.560(4) Å
c = 11.854(4) Å
α = 93.139(10)°
β = 91.457(7)°
γ = 105.810(11)°
V = 1054.3(7) $Å^3$

R_1 = 0.0694

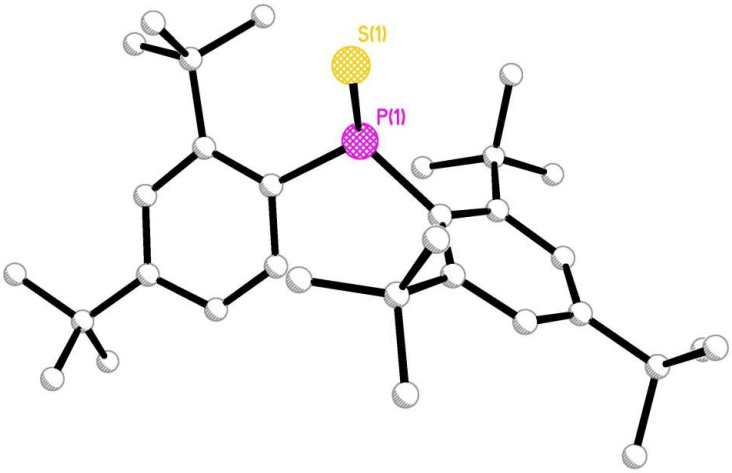


CFPK12ROB-2

P-1

a = 9.398(5) Å
b = 12.868(7) Å
c = 14.381(7) Å
α = 108.860(7)°
β = 100.484(9)°
γ = 105.905(8)°
V = 1511.2(13) $Å^3$

R_1 = 0.1342

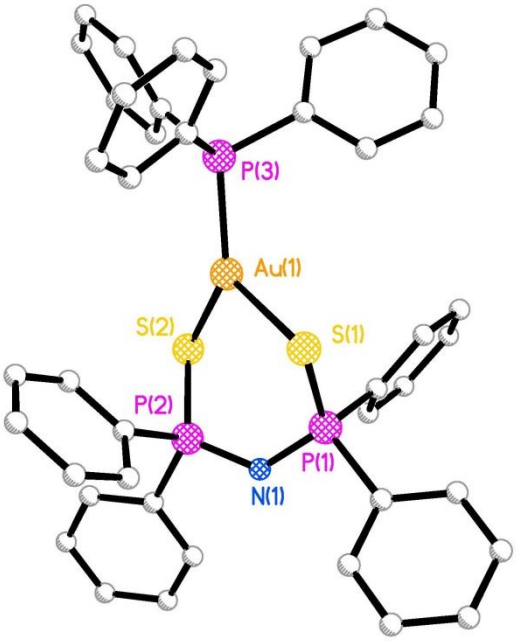


COMP1

P-1

a = 8.9300(7) Å
b = 12.0100(10) Å
c = 18.480(2) Å
α = 78.000(6)°
β = 80.000(6)°
γ = 74.000(6)°
V = 1849.2(3) $Å^3$

R_1 = 0.0374

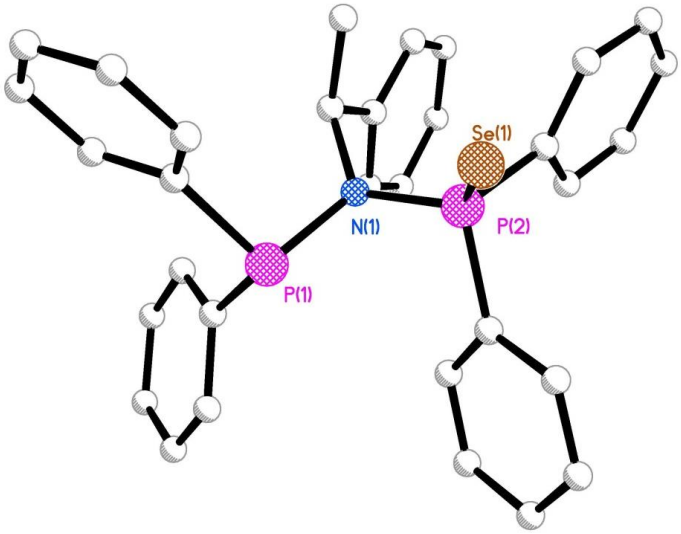


COMP-2-FS

$P2_12_12_1$

a = 10.679(2) Å
b = 14.996(3) Å
c = 16.908(4) Å
V = 2707.9(9) $Å^3$

R_1 = 0.0899

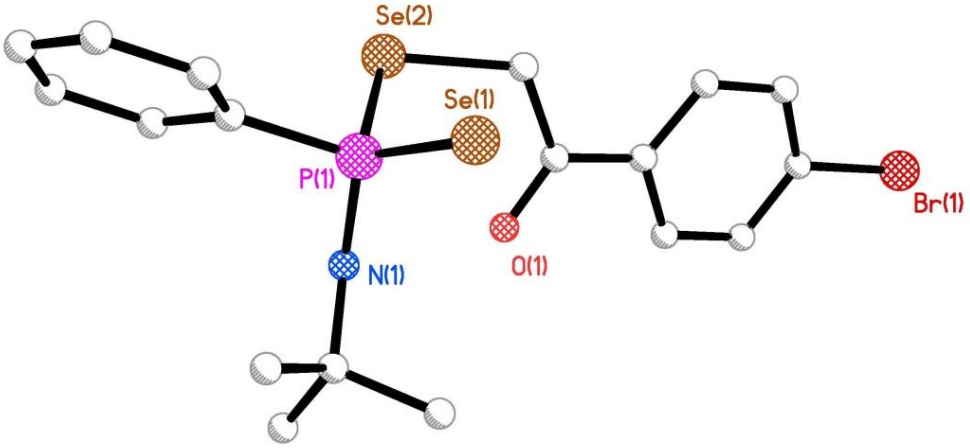


HDW-229_Off

P-1

a = 8.167(8) Å
b = 10.242(10) Å
c = 12.625(13) Å
α = 81.19(3)°
β = 79.35(3)°
γ = 75.78(3)°
V = 1000(2) Å^3

R_1 = 0.0522

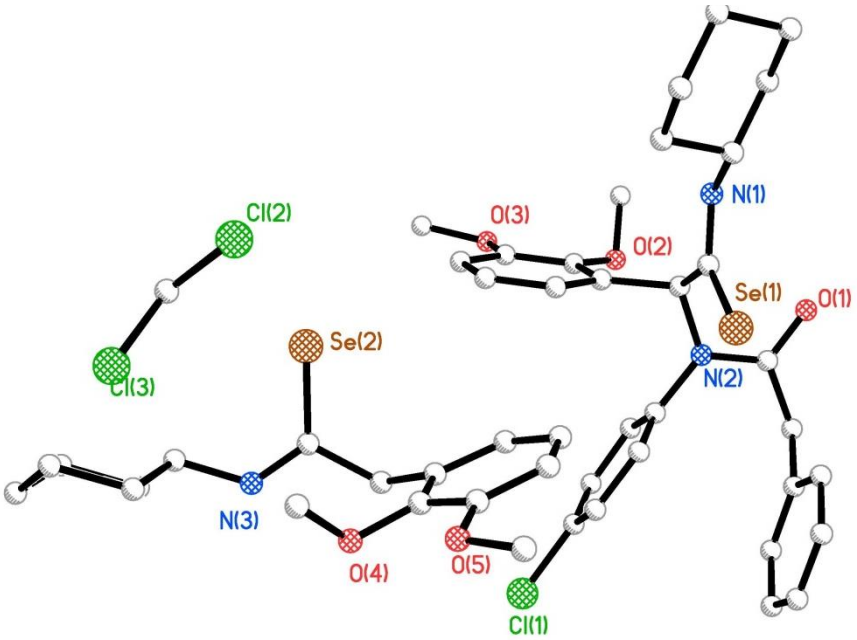


HDW-230_Off

P-1

a = 11.419(4) Å
b = 11.488(4) Å
c = 18.648(6) Å
α = 82.268(10)°
β = 80.837(10)°
γ = 73.983(9)°
V = 2310.7(12) Å^3

