

New Journal of Chemistry

Chalcogen bonding interactions in chelating, chiral bis(selenocyanates)

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SUPPLEMENTARY INFORMATION

Crystallography.

ORTEP drawings of the reported structures

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Theoretical calculations

Optimized molecular structures

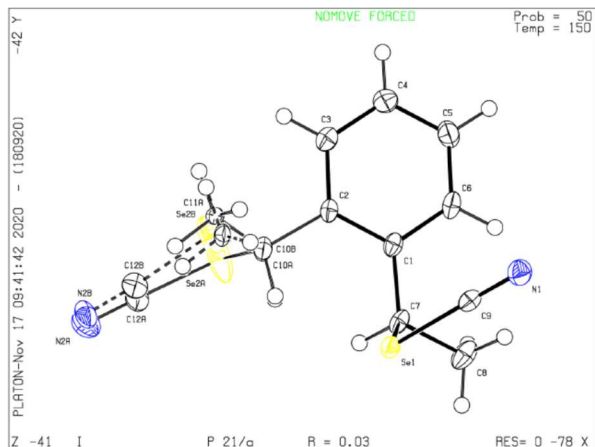
pages 7-12

Cartesian coordinates of the optimized structures

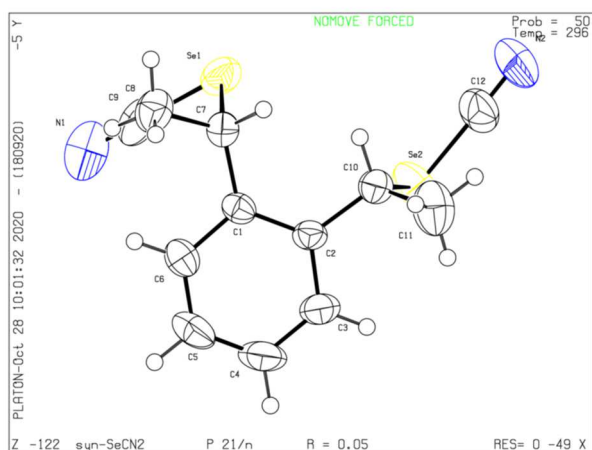
pages 12-18

Crystallography. ORTEP drawings of the reported structures

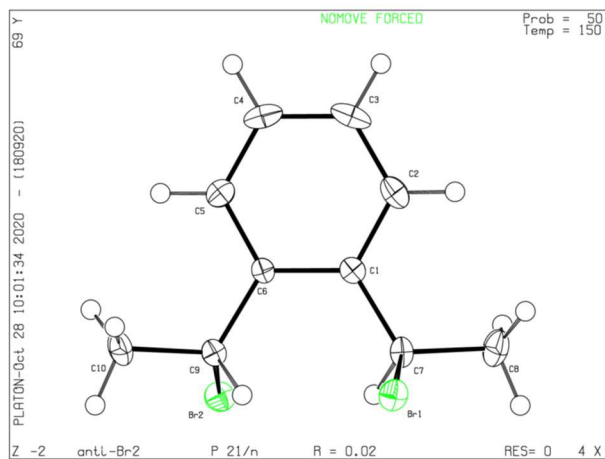
anti-1



