Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Metal-metal bond passing through the arene ligand: Theoretical study on inverse sandwiches X[Sc-C_8H_8-Sc]$_n$X (X= F, Cl, Br; n = 1, 2)

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This supplementary material belongs to *New Journal of Chemistry,* and is uploaded in November, 2014.

Part 1 Bond Analysis

1. The Sc-Sc interaction in triplet X[Sc-C_8H_8-Sc]X (X=F, Cl, Br)

The Sc-Sc bond is not totally broken in the triplet state. In triplet X[Sc-C_8H_8-Sc]X, the Mayer and Wiberg bond orders of Sc-Sc are 0.26, 0.27 for X=F, 0.27 and 0.29 for X=Cl, 0.28 and 0.29 for X=Br. Figure 1 shows the α-HOMO and β-HOMO (α is lower in energy than β) of X[Sc-C_8H_8-Sc]X, Figure 2 shows the LOL plot of Sc-Sc in X[Sc-C_8H_8-Sc]X, Figure 3 shows the value of orbital wave-function of α-HOMO and β-HOMO. From LOL values, the minima of 0.266 for X=F, 0.320 for X=Cl and 0.332 for X=Br are found in the middle area between two Sc atoms. Thus, although weak, the Sc-Sc interaction also exist in triplet X[Sc-C_8H_8-Sc]X.

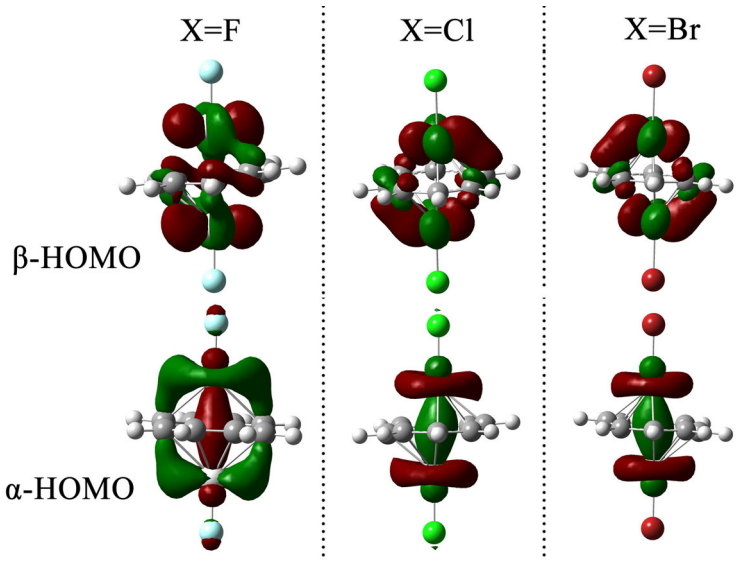

Figure 1 The α-HOMO and β-HOMO of X[Sc-C_8H_8-Sc]X (X=F, Cl, Br)

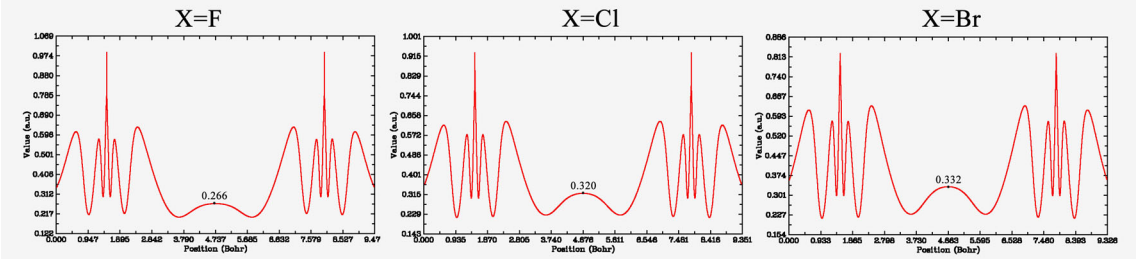

Figure 2 The LOL values of Sc-Sc interaction of X[Sc-C_8H_8-Sc]X (X=F, Cl, Br)