R_1 = 0.0928

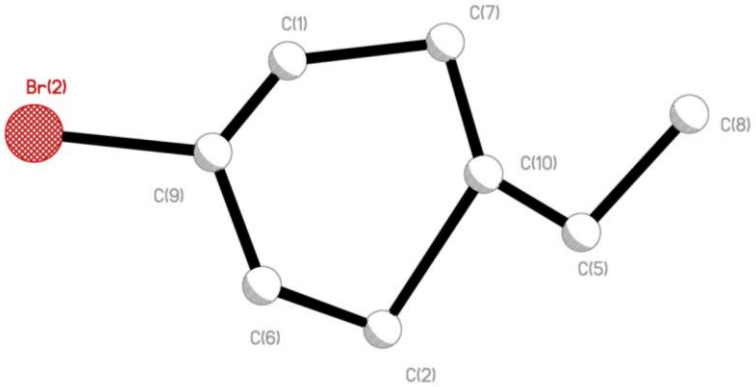


HDW-232_Off

Cmc2$_1$

a = 37.130(13) Å
b = 6.941(3) Å
c = 6.080(2) Å
V = 1567.0(10) Å^3

R_1 = 0.0598

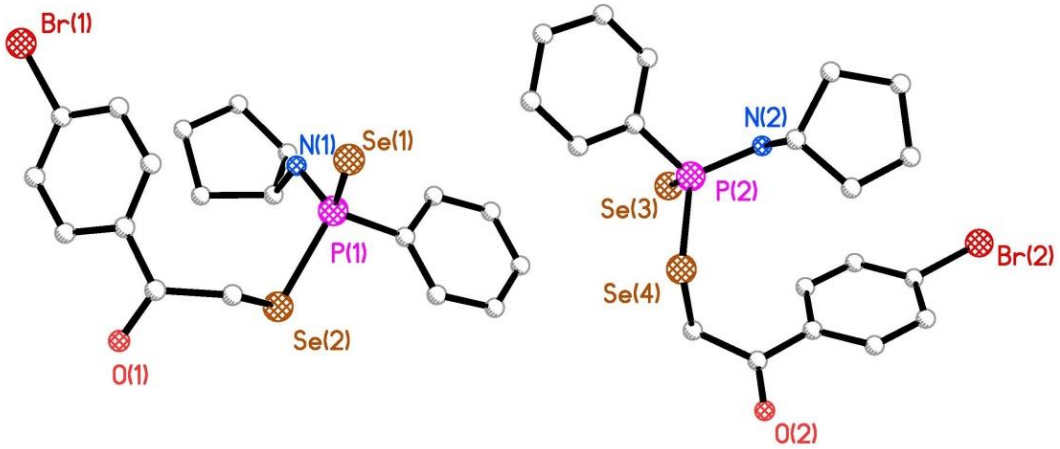


HDW-235_Off

$P2_1/c$

a = 6.956(6) Å
b = 17.86(2) Å
c = 32.53(3) Å
β = 92.038(11)°
V = 4040(6) $Å^3$

R_1 = 0.0659

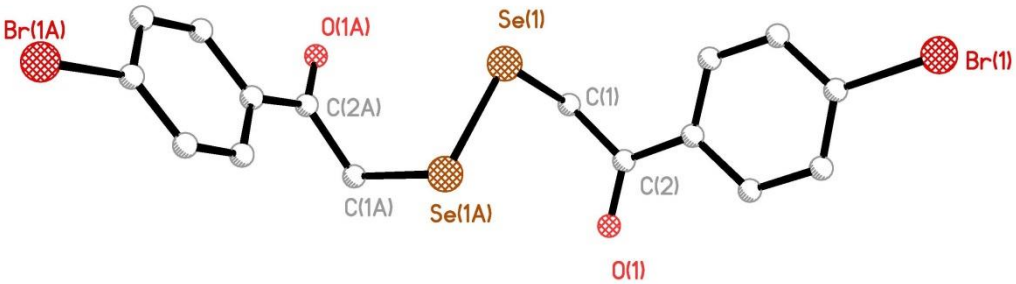


HDW-237_Off

C2

a = 31.56(10) Å
b = 4.98(2) Å
c = 5.46(2) Å
β = 91.83(4)°
V = 858(5) $Å^3$

R_1 = 0.0593

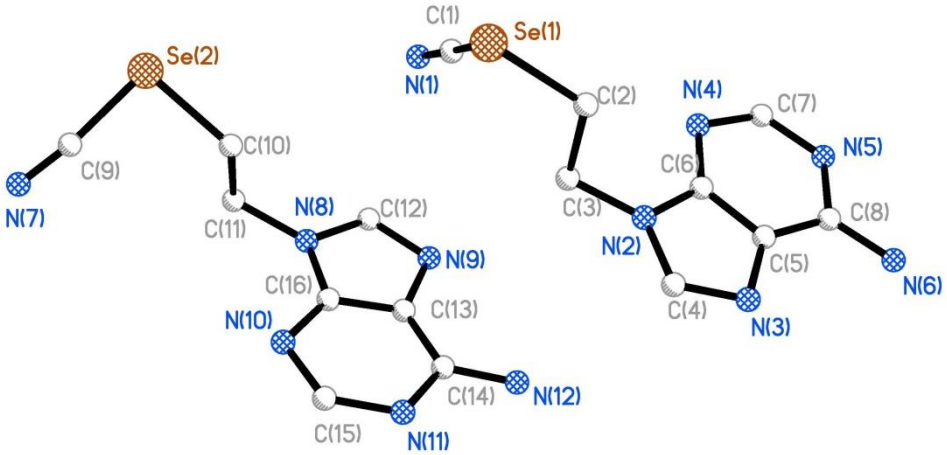


HDW-240_Off

$P2_1/c$

a = 12.931(5) Å
b = 18.361(7) Å
c = 8.275(3) Å
V = 1868.8(12) $Å^3$

R_1 = 0.1137

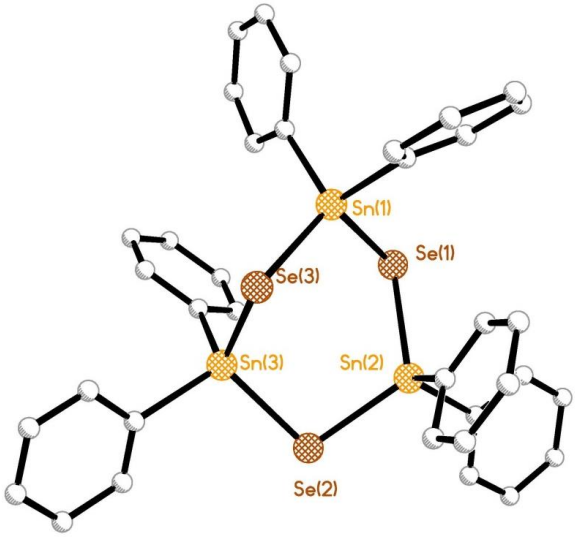


HDW-243_Off

$P2_1/n$

a = 9.861(3) Å
b = 16.525(4) Å
c = 21.478(6) Å
β = 93.910(8)°
V = 3475.4(16) $Å^3$

R_1 = 0.1245

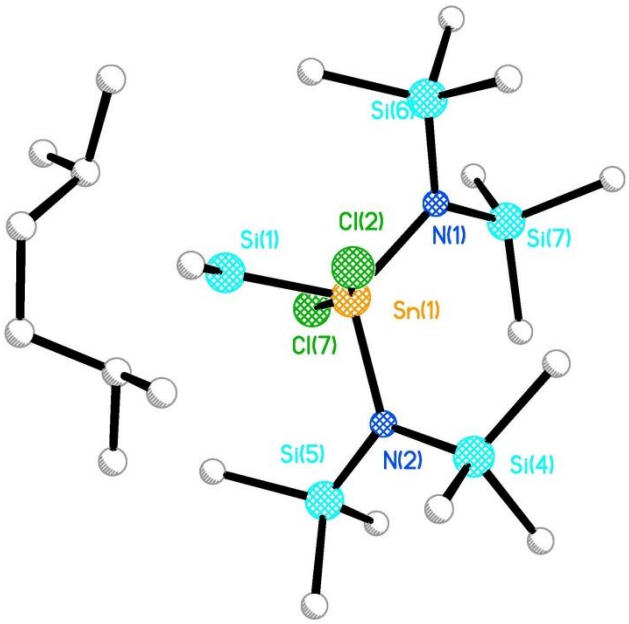


MLDW1

P-1

a = 11.531(6) Å
b = 12.048(6) Å
c = 13.895(6) Å
α = 91.596(3)°
β = 101.678(2)°
γ = 116.793(6)°
V = 1671.8(13) $Å^3$

R_1 = 0.0637

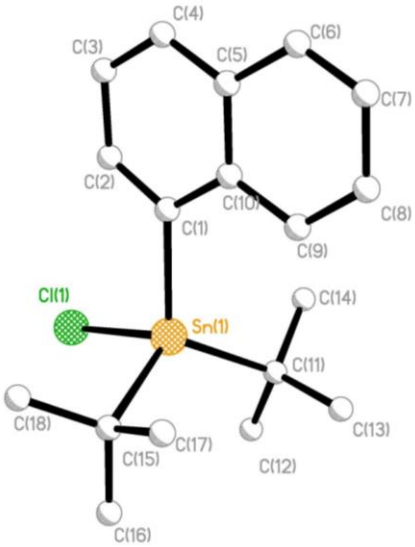


MLDW3

Pbca

a = 14.73(2) Å
b = 15.26(2) Å
c = 16.26(2) Å
V = 3656(7) $Å^3$

R_1 = 0.1330

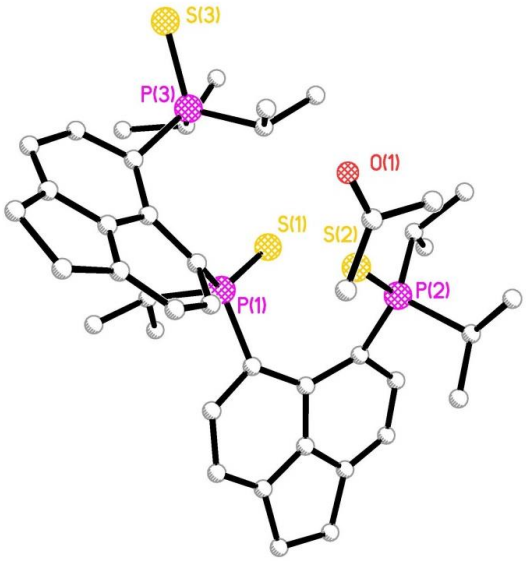


MRPK23-8

$P2_1/c$

a = 16.969(5) Å
b = 13.057(3) Å
c = 20.051(6) Å
β = 111.872(6)°
V = 4123(2) $Å^3$