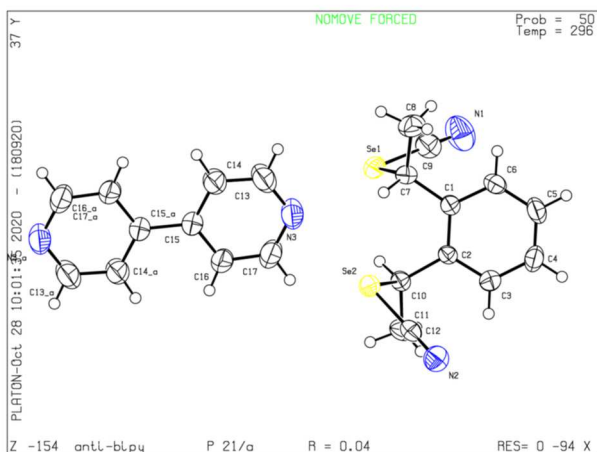
syn-1



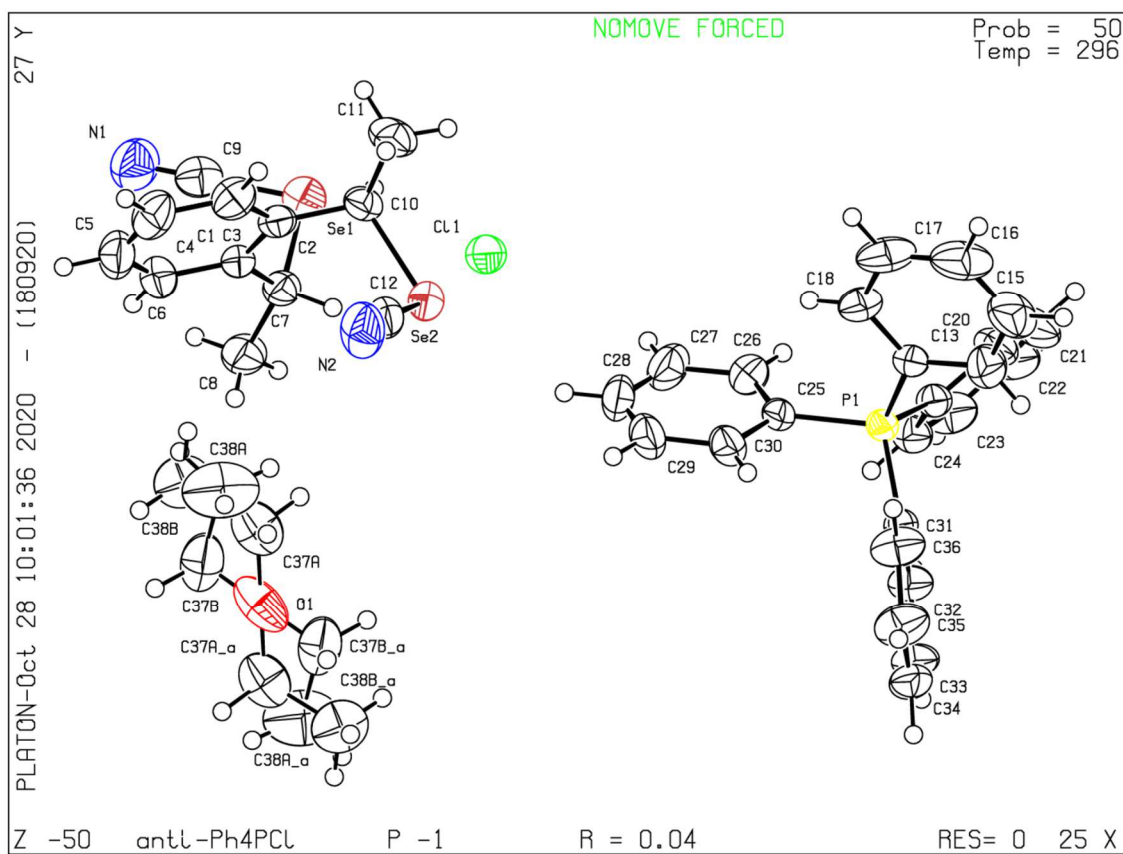
anti-2



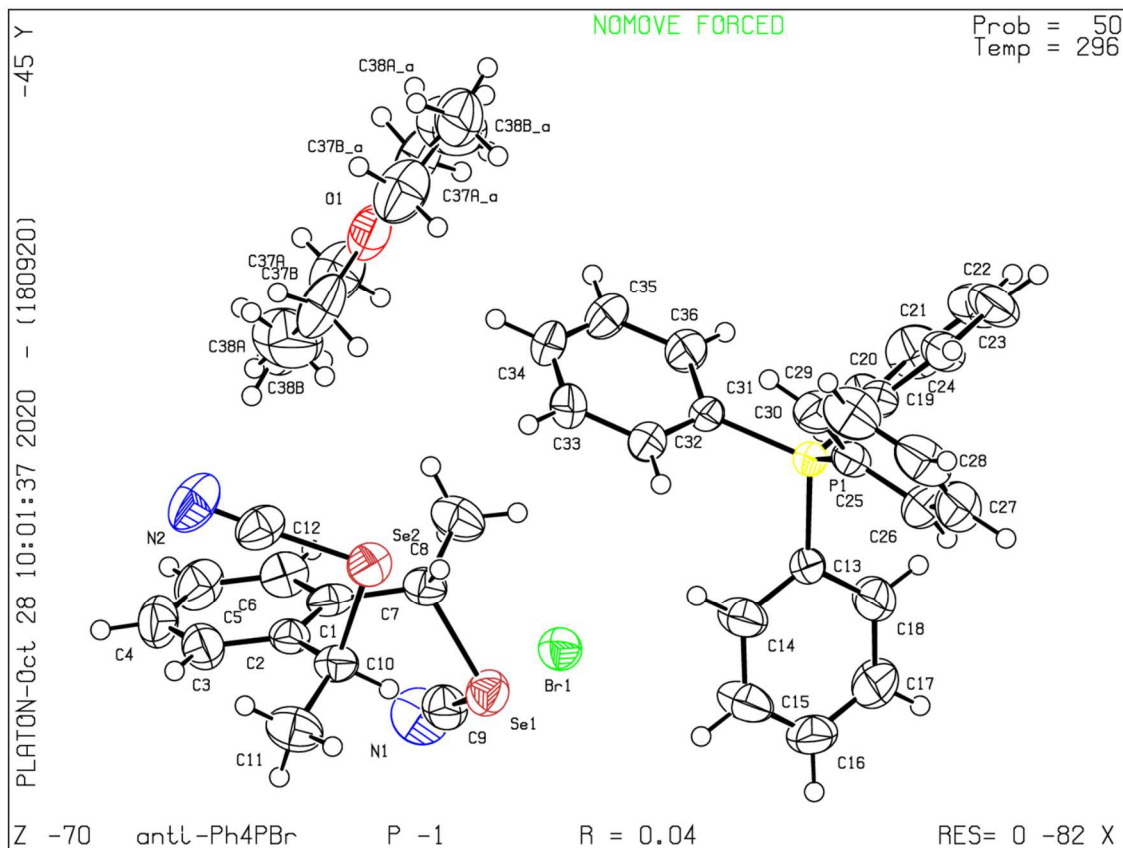
(anti-1)₂•bipy



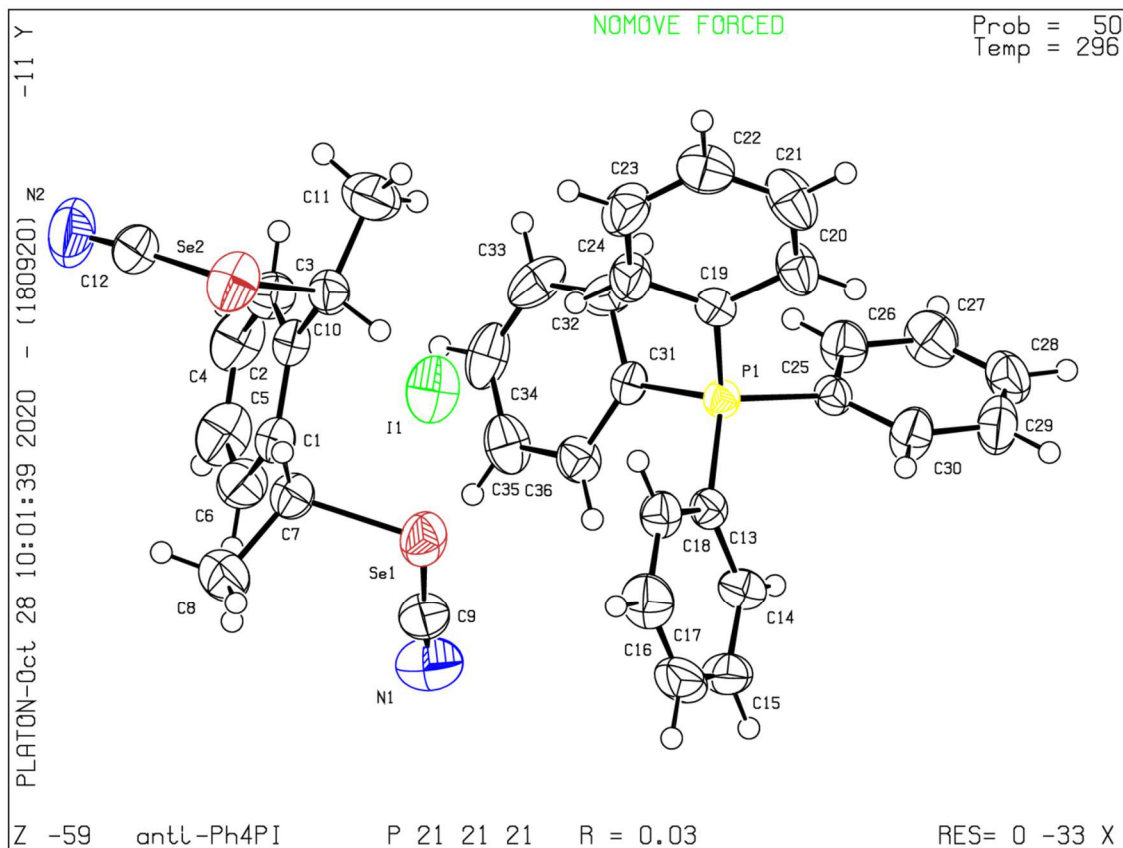
Ph₄PCl(anti-1)•0.5 Et₂O



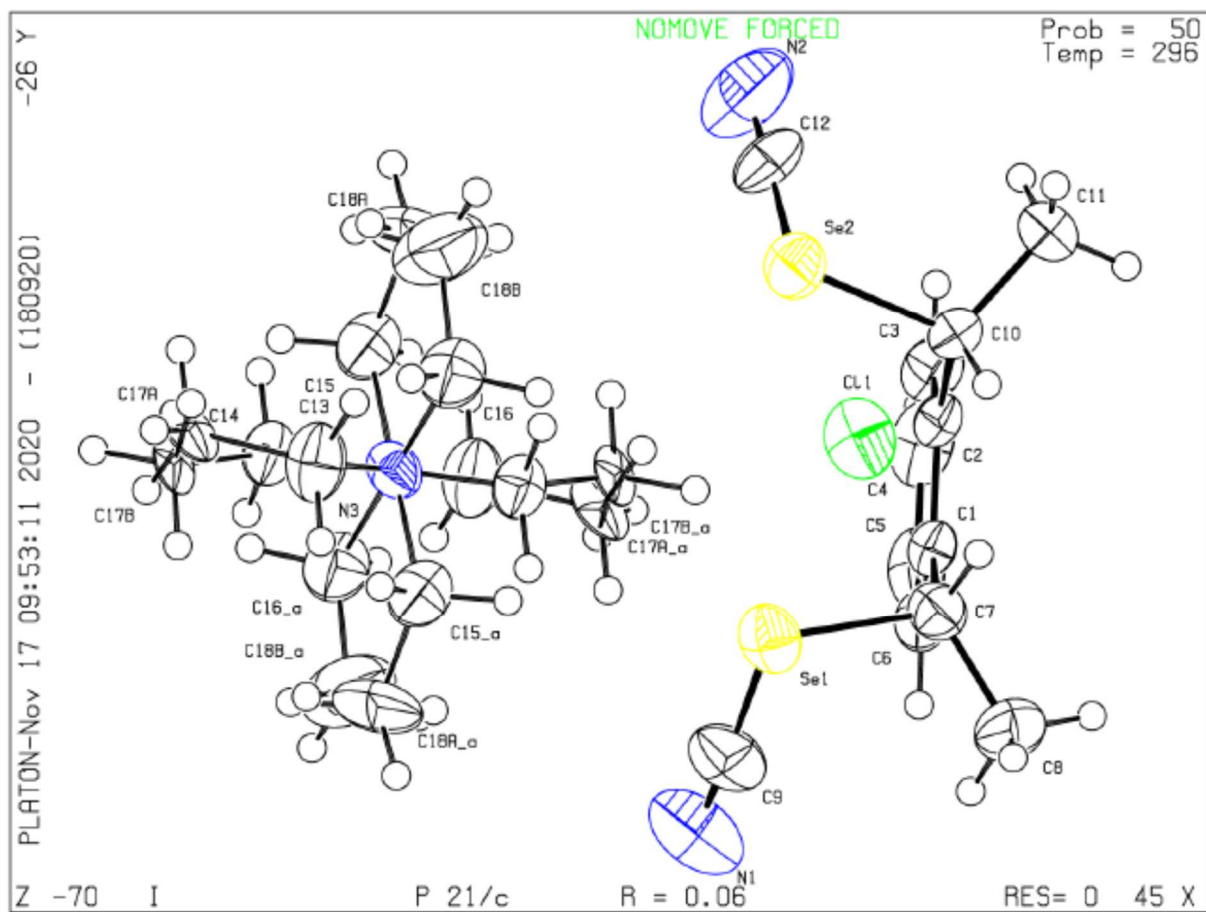
Ph₄PBr(*anti*-1)•0.5 Et₂O



Ph₄PI(*anti*-1)