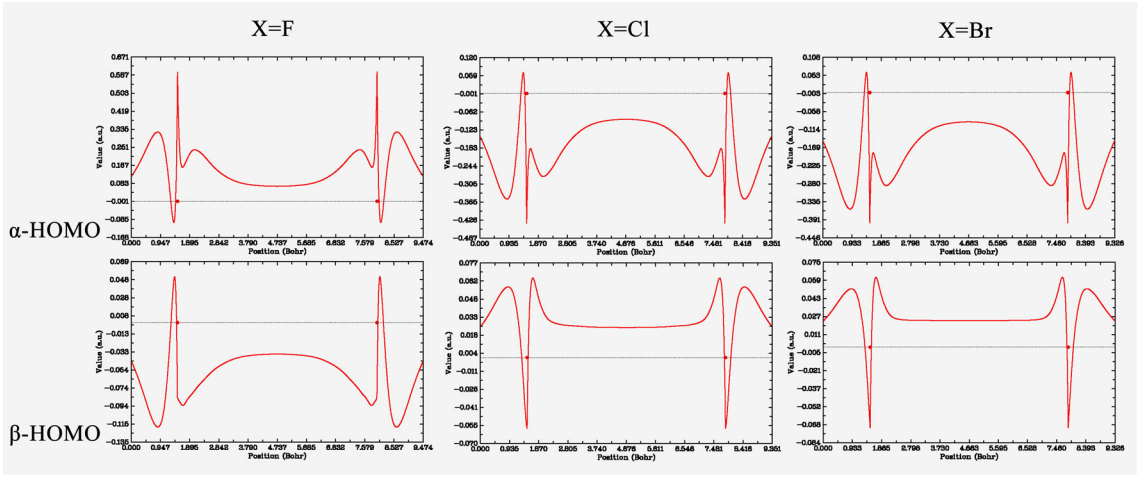

Figure 3 The wave-function values of α-HOMO and β-HOMO of X[Sc-C_8H_8-Sc]X (X=F, Cl, Br)

2. The Sc-Sc interaction in triplet X[Sc-C_8H_8-Sc]$_2$X (X=F, Cl, Br)

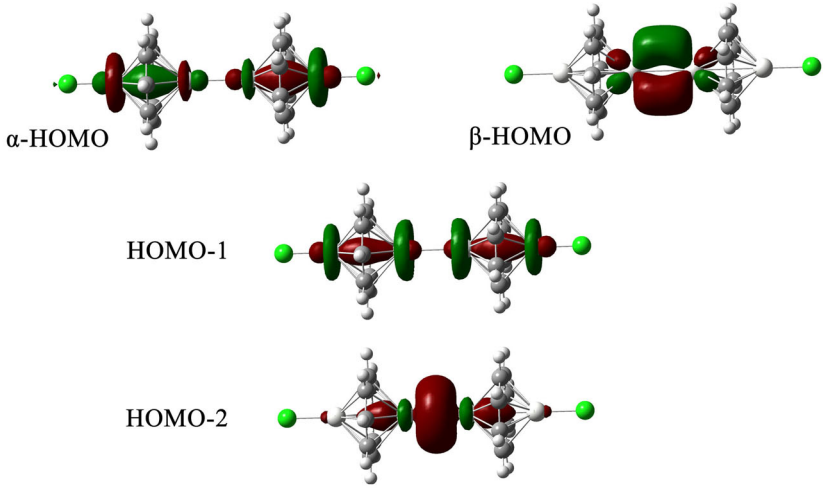

Figure 4. α-HOMO, β-HOMO, HOMO-1 and HOMO-2 of X[Sc-C_8H_8-Sc]$_2$X (X=F, Cl, Br)

In singlet X[Sc-C_8H_8-Sc]$_2$X, the central Sc-Sc is single bond, but in the triplet, it could be roughly seemed as one and a half bond. Figure 4 shows theα-HOMO, β-HOMO, HOMO-1 and HOMO-2 (α is lower in energy than β) of X[Sc-C_8H_8-Sc]$_2$X. Between the central Sc atoms, HOMO-2 is a $\sigma_{Sc\text{-}Sc}$ single bond, and β-HOMO could be seemed as $\pi_{Sc\text{-}Sc}$ half bond. The Mayer bond orders of the central and terminal Sc-Sc bonds in singlet X[Sc-C_8H_8-Sc]$_2$X are 0.98 and 0.69 for F, 0.94 and 0.71 for Cl, 0.93 and 0.72 for Br, respectively; in triplet, the values are 1.18 and 0.45 for F, 1.16 and 0.43 for Cl, 1.15 and 0.44 for Br, respectively. The stronger central Sc-Sc bond is in the triplet than in the singlet. This might be the reason for why the longer and shorter central Sc-Sc bond of X[Sc-C_8H_8-Sc]$_2$X in the singlet and triplet spin states.