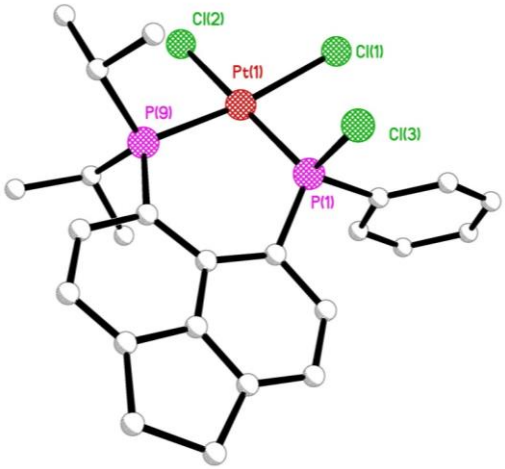
R_1 = 0.1315



MRPK-51-2
$P2_1/c$

a = 9.551(2) Å
b = 15.931(4) Å
c = 16.866(5) Å
β = 100.242(7)°
V = 2525.5(11) $Å^3$

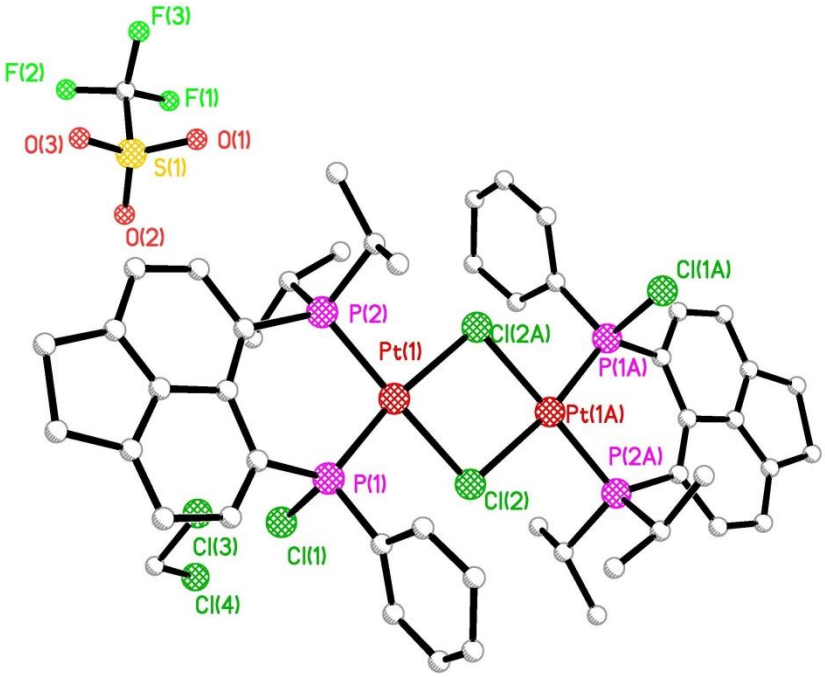
R_1 = 0.0577



MRPK-54-1
P-1

a = 8.591(3) Å
b = 12.764(4) Å
c = 15.447(7) Å
α = 101.95(5)°
β = 101.91(4)°
γ = 106.94(5)°
V = 1519.4(12) $Å^3$

R_1 = 0.1052

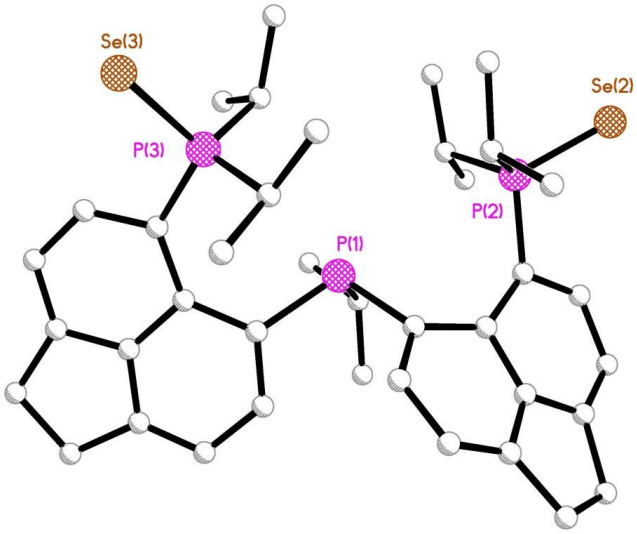


MRPK56-OFF

$P2_1/n$

a = 12.3969(13) Å
b = 21.308(3) Å
c = 13.836(2) Å
β = 92.761(3)°
V = 3650.5(7) $Å^3$

R_1 = 0.0451

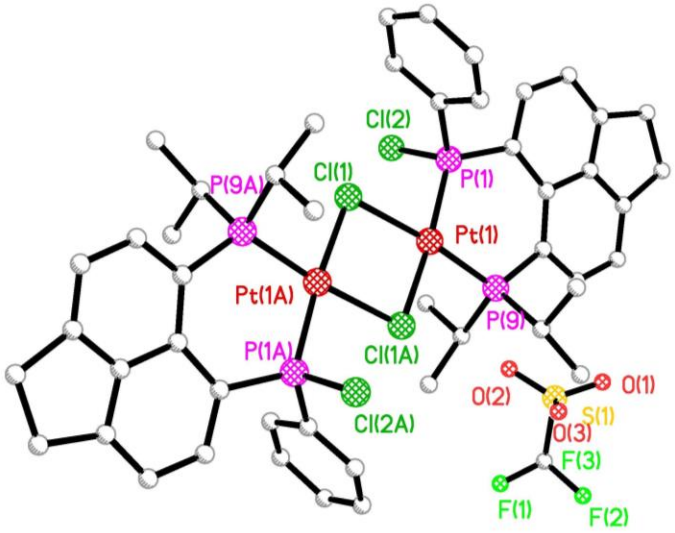


MRPK-57-FS

P-1

a = 8.540(1) Å
b = 12.702(2) Å
c = 15.366(2) Å
α = 102.196(8)°
β = 101.379(7)°
γ = 106.672(8)°
V = 1500.3(4) $Å^3$

R_1 = 0.0530

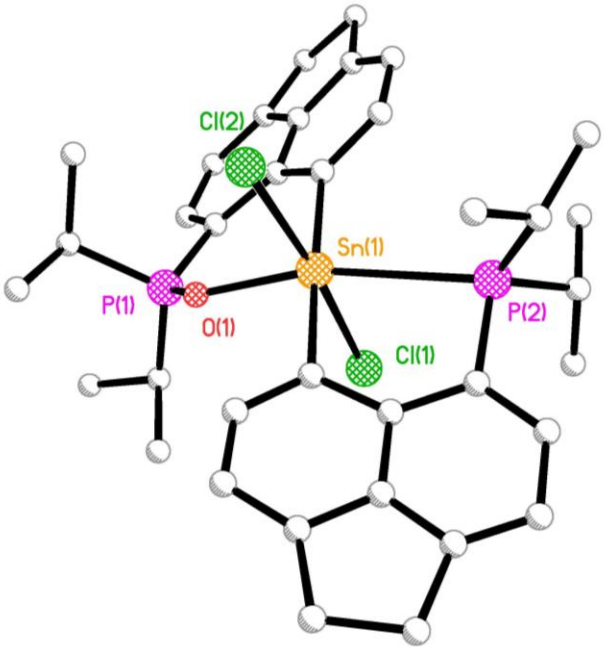


MRPK-64-FS

P2/c

a = 18.192(7) Å
b = 13.185(5) Å
c = 15.021(5) Å
β = 111.193(8)°
V = 3359(2) $Å^3$

R_1 = 0.1173

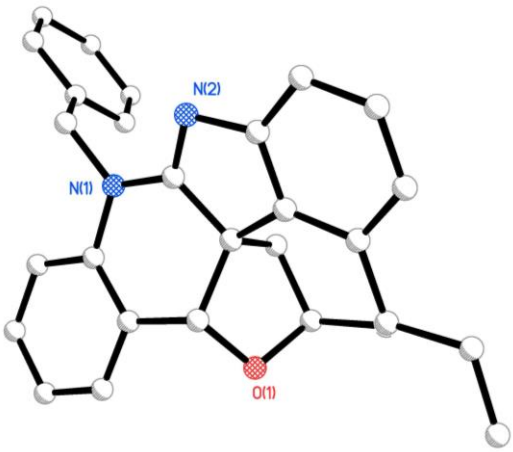


RWNW5-1

P-1

a = 9.505(2) Å
b = 11.215(2) Å
c = 11.558(2) Å
α = 66.711(5)°
β = 66.693(5)°
γ = 76.410(5)°
V = 1034.8(3) $Å^3$

R_1 = 0.0736

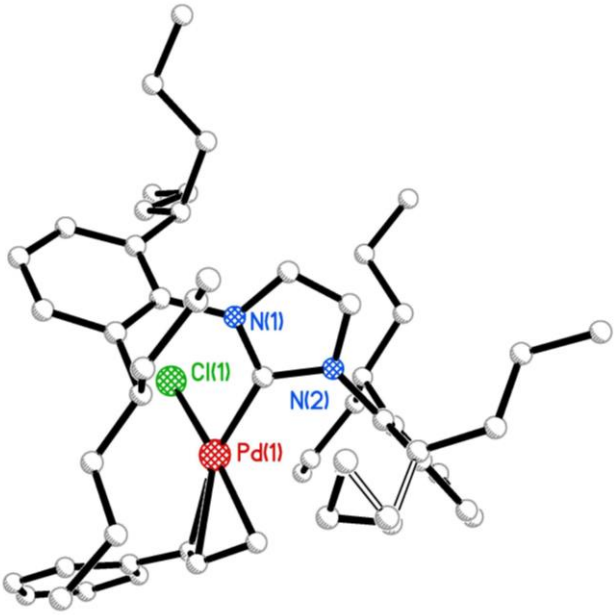


SNAC-13-Off

C2/c

a = 26.213(3) Å
b = 12.4787(9) Å
c = 32.038(5) Å
β = 113.478(12)°
V = 9612(2) $Å^3$