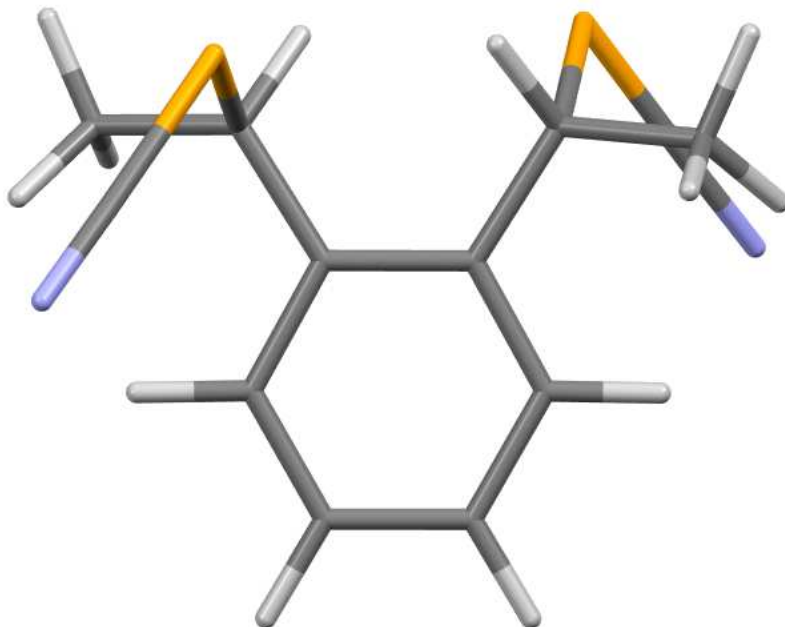
Et₄NCl(syn-1)₂



Theoretical calculations

Optimized molecular structures as stick drawings: carbon=grey; hydrogen=light-grey; selenium=orange; nitrogen=blue; fluorine=light-green.