Part 2 Coordination Information

1. The detailed Cartesian coordinates of X[Sc-C_8H_8-Sc]X (X = F, Cl, Br) obtained at

PBEPBE/ TZVP level.

singlet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 1

C	0.00084300	-1.01574900	1.55320300
C	-0.00008300	0.38003900	1.81696000
C	-0.00101600	1.55312900	1.01593600
C	0.00182200	-1.81677900	0.38011600
C	-0.00182000	1.81689100	-0.37985200
C	0.00098400	-1.55301600	-1.01567100
C	0.00008200	-0.37992900	-1.81670100
H	0.00158700	-1.61571400	2.46927300
H	-0.00017300	0.60384200	2.88879900
H	-0.00183600	2.46919700	1.61590400
H	0.00273300	-2.88861700	0.60391900
H	0.00179900	-2.46908500	-1.61563900
C	-0.00081100	1.01585900	-1.55293700
H	-0.00273200	2.88872700	-0.60365900
H	-0.00154600	1.61582300	-2.46900800
H	0.00017300	-0.60373200	-2.88853900
Sc	-1.63123600	-0.00120000	0.00026500
Sc	1.63123600	0.00128000	-0.00007700
F	3.53333200	-0.00004700	-0.00066400
F	-3.53333300	-0.00048400	-0.00059500

State=1-A\HF=-2030.0967855\RMSD=8.088e-09\RMSF=8.139e-05\ZeroPoint=0.1349022\Thermal=0.1481907\

triplet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 3

C	-1.17551400	0.31389100	-1.41558100
C	-0.90205100	1.48393900	-0.66545700
C	-0.02618200	1.80895200	0.42043200
C	-0.67892400	-1.03011100	-1.39693700
C	0.67892500	1.03116000	1.39735300
C	0.02618100	-1.80790300	-0.42001600
C	0.90205100	-1.48289000	0.66587300
H	-1.84106400	0.50236600	-2.25990700
H	-1.40728000	2.36456700	-1.06663700
H	-0.06835800	2.86927400	0.67781700
H	-1.09984700	-1.63970600	-2.19899300
H	0.06835700	-2.86822500	-0.67740000
C	1.17551400	-0.31284200	1.41599600
H	1.09984800	1.64075600	2.19940900
H	1.84106500	-0.50131600	2.26032200
H	1.40727900	-2.36351800	1.06705400
Sc	1.22898800	0.40391600	-1.12284200
Sc	-1.22898900	-0.40286700	1.12325900
F	-2.53977200	-0.89026400	2.38417600
F	2.53977300	0.89131500	-2.38375800

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singlet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 1

C	-0.00011700	1.26152800	-1.36503000
C	-0.00005800	1.85707000	-0.07309000
C	0.00005200	1.36513900	1.26144600
C	-0.00082100	-0.07302700	-1.85694000
C	0.00082100	0.07317900	1.85696400
C	-0.00005900	-1.36498700	-1.26142200
C	0.00005800	-1.85691800	0.07311400
H	-0.00076200	2.00503900	-2.16905100
H	-0.00007800	2.95134200	-0.11604100
H	0.00063400	2.16912800	2.00499200
H	-0.00069700	-0.11597400	-2.95121400
H	-0.00064500	-2.16897700	-2.00496700
C	0.00012300	-1.26137600	1.36505400
H	0.00069700	0.11612400	2.95123800
H	0.00077500	-2.00488900	2.16907400
H	0.00007800	-2.95118900	0.11606400
Cl	-3.92962200	-0.00020700	0.00001900
Cl	3.92962200	-0.00020000	-0.00008300
Sc	1.59281800	0.00008800	-0.00035400
Sc	-1.59281900	0.00003900	0.00037400

State=1-A\HF=-2750.5736401\RMSD=3.369e-09\RMSF=7.371e-05\ZeroPoint=0.1347754\Thermal=0.1479465\

triplet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 3

C	-1.22244000	0.28737000	-1.37278000
C	-0.92797300	1.46453600	-0.62337000
C	-0.10087800	1.79552800	0.48861400
C	-0.67732100	-1.03614300	-1.42128900
C	0.67733200	1.03718900	1.42170300
C	0.10088600	-1.79448100	-0.48819800
C	0.92797200	-1.46349400	0.62379500
H	-1.92060600	0.48551300	-2.18861100
H	-1.47894200	2.33176800	-0.99402200
H	-0.19476000	2.84560500	0.77267100
H	-1.08250400	-1.63967100	-2.23594700
H	0.19476000	-2.84455900	-0.77225000
C	1.22244200	-0.28632700	1.37320400
H	1.08251000	1.64071700	2.23636400
H	1.92059800	-0.48447400	2.18904200
H	1.47892900	-2.33073000	0.99445600
Sc	1.22745200	0.29097200	-1.11019700