R_1 = 0.0633

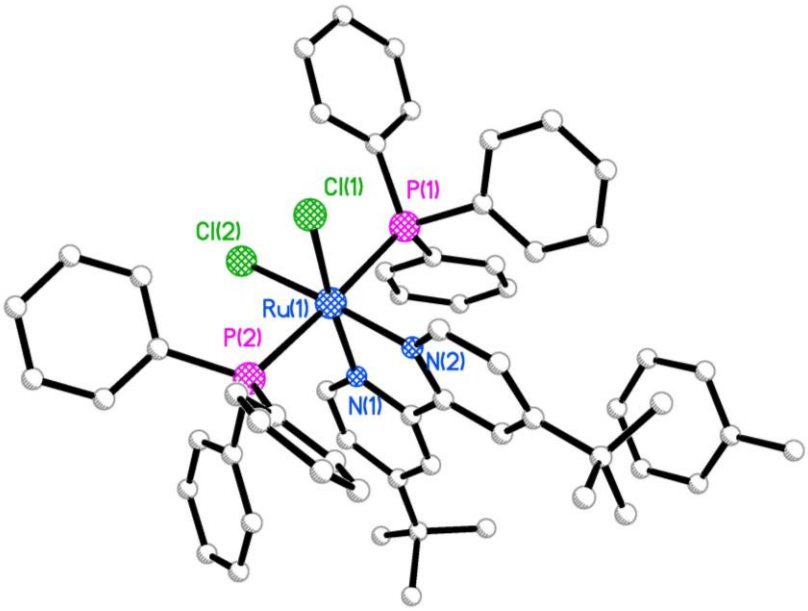


SNCU-25_Off

$P2_1/n$

a = 12.060(3) Å
b = 28.536(5) Å
c = 15.392(3) Å
β = 102.698(5)°
V = 5167(2) $Å^3$

R_1 = 0.0773

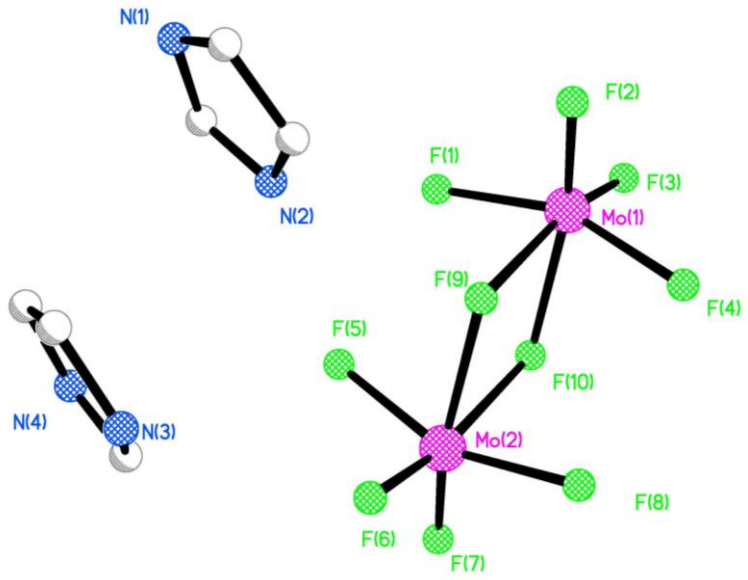


SRPL-88-1

$P2_1/n$

a = 11.593(10) Å
b = 9.521(8) Å
c = 12.996(12) Å
β = 98.23(3)°
V = 1420(2) $Å^3$

R_1 = 0.0913

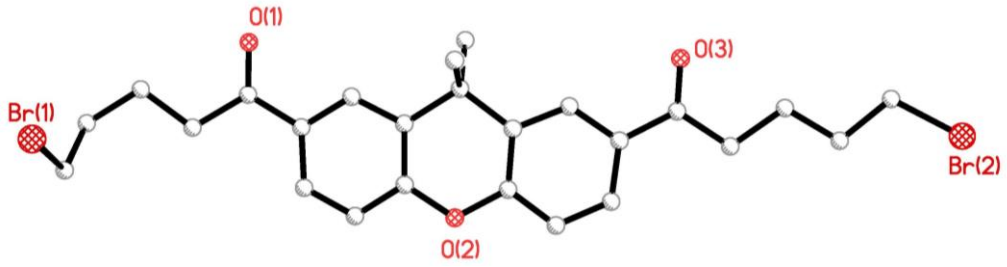


SVBB4-1-off

C2/m

a = 6.940(3) Å
b = 9.472(4) Å
c = 20.800(9) Å
β = 96.212(12)°
V = 1359.3(10) $Å^3$

R_1 = 0.0472

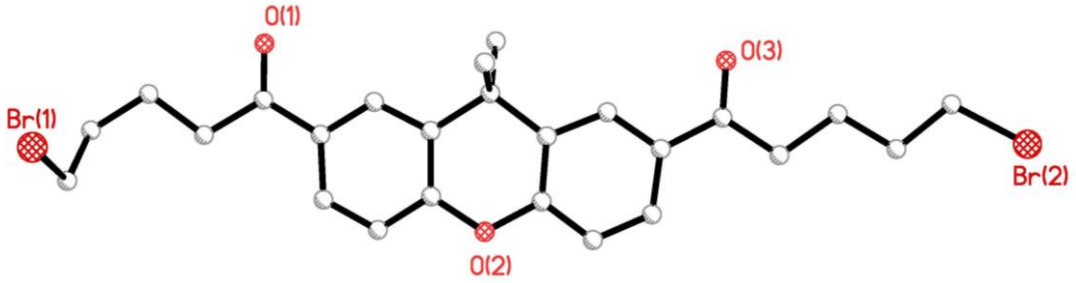


USPK1-off

P-1

a = 9.8630(7) Å
b = 10.952(2) Å
c = 12.138(2) Å
α = 84.904(13)°
β = 67.383(10)°
γ = 69.892(10)°
V = 1135.2(3) $Å^3$

R_1 = 0.0319

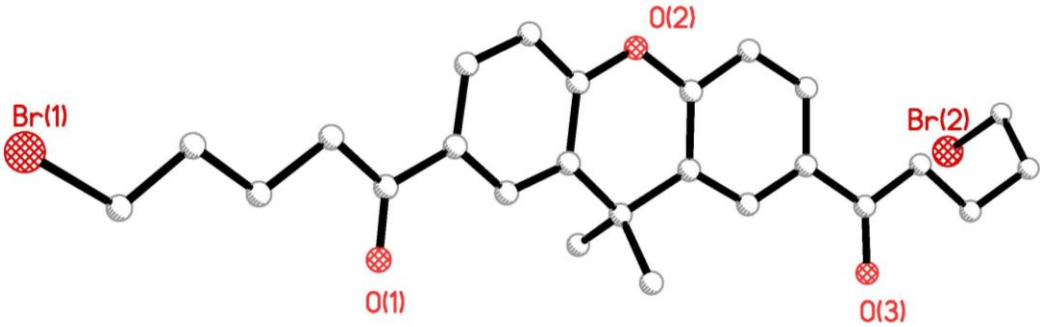


USPK2-1

P-1

a = 9.846(2) Å
b = 10.928(3) Å
c = 12.148(3) Å
α = 84.92(3)°
β = 67.30(2)°
γ = 69.93(2)°
V = 1131.2(5) $Å^3$

R_1 = 0.0882

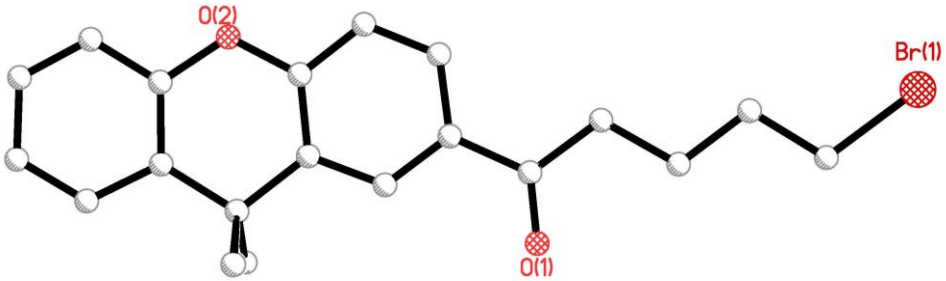


USPK3-Off

$P2_1/c$

a = 11.553(3) Å
b = 12.528(3) Å
c = 12.432(4) Å
β = 106.320(5)°
V = 1726.9(7) $Å^3$

R_1 = 0.0503

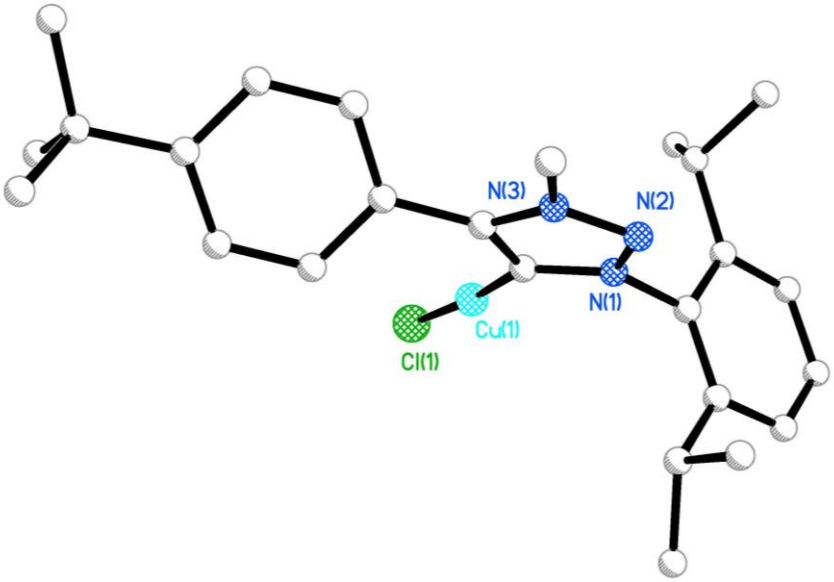


YBCC24_Off

$P2_1/n$

a = 6.426(2) Å
b = 28.842(7) Å
c = 13.413(3) Å
β = 99.157(7)°
V = 2454.1(10) $Å^3$