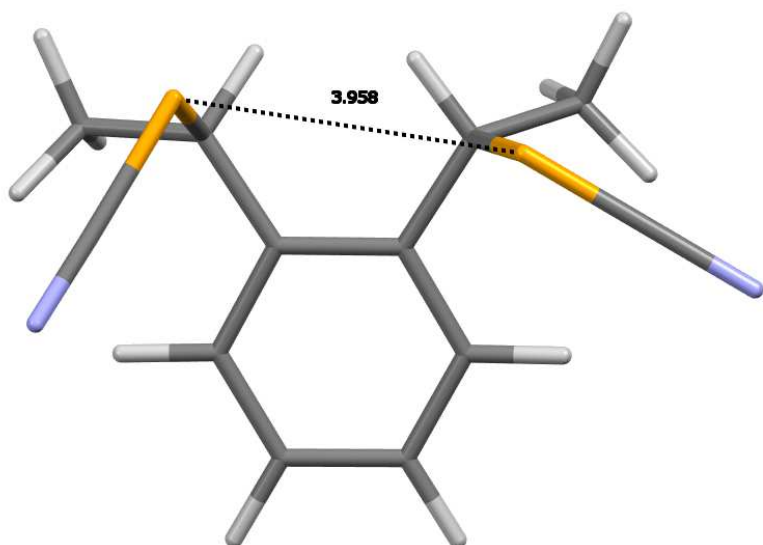
anti-1



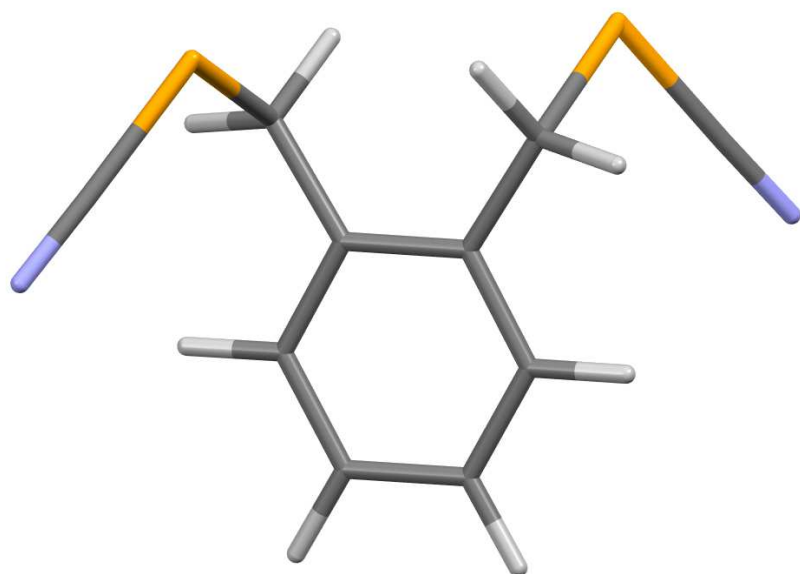
syn-1 Cs



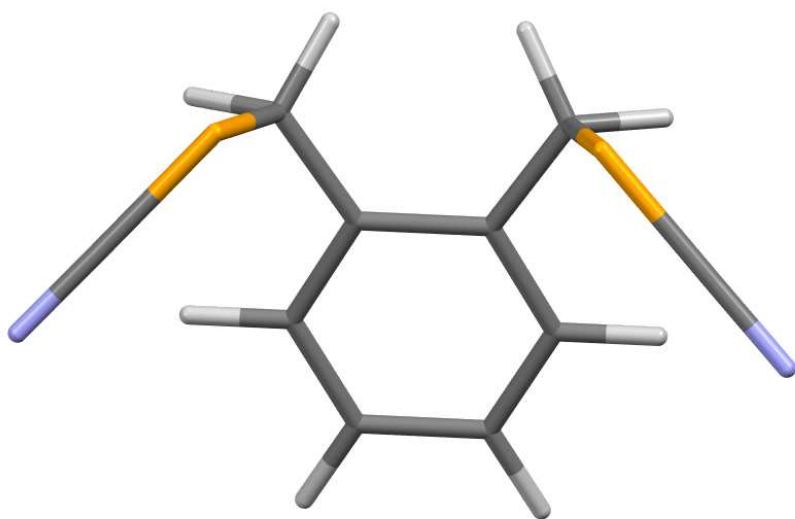
syn-1 C1



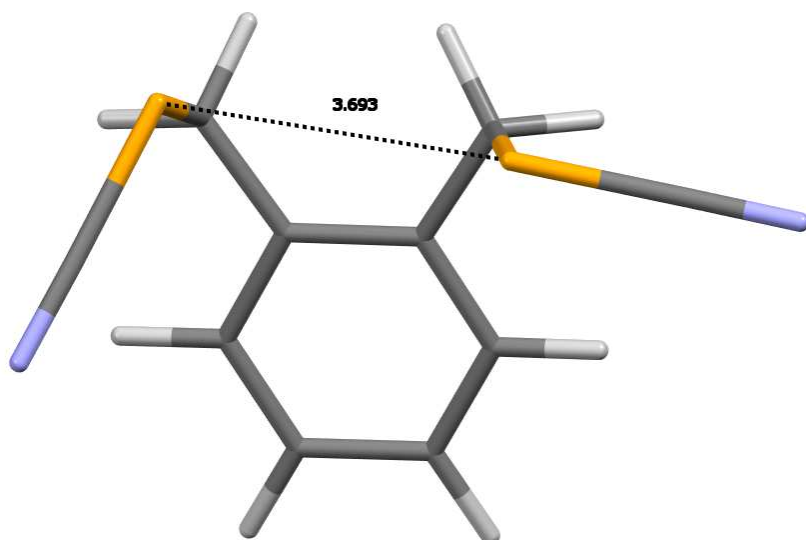
anti-A



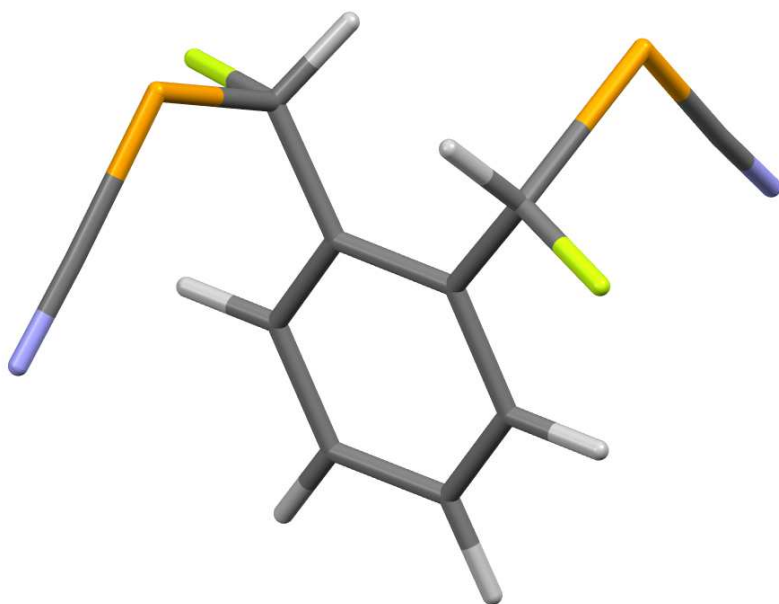
syn-A Cs



syn-A C1



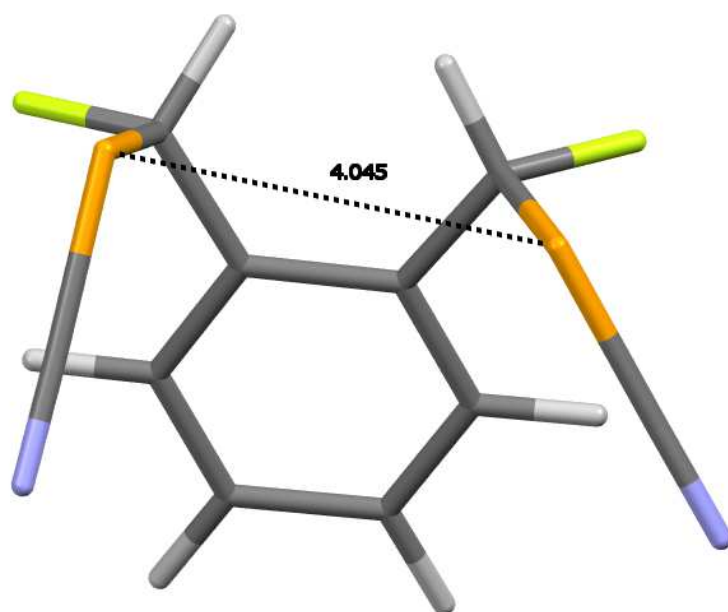
fluorine-substituted *anti*-3



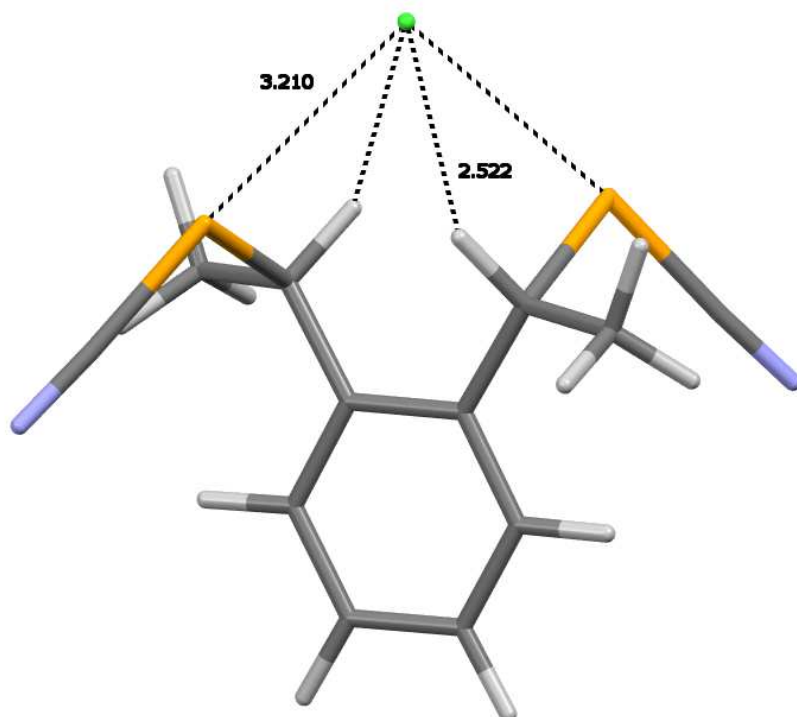
fluorine-substituted *syn*-3 Cs



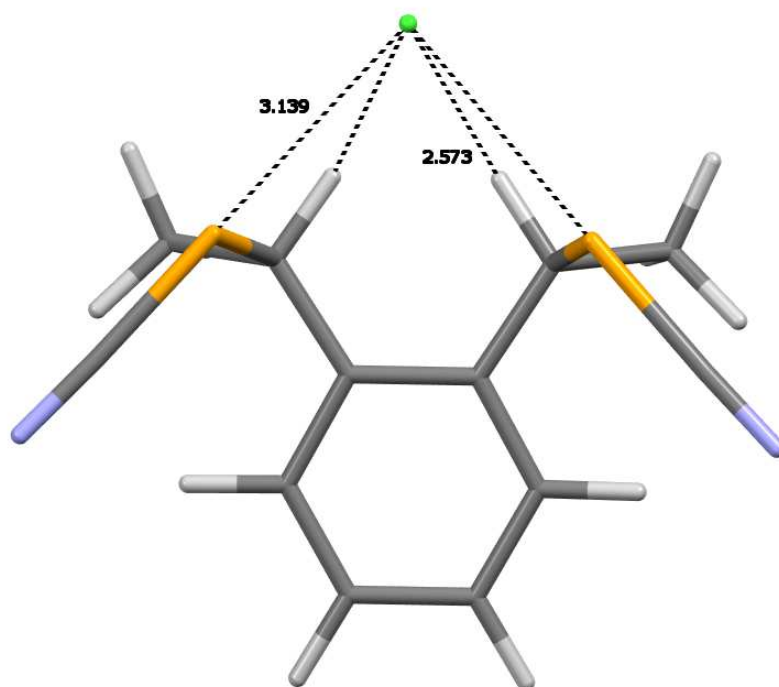
fluorine-substituted *syn*-3 C1



(*anti*-1)Cl⁻



(*syn*-1)Cl⁻



Cartesian coordinates of the optimized structures:

anti-1

C	0.31466900	0.63604200	0.82794700
C	-0.31466900	-0.63604200	0.82794700
C	-0.62857000	-1.23080500	2.05467100
H	-1.12692200	-2.19063600	2.07314800
C	-0.31982100	-0.61635700	3.26460500
H	-0.57847600	-1.10374500	4.19723800
C	0.31982100	0.61635700	3.26460500
H	0.57847600	1.10374500	4.19723800
C	0.62857000	1.23080500	2.05467100
H	1.12692200	2.19063600	2.07314800
C	0.63673000	1.36986800	-0.44802600
H	-0.03616100	1.05893500	-1.24746000
C	0.63673000	2.89454000	-0.38361700
H	-0.32175500	3.24047100	0.01524000
H	0.76947400	3.31557500	-1.38104600
H	1.43146300	3.28670000	0.25205200
C	3.51136400	1.25226400	0.10590200
C	-0.63673000	-1.36986800	-0.44802600
H	0.03616100	-1.05893500	-1.24746000
C	-0.63673000	-2.89454000	-0.38361700
H	0.32175500	-3.24047100	0.01524000
H	-0.76947400	-3.31557500	-1.38104600
H	-1.43146300	-3.28670000	0.25205200
C	-3.51136400	-1.25226400	0.10590200

N	4.22442200	1.59494100	0.95321800
N	-4.22442200	-1.59494100	0.95321800