Sc	-1.22744600	-0.28990700	1.11059500
Cl	2.98198100	0.75753100	-2.58117100
Cl	-2.98199500	-0.75644500	2.58155100

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singlet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 1

C	-0.00118400	1.35853600	-1.27026900
C	0.00003600	1.85912100	0.06201500
C	0.00094700	1.27085100	1.35816800
C	-0.00246000	0.06237600	-1.85852300
C	0.00245700	-0.06144100	1.85873900
C	-0.00097500	-1.26991500	-1.35795400
C	-0.00004000	-1.85817800	-0.06180000
H	-0.00253000	2.15795300	-2.01863300
H	-0.00012300	2.95356100	0.09808900
H	0.00239500	2.01920000	2.15759900
H	-0.00299900	0.09844600	-2.95296300
H	-0.00242100	-2.01826500	-2.15738100
C	0.00120300	-1.35760000	1.27048500
H	0.00299300	-0.09751200	2.95317900
H	0.00254600	-2.15702000	2.01884400
H	0.00011700	-2.95261700	-0.09787500
Sc	1.58289900	0.00047200	-0.00144000
Sc	-1.58289700	0.00040900	0.00164300
Br	4.07304900	-0.00061700	-0.00023300
Br	-4.07304600	-0.00066100	-0.00006100

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triplet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 3

C	-1.21931900	0.28855300	-1.37798800
C	-0.92586200	1.46455600	-0.62706000
C	-0.09649200	1.79515300	0.48472100
C	-0.67898800	-1.03711700	-1.42072400
C	0.67897900	1.03817100	1.42114200
C	0.09648600	-1.79410000	-0.48430700
C	0.92586300	-1.46349900	0.62746900
H	-1.91413900	0.48711300	-2.19662200
H	-1.47315000	2.33358200	-0.99928400
H	-0.18799000	2.84629200	0.76610100
H	-1.08262800	-1.64169700	-2.23541200
H	0.18799000	-2.84523700	-0.76569200
C	1.21931600	-0.28749700	1.37840100

H	1.08262100	1.64275100	2.23582800
H	1.91414400	-0.48605500	2.19702900
H	1.47316100	-2.33252200	0.99968400
Sc	1.22008400	0.29553500	-1.10684400
Sc	-1.22008800	-0.29449800	1.10727600
Br	-3.08825700	-0.81166100	2.67561300
Br	3.08826900	0.81267700	-2.67516700

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4. The detailed Cartesian coordinates of XSc-C_8H_8-ScX (X = F, Cl, Br) obtained at PBEPBE/ TZVPP level.

singlet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 1

C	0.00071200	1.27151100	-1.35263200
C	0.00006600	1.85542200	-0.05737400
C	-0.00041100	1.35287600	1.27133400
C	-0.00521500	-0.05720300	-1.85516500
C	0.00521800	0.05761100	1.85523200
C	0.00030800	-1.35247300	-1.27127300
C	-0.00006900	-1.85500700	0.05744000
H	-0.00206100	2.02117500	-2.14989200
H	0.00021200	2.94923700	-0.09103600
H	0.00241200	2.15012700	2.02100600
H	-0.00432200	-0.09086500	-2.94898100
H	-0.00255400	-2.14972900	-2.02094200
C	-0.00061000	-1.27110800	1.35270400
H	0.00432800	0.09127000	2.94904700
H	0.00221800	-2.02077800	2.14995800
H	-0.00021200	-2.94882600	0.09110000
Sc	1.63447400	-0.00002900	-0.00172900
Sc	-1.63447500	0.00029200	0.00177100
F	3.52809400	-0.00097600	-0.00053800
F	-3.52809400	-0.00090100	0.00023200

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triplet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 3

C	-1.17388000	0.31341800	-1.41484200
C	-0.89883300	1.48414900	-0.66731600
C	-0.02498500	1.81054000	0.41981300
C	-0.67992700	-1.03144100	-1.39588900
C	0.67992400	1.03249100	1.39630900
C	0.02499100	-1.80948900	-0.41939900
C	0.89883600	-1.48309800	0.66773300
H	-1.83900700	0.50206600	-2.25868500