R_1 = 0.0549

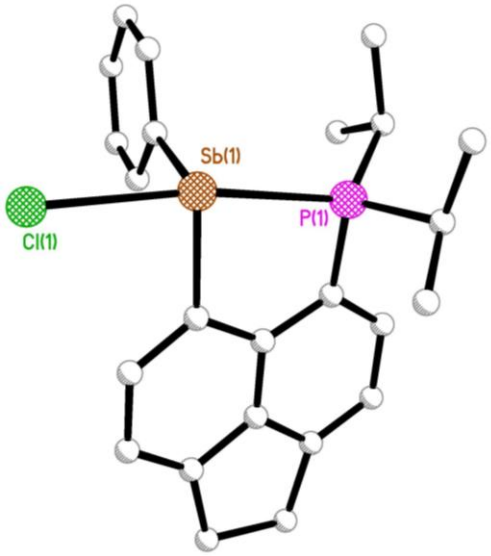


BCPK-45-fs

P-1

a = 8.2454(9) Å
b = 9.2117(11) Å
c = 16.0081(18) Å
α = 102.952(7)°
β = 91.493(6)°
γ = 111.372(8)°
V = 1095.7(2) $Å^3$

R_1 = 0.0260

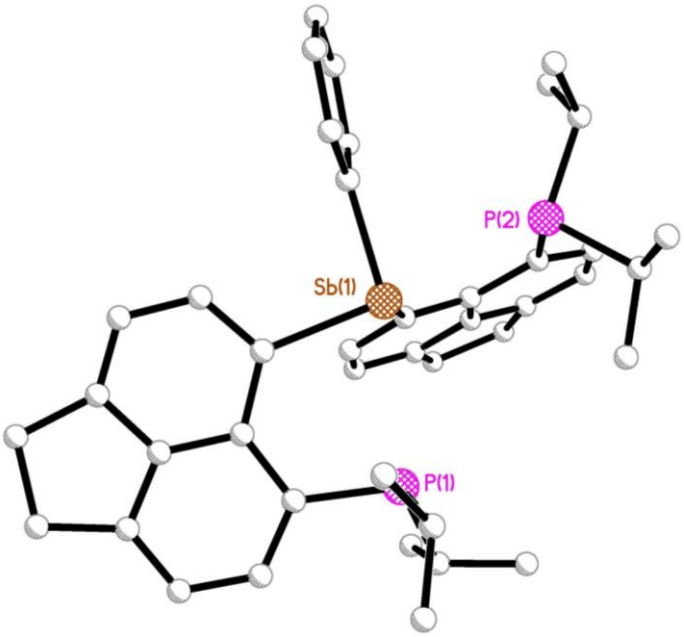


BCPK-54-FS

P-1

a = 9.309(1) Å
b = 11.219(2) Å
c = 18.514(3) Å
α = 75.934(6)°
β = 85.019(6)°
γ = 75.907(6)°
V = 1818.4(4) $Å^3$

R_1 = 0.0704

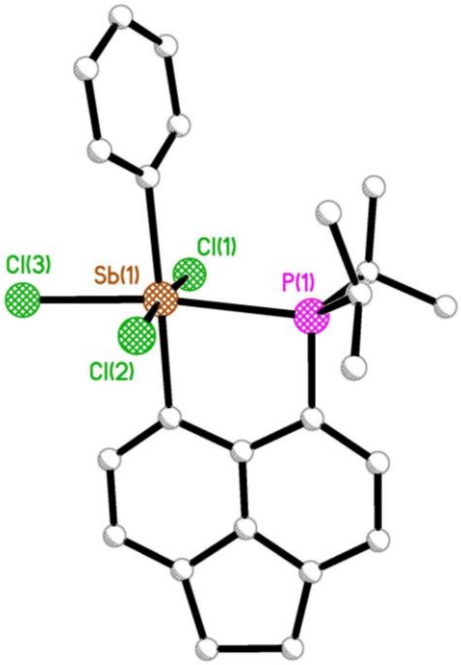


BCPK-62

$Pca2_1$

a = 16.3311(11) Å
b = 7.9541(5) Å
c = 18.1635(13) Å
V = 2359.4(3) $Å^3$

R_1 = 0.0386

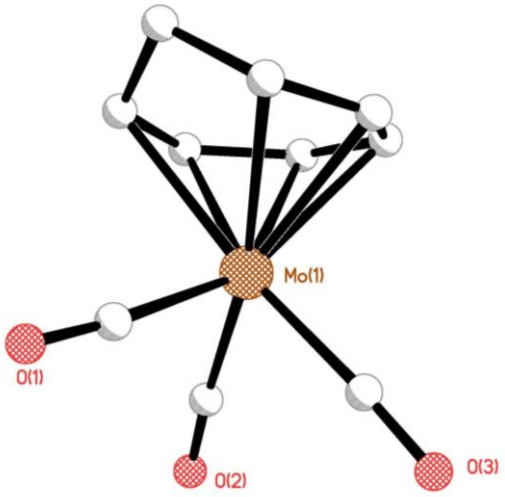


BCPK-65-2-FS

$P2_1/n$

a = 12.152(5) Å
b = 7.062(3) Å
c = 12.323(5) Å
β = 114.08(2)°
V = 965.5(7) $Å^3$

R_1 = 0.0355

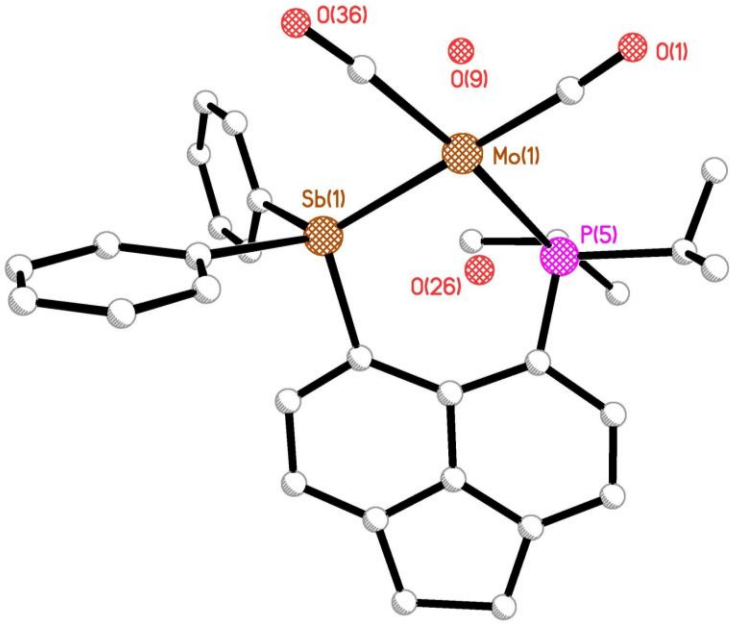


BCPK-72-FS

$P2_1/c$

a = 17.11(2) Å
b = 13.72(2) Å
c = 15.36(2) Å
β = 106.66(2)°
V = 3453(7) $Å^3$

R_1 = 0.0896

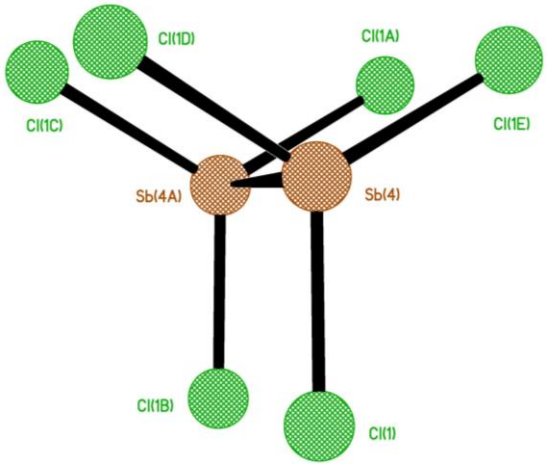


BCPK-80

$P6_3/mmc$

a = 7.243(4) Å
c = 8.389(5) Å
V = 381.2(4) $Å^3$

R_1 = 0.0631

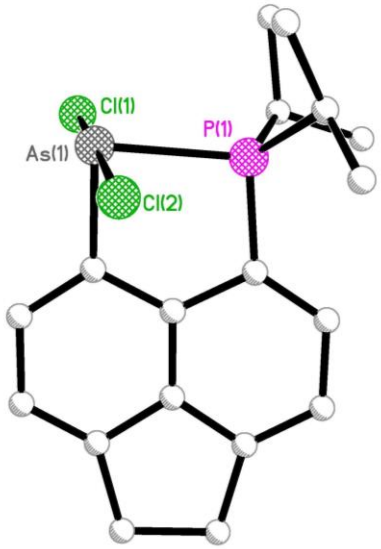


BCPK-82-FS

$P2_1/c$

a = 11.633(3) Å
b = 11.096(3) Å
c = 14.877(4) Å
β = 108.181(8)°
V = 1824.4(8) $Å^3$