Se	2.40758700	0.71392600	-1.26795800
Se	-2.40758700	-0.71392600	-1.26795800

syn-1 Cs

C	1.12478400	0.50033400	0.70937400
C	1.12478400	0.50033400	-0.70937400
C	2.17816100	-0.13787100	-1.38073200
H	2.18960800	-0.15223700	-2.46262800
C	3.20516600	-0.77378400	-0.69572600
H	3.99712700	-1.26615800	-1.24772500
C	3.20516600	-0.77378400	0.69572600
H	3.99712700	-1.26615800	1.24772500
C	2.17816100	-0.13787100	1.38073200
H	2.18960800	-0.15223700	2.46262800
C	0.05239700	1.16849200	1.53288100
H	-0.56385500	1.82488500	0.92038000
C	0.53063700	1.95937500	2.74888200
H	0.99249000	1.32461000	3.50564100
H	-0.30386700	2.48439200	3.21609200
H	1.27343200	2.69664700	2.42874800
C	-0.46052300	-1.06377200	3.36984600
C	0.05239700	1.16849200	-1.53288100
H	-0.56385500	1.82488500	-0.92038000
C	0.53063700	1.95937500	-2.74888200
H	1.27343200	2.69664700	-2.42874800
H	-0.30386700	2.48439200	-3.21609200
H	0.99249000	1.32461000	-3.50564100
C	-0.46052300	-1.06377200	-3.36984600
N	0.12336400	-1.63824800	4.19050600
N	0.12336400	-1.63824800	-4.19050600
Se	-1.41859400	-0.15767800	2.08272100
Se	-1.41859400	-0.15767800	-2.08272100

syn-1 C1

C	1.13057900	0.45269700	0.62493200
C	1.22821300	0.58807800	-0.78283000
C	2.32516500	0.00869800	-1.43659000
H	2.41090900	0.08803600	-2.51182900
C	3.31626300	-0.67127000	-0.73911400
H	4.14786400	-1.11115800	-1.27689900
C	3.23127600	-0.78096800	0.64507200
H	3.99671100	-1.30566200	1.20473400
C	2.14801100	-0.22175900	1.31128000
H	2.08085300	-0.33357700	2.38655700
C	-0.03251000	0.99992400	1.41403500