R_1 = 0.0449

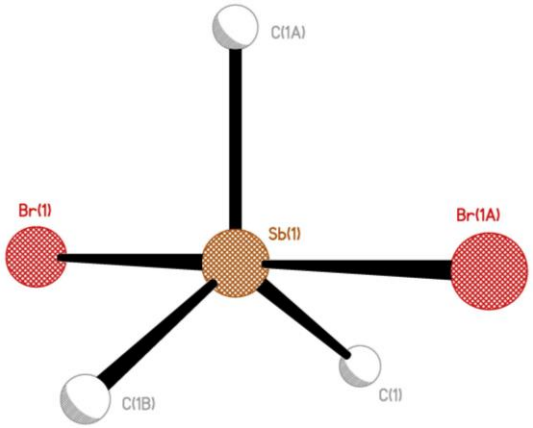


BCPK-84-fs

$P6_3/mmc$

a = 7.321(6) Å
c = 8.855(4) Å
V = 411.0(6) $Å^3$

R_1 = 0.0300

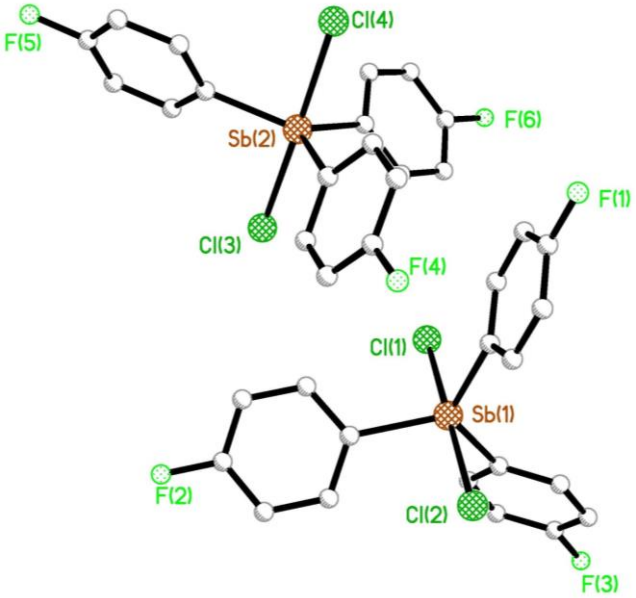


BCPK-94-fs

$P2_1/c$

a = 15.279(2) Å
b = 18.049(2) Å
c = 15.165(1) Å
β = 123.1420(8)°
V = 3501.5(5) $Å^3$

R_1 = 0.0365

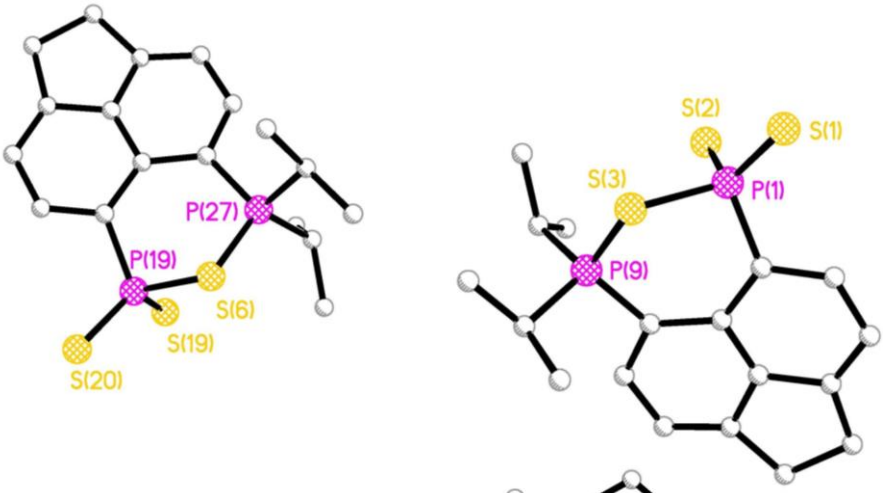


Brian36-off

P-1

a = 7.9678(13) Å
b = 14.172(3) Å
c = 16.796(3) Å
α = 90.762(10)°
β = 91.000(7)°
γ = 92.000(8)°
V = 1894.9(6) $Å^3$

R_1 = 0.0705

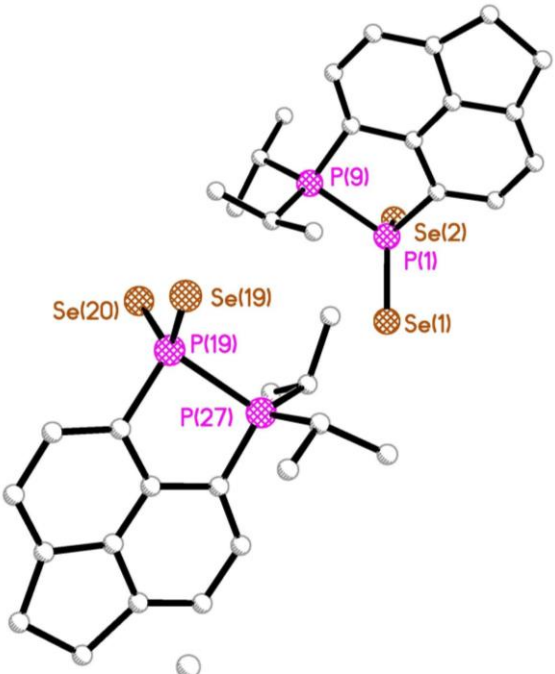


Brian38-off

P-1

a = 8.3216(12) Å
b = 15.389(2) Å
c = 16.939(2) Å
α = 64.679(4)°
β = 78.050(6)°
γ = 80.604(5)°
V = 1911.5(5) $Å^3$

R_1 = 0.0751

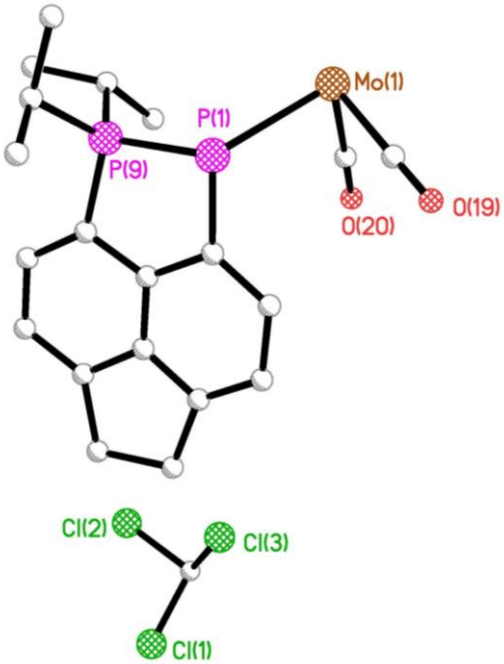


Brian48off

C2/c

a = 21.2672(2) Å
b = 11.072(11) Å
c = 19.143(2) Å
β = 90.793(9)°
V = 4507(5) $Å^3$

R_1 = 0.1156

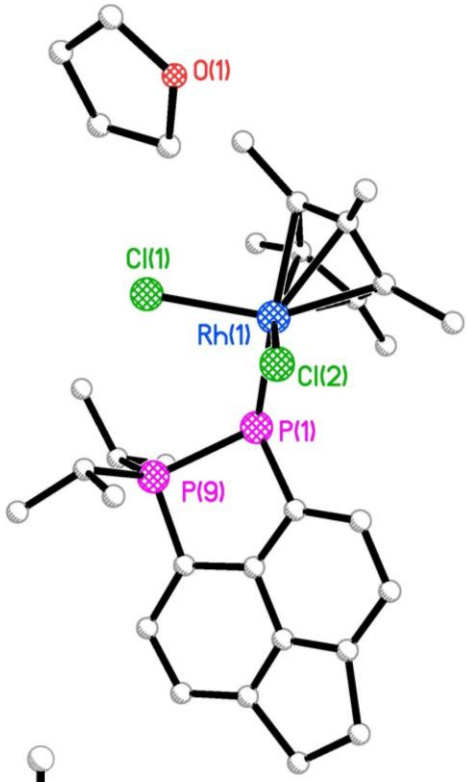


Brian49minioff

$P2_1/c$

a = 15.138(3) Å
b = 13.808(3) Å
c = 16.874(3) Å
β = 99.36(2)°
V = 3479.9(11) $Å^3$

R_1 = 0.2071

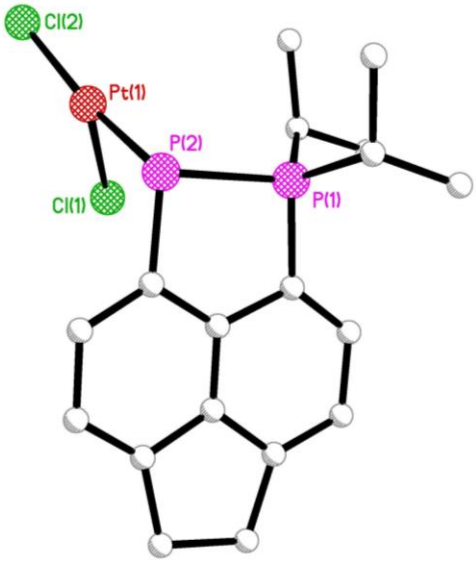


BSPK32

P-1

a = 8.492(2) Å
b = 10.601(3) Å
c = 13.737(3) Å
α = 85.39(3)°
β = 73.92(2)°
γ = 79.53(2)°
V = 1167.9(5) $Å^3$