H	-0.71524600	1.55776400	0.77730600
C	0.33205800	1.87171000	2.61321600
H	0.90596000	1.32788600	3.36400600
H	-0.56431200	2.26765200	3.09341900
H	0.94383400	2.71104000	2.26772000
C	-0.48734700	-1.00476600	3.51840400
C	0.21415900	1.35346600	-1.59624800
H	-0.23260300	2.15026100	-1.00026900
C	0.69497800	1.94914100	-2.91675500
H	1.57844000	2.57019800	-2.73890300
H	-0.08451000	2.57373400	-3.35490000
H	0.95844800	1.18448700	-3.64852300
C	-0.68974100	-1.11825600	-2.87892800
N	0.02248200	-1.33619000	4.50596200
N	-0.20704000	-1.97419500	-3.49353300
Se	-1.32363800	-0.50499300	1.95066000
Se	-1.48860200	0.24599700	-1.93198200

anti-A

C	-0.45561000	0.54015100	0.84120300
C	0.45561000	-0.54015100	0.84120300
C	0.88581800	-1.06392600	2.06452800
H	1.57608700	-1.90014000	2.06752100
C	0.44377700	-0.53531400	3.27413000
H	0.79265200	-0.95984200	4.20800700
C	-0.44377700	0.53531400	3.27413000
H	-0.79265200	0.95984200	4.20800700
C	-0.88581800	1.06392600	2.06452800
H	-1.57608700	1.90014000	2.06752100
C	-0.99783600	1.14065800	-0.41503300
H	-1.17741800	0.41205400	-1.20609300
C	0.35634500	3.67347200	0.03469800
C	0.99783600	-1.14065800	-0.41503300
H	1.17741800	-0.41205400	-1.20609300
C	-0.35634500	-3.67347200	0.03469800
N	0.44377700	4.45927700	0.88195900
N	-0.44377700	-4.45927700	0.88195900
Se	0.23483100	2.45773800	-1.34711200
Se	-0.23483100	-2.45773800	-1.34711200
H	-1.91857800	1.69066100	-0.23849100
H	1.91857800	-1.69066100	-0.23849100

syn-A Cs

C	1.18891300	0.77157300	0.70711700
C	1.18891300	0.77157300	-0.70711700
C	2.29660600	0.24316400	-1.38362100
H	2.30295700	0.24712700	-2.46775800
C	3.38036300	-0.29065400	-0.69617800
H	4.22048400	-0.69803800	-1.24609900

C	3.38036300	-0.29065400	0.69617800
H	4.22048400	-0.69803800	1.24609900
C	2.29660600	0.24316400	1.38362100
H	2.30295700	0.24712700	2.46775800
C	0.07500400	1.33735100	1.52863200
H	-0.49756100	2.11820800	1.03008500
C	-0.39782700	-0.93488100	3.26409500
C	0.07500400	1.33735100	-1.52863200
H	-0.49756100	2.11820800	-1.03008500
C	-0.39782700	-0.93488100	-3.26409500
N	0.20274900	-1.54453900	4.04594100
N	0.20274900	-1.54453900	-4.04594100
Se	-1.38619400	0.01928200	2.03388300
Se	-1.38619400	0.01928200	-2.03388300
H	0.42711400	1.72956900	-2.47948000
H	0.42711400	1.72956900	2.47948000

syn-A C1

C	1.25848700	0.66875600	0.59735900
C	1.30278000	0.84240600	-0.80376100
C	2.44635400	0.43565100	-1.50320900
H	2.47866600	0.55995400	-2.57995700
C	3.53730800	-0.12030200	-0.84461200
H	4.40976700	-0.42784400	-1.40876400
C	3.50002300	-0.27571400	0.53888400
H	4.34559400	-0.70211400	1.06573300
C	2.36927300	0.11653500	1.24609900
H	2.33922000	-0.01311800	2.32274100
C	0.06603100	1.04622600	1.41590500
H	-0.55345000	1.82113500	0.97224400
C	-0.81362900	-0.74498600	3.50914900
C	0.19000200	1.46757800	-1.58259400
H	-0.26553800	2.32755100	-1.08996400
C	-0.56380900	-1.06865200	-2.78283200
N	-0.56976300	-0.91802500	4.62947000
N	-0.04582500	-1.92676200	-3.36385700
Se	-1.22318300	-0.50489500	1.71954500
Se	-1.43284000	0.28693100	-1.88079500
H	0.51113300	1.77029600	-2.57587400
H	0.33861500	1.35571600	2.42149000

anti-3

C	-0.46745200	0.52962100	0.86200300
C	0.46745200	-0.52962100	0.86200300
C	0.91291500	-1.04664900	2.08026500
H	1.62878400	-1.85730900	2.07950900
C	0.45591800	-0.52425600	3.28645200
H	0.81488100	-0.93983700	4.22029300
C	-0.45591800	0.52425600	3.28645200
H	-0.81488100	0.93983700	4.22029300