R_1 = 0.0583

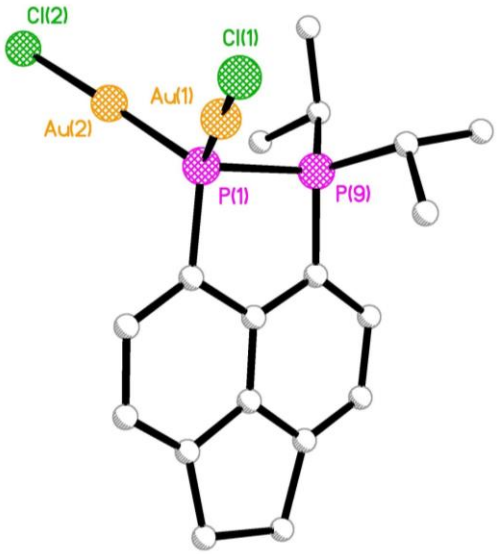


BSPK32mini

C2/c

a = 19.14(3) Å
b = 12.79(2) Å
c = 22.67(3) Å
β = 105.50(2)°
V = 5346(11) $Å^3$

R_1 = 0.0662

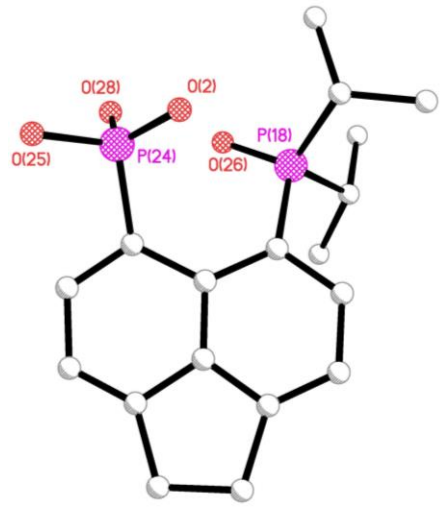


BSPK-34-1TS_Off

P-1

a = 8.987(5) Å
b = 15.110(9) Å
c = 15.777(10) Å
α = 115.74(2)°
β = 91.98(3)°
γ = 90.05(3)°
V = 1928(2) Å^3

R_1 = 0.1525

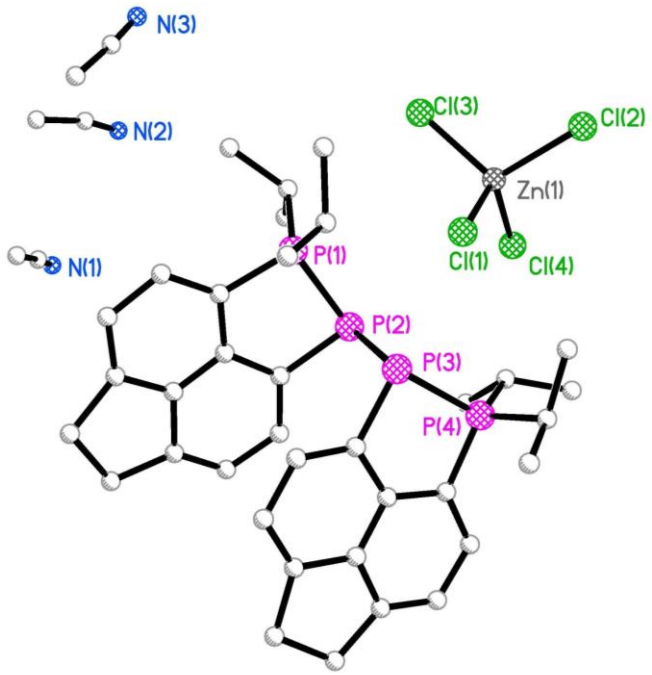


BSPK37

$P2_12_12_1$

a = 12.941(4) Å
b = 16.141(4) Å
c = 21.948(6) Å
V = 4584(2) Å^3

R_1 = 0.0863

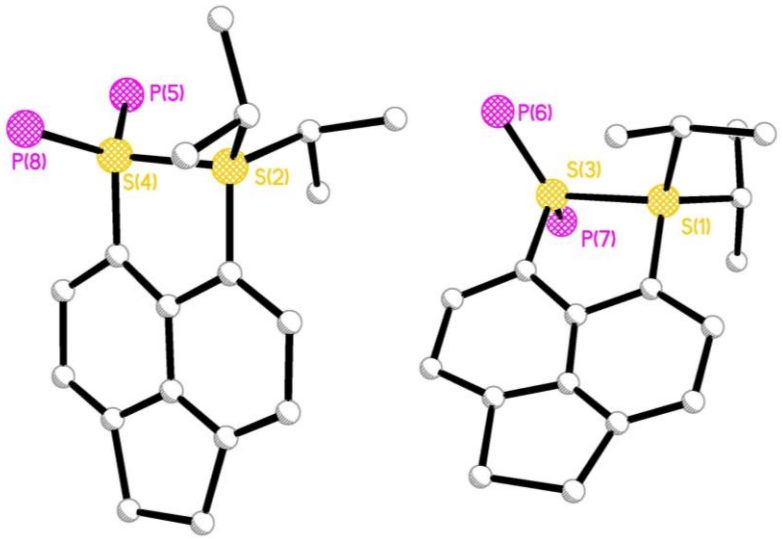


BSPK40

P-1

a = 8.267(3) Å
b = 14.8752(10) Å
c = 16.6453(12) Å
α = 65.56(5)°
β = 79.92(5)°
γ = 81.64(5)°
V = 1828.7(9) Å^3

R_1 = 0.0732

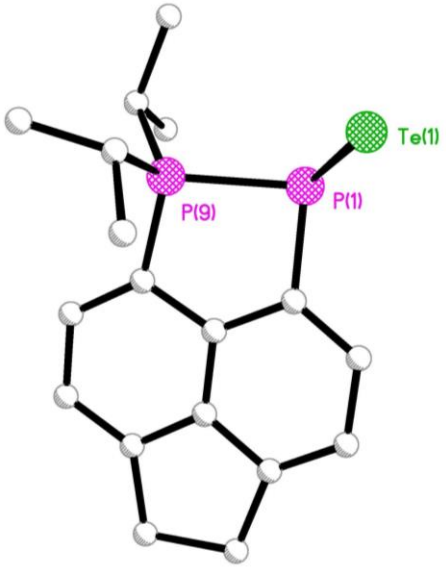


BSPK45fs

P-1

a = 8.043(5) Å
b = 8.499(6) Å
c = 14.948(9) Å
α = 74.38(2)°
β = 76.84(2)°
γ = 65.54(2)°
V = 888(1) $Å^3$

R_1 = 0.0434

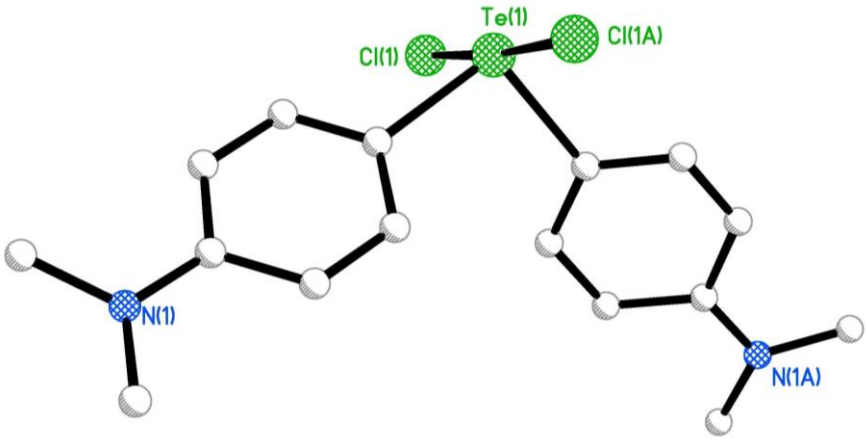


LD066-1

P2/n

a = 8.842(4) Å
b = 5.931(2) Å
c = 16.345(8) Å
β = 96.922(12)°
V = 850.9(7) $Å^3$

R_1 = 0.0634

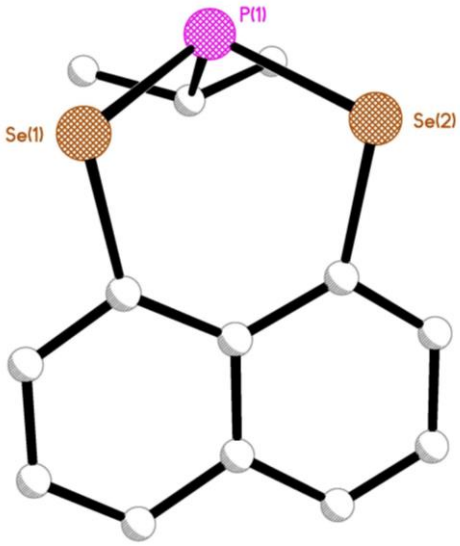


PSDW1

P-1

a = 7.671(2) Å
b = 9.404(2) Å
c = 10.484(3) Å
α = 106.421(8)°
β = 104.690(8)°
γ = 106.308(8)°
V = 649.1(3) $Å^3$

R_1 = 0.0296

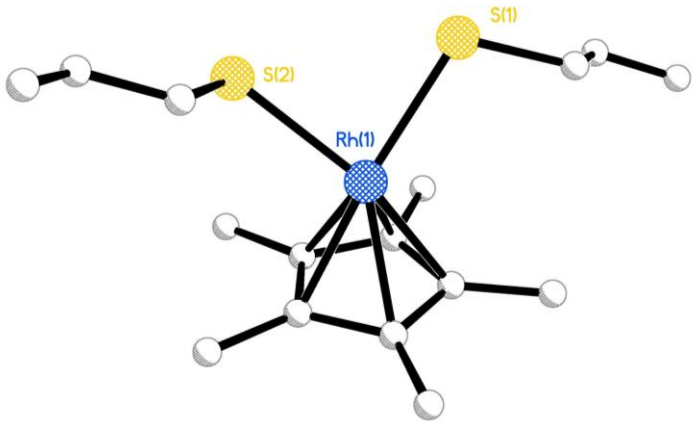


PNPK01-FS

P-1

a = 8.0024(17) Å
b = 10.504(3) Å
c = 10.821(3) Å
α = 61.575(7)°
β = 69.414(7)°
γ = 79.266(7)°
V = 748.7(3) $Å^3$

R_1 = 0.0272

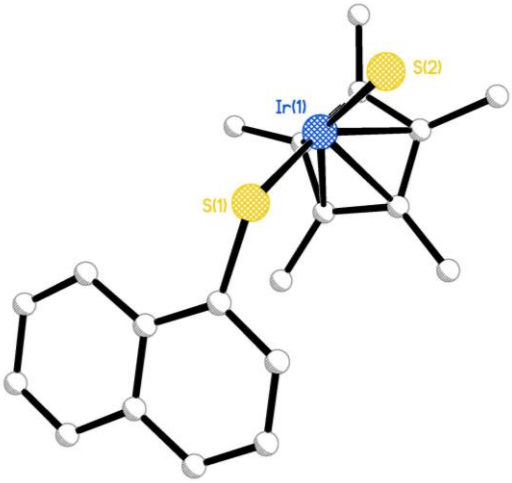


PNPK02-FS

$P2_1/n$

a = 9.8117(9) Å
b = 16.2184(13) Å
c = 10.8329(8) Å
β = 90.330(6)°
V = 1723.8(2) $Å^3$

R_1 = 0.0177



PSC20-fs

$P2_1/c$

a = 21.259(3) Å
b = 7.2032(9) Å
c = 20.189(3) Å
β = 116.264(9)°
V = 2772.5(7) $Å^3$

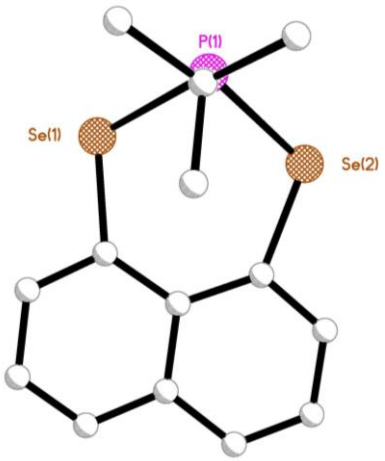
R_1 = 0.0691

PSC21-1-FS

P-1

a = 7.388(2) Å
b = 10.374(2) Å
c = 10.810(2) Å
α = 107.355(8)°
β = 107.255(8)°
γ = 106.126(8)°
V = 691.6(3) $Å^3$

R_1 = 0.0328

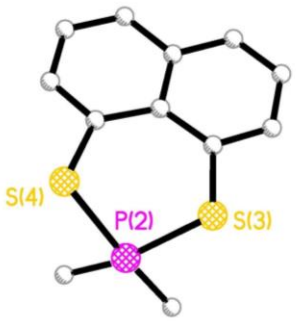


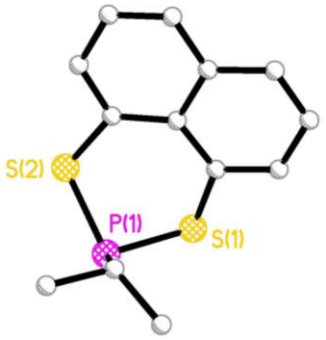
PSC22-FS

$P2_1/c$

a = 18.0397(17) Å
b = 9.8619(10) Å
c = 15.5876(15) Å
β = 114.111(8)°
V = 2531.2(5) $Å^3$

R_1 = 0.0462



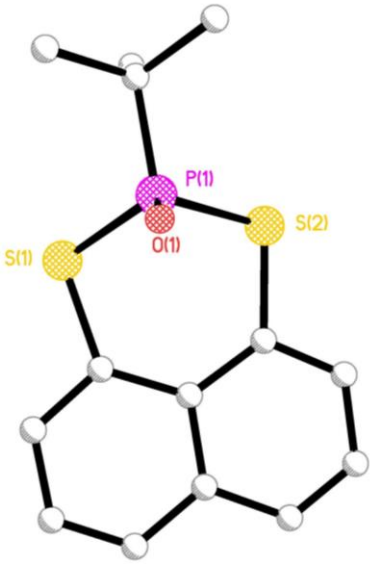


PSC23-fs

$P2_12_12_1$

a = 7.157(2) Å
b = 13.296(3) Å
c = 14.276(3) Å
V = 1358.5(4) $Å^3$

R_1 = 0.0640

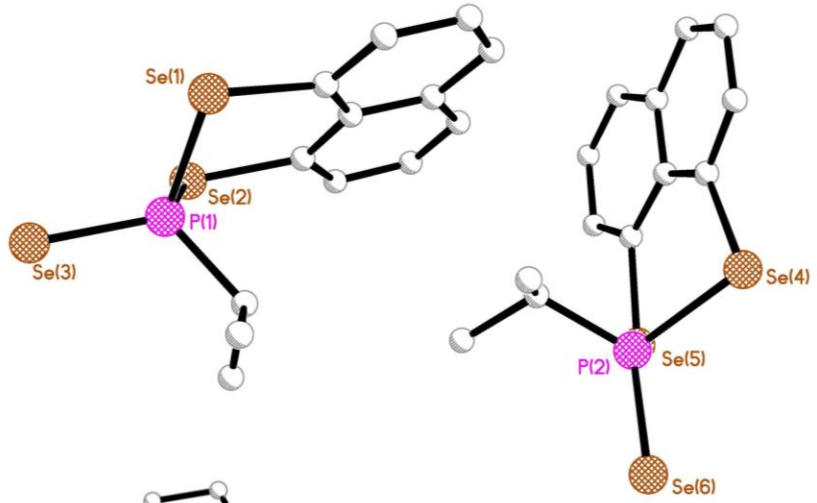


PSC26-FS

P-1

a = 9.201(1) Å
b = 12.861(2) Å
c = 13.126(2) Å
α = 70.831(8)°
β = 89.618(7)°
γ = 78.617(7)°
V = 1435.4(4) $Å^3$

R_1 = 0.0267

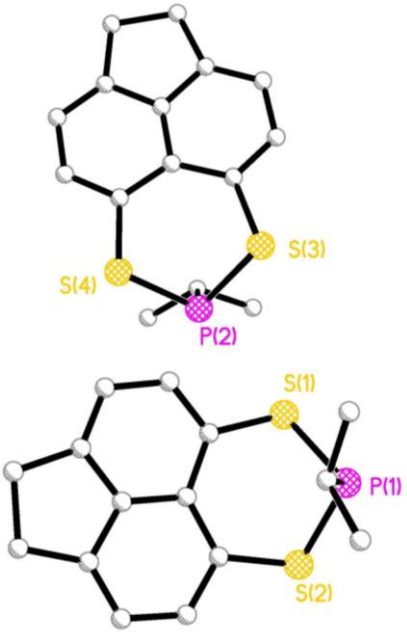


PSC36-fs

P-1

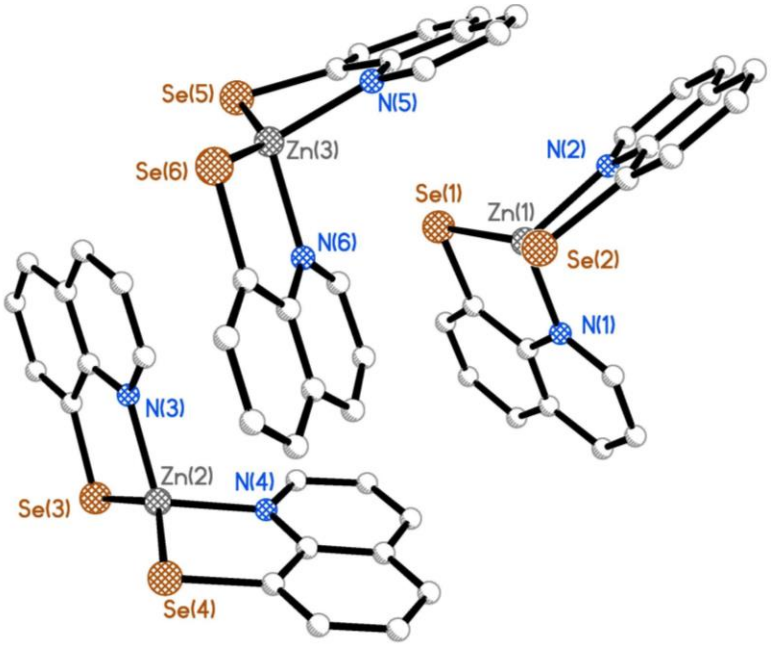
a = 7.474(1) Å
b = 9.595(2) Å
c = 19.319(3) Å
α = 88.766(7)°
β = 82.404(6)°
γ = 85.599(6)°
V = 1369.0(3) $Å^3$

R_1 = 0.0699



NBDW2-off

$P2_1/c$

a = 12.2296(9) Å
b = 16.2379(11) Å
c = 25.1151(18) Å
β = 103.0270(14)°
V = 4859.1(6) $Å^3$

R_1 = 0.0271