C	-0.91291500	1.04664900	2.08026500
H	-1.62878400	1.85730900	2.07950900
C	-1.01725800	1.11155600	-0.40467800
H	-1.19163900	0.36610700	-1.18249100
C	0.91291500	3.26478600	0.12164200
C	1.01725800	-1.11155600	-0.40467800
H	1.19163900	-0.36610700	-1.18249100
C	-0.91291500	-3.26478600	0.12164200
N	1.37110400	3.83881500	1.01717200
N	-1.37110400	-3.83881500	1.01717200
Se	0.22618500	2.40817400	-1.36078500
Se	-0.22618500	-2.40817400	-1.36078500
F	2.21009200	-1.76477000	-0.18277100
F	-2.21009200	1.76477000	-0.18277100

syn-3 Cs

C	-1.13252300	-0.60541400	0.70646500
C	-1.13252300	-0.60541400	-0.70646500
C	-2.21104200	-0.03064700	-1.38807300
H	-2.22130300	-0.04647600	-2.46956700
C	-3.27073700	0.54238700	-0.69574700
H	-4.09241200	0.98595900	-1.24500700
C	-3.27073700	0.54238700	0.69574700
H	-4.09241200	0.98595900	1.24500700
C	-2.21104200	-0.03064700	1.38807300
H	-2.22130300	-0.04647600	2.46956700
C	-0.04155400	-1.22845000	1.52196200
H	0.52663400	-1.99201300	0.98959600
C	0.42174600	1.41290100	2.71472600
C	-0.04155400	-1.22845000	-1.52196200
H	0.52663400	-1.99201300	-0.98959600
C	0.42174600	1.41290100	-2.71472600
N	-0.17695100	2.31117600	3.13488400
N	-0.17695100	2.31117600	-3.13488400
Se	1.45314900	0.02082400	2.08564900
Se	1.45314900	0.02082400	-2.08564900
F	-0.55296400	-1.81982100	2.66102700
F	-0.55296400	-1.81982100	-2.66102700

syn-3 C1

C	-1.11326700	-0.55795000	0.62983500
C	-1.19503400	-0.63924700	-0.77794900
C	-2.30918200	-0.09962100	-1.42909400
H	-2.37445800	-0.16567200	-2.50667700
C	-3.33921400	0.49229500	-0.70756600
H	-4.19206300	0.90573700	-1.23240100
C	-3.27514400	0.54137700	0.68159500
H	-4.07881700	0.98977100	1.25313300
C	-2.16999800	0.01862700	1.34241100

H	-2.12341900	0.05405000	2.42245000
C	0.06287800	-1.07693600	1.39725000
H	0.68974800	-1.76590400	0.83110700
C	0.33596700	1.41700800	2.90371700
C	-0.16120800	-1.33408000	-1.61260000
H	0.30160200	-2.18624500	-1.11257000
C	0.63466300	1.38823500	-2.37609700
N	-0.30984400	2.13214300	3.54688300
N	0.15818700	2.42533800	-2.57286500
Se	1.43900100	0.32595200	1.90733700
Se	1.47166200	-0.23093600	-2.09859200
F	-0.33873400	-1.72667200	2.54704500
F	-0.70924200	-1.80642100	-2.78855000

(*anti-1*)Cl⁻

C	-0.16668200	0.69047000	-1.21454200
C	0.16668200	-0.69047000	-1.21454200
C	0.34318700	-1.33687700	-2.44337700
H	0.62117100	-2.38257600	-2.45719300
C	0.17822500	-0.67142200	-3.65509200
H	0.32684300	-1.20399700	-4.58825500
C	-0.17822500	0.67142200	-3.65509200
H	-0.32684300	1.20399700	-4.58825500
C	-0.34318700	1.33687700	-2.44337700
H	-0.62117100	2.38257600	-2.45719300
C	-0.29207700	1.47660000	0.06567800
H	0.32237000	1.04540000	0.85426800
C	0.00000000	2.97134300	-0.01905700
H	0.98681800	3.12648600	-0.46882300
H	0.00890200	3.39643400	0.98557200
H	-0.73613900	3.51790600	-0.61234400
C	-3.12363900	1.93207100	-0.37874600
C	0.29207700	-1.47660000	0.06567800
H	-0.32237000	-1.04540000	0.85426800
C	0.00000000	-2.97134300	-0.01905700
H	-0.98681800	-3.12648600	-0.46882300
H	-0.00890200	-3.39643400	0.98557200
H	0.73613900	-3.51790600	-0.61234400
C	3.12363900	-1.93207100	-0.37874600
N	-3.81072400	2.40821900	-1.18549800
N	3.81072400	-2.40821900	-1.18549800
Se	-2.09205100	1.17754400	0.99631600
Se	2.09205100	-1.17754400	0.99631600
Cl	0.00000000	0.00000000	3.12721700

(*syn-1*)Cl⁻

C	1.28260600	0.64555800	0.70994800
C	1.28260600	0.64555800	-0.70994800
C	2.45888300	0.27281500	-1.37895800

H	2.46790300	0.25695200	-2.46097100
C	3.60869200	-0.10293100	-0.69593100
H	4.49351400	-0.39812800	-1.24953300
C	3.60869200	-0.10293100	0.69593100
H	4.49351400	-0.39812800	1.24953300
C	2.45888300	0.27281500	1.37895800
H	2.46790300	0.25695200	2.46097100
C	0.08177100	1.05389100	1.52906400
H	-0.68061100	1.53077100	0.91893900
C	0.37420900	1.94027900	2.73797700
H	0.95920400	1.43352700	3.50760500
H	-0.56271100	2.27156400	3.18907700
H	0.93598400	2.82341300	2.41314000
C	0.16225600	-1.22210300	3.33348600
C	0.08177100	1.05389100	-1.52906400
H	-0.68061100	1.53077100	-0.91893900
C	0.37420900	1.94027900	-2.73797700
H	0.93598400	2.82341300	-2.41314000
H	-0.56271100	2.27156400	-3.18907700
H	0.95920400	1.43352700	-3.50760500
C	0.16225600	-1.22210300	-3.33348600
N	0.86778600	-1.66913400	4.14156900
N	0.86778600	-1.66913400	-4.14156900
Se	-1.06448500	-0.55143900	2.07488000
Se	-1.06448500	-0.55143900	-2.07488000
Cl	-2.97715300	0.82232100	0.00000000