H	-1.40379900	2.36364000	-1.06961600
H	-0.06587800	2.87086000	0.67504600
H	-1.10100300	-1.63961200	-2.19823000
H	0.06588600	-2.86980800	-0.67463500
C	1.17387800	-0.31236900	1.41526300
H	1.10099500	1.64066100	2.19865300
H	1.83900200	-0.50101700	2.25910800
H	1.40380300	-2.36258900	1.07003100
Sc	1.21779200	0.39945200	-1.10799800
Sc	-1.21779200	-0.39840300	1.10841000
F	-2.52061800	-0.89053200	2.36847600
F	2.52061500	0.89158100	-2.36806800

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singlet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 1

C	0.00049100	-1.14912700	1.46140700
C	-0.00011000	0.22043900	1.84615400
C	-0.00075800	1.46118500	1.14956900
C	0.00428400	-1.84573900	0.22066800
C	-0.00426600	1.84595300	-0.21999900
C	0.00049600	-1.46094400	-1.14888200
C	0.00011500	-0.22022800	-1.84552200
H	0.00260100	-1.82627600	2.32152500
H	-0.00022300	0.34993300	2.93312900
H	-0.00291500	2.32129800	1.82672300
H	0.00401400	-2.93270700	0.35015900
H	0.00249700	-2.32106500	-1.82603400
C	-0.00017700	1.14932300	-1.46071800
H	-0.00397300	2.93292000	-0.34949900
H	-0.00206900	1.82648100	-2.32083400
H	0.00026000	-0.34972200	-2.93248700
Sc	-1.58821100	-0.00188600	0.00041600
Sc	1.58819300	0.00208000	0.00018900
Cl	3.92764800	-0.00012500	-0.00093100
Cl	-3.92766300	-0.00047000	-0.00091900

State=1-A\HF=-2750.6119926\RMSD=6.990e-09\RMSF=4.888e-04\ZeroPoint=0.1346807\Thermal=0.1477434\

triplet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 3

C	-1.22358800	0.28675900	-1.37230100
C	-0.92479200	1.46367900	-0.62526300
C	-0.09638100	1.79584500	0.48546000
C	-0.68046400	-1.03760800	-1.42057000
C	0.68048500	1.03865200	1.42098200

C	0.09639700	-1.79479900	-0.48504400
C	0.92479000	-1.46264400	0.62569800
H	-1.92199300	0.48585800	-2.18694600
H	-1.47348600	2.33131900	-0.99683700
H	-0.18817900	2.84651000	0.76581100
H	-1.08599800	-1.64138700	-2.23403900
H	0.18818100	-2.84546800	-0.76538600
C	1.22359300	-0.28572300	1.37273200
H	1.08601100	1.64242900	2.23445700
H	1.92197700	-0.48482900	2.18739300
H	1.47346000	-2.33029200	0.99728900
Sc	1.20973200	0.28769800	-1.09995000
Sc	-1.20972100	-0.28661900	1.10033100
Cl	2.97247000	0.76425400	-2.56108200
Cl	-2.97249800	-0.76313400	2.56142800

HF=-2750.5900112\S2=2.006468\S2-1=0.\S2A=2.000021\RMSD=5.980e-09\RMSF=3.574e-05\ZeroPoint=0.132276\Thermal=0.146618\

singlet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 1

C	-0.00128600	1.34998000	-1.27639000
C	0.00000300	1.85741300	0.05169900
C	0.00087200	1.27698500	1.34959900
C	-0.00257500	0.05207400	-1.85679100
C	0.00257200	-0.05111200	1.85700700
C	-0.00090800	-1.27602600	-1.34938700
C	-0.00000700	-1.85644100	-0.05148300
H	-0.00273100	2.14412300	-2.02879800
H	-0.00016800	2.95101000	0.08121900
H	0.00239300	2.02936600	2.14376700
H	-0.00307500	0.08158700	-2.95038800
H	-0.00242600	-2.02840800	-2.14355100
C	0.00131200	-1.34902100	1.27660800
H	0.00307000	-0.08062600	2.95060400
H	0.00275300	-2.14316600	2.02901100
H	0.00016100	-2.95003800	-0.08100400
Sc	1.57897000	0.00044600	-0.00146000
Sc	-1.57896700	0.00045900	0.00166200
Br	4.07846500	-0.00061200	-0.00024400
Br	-4.07846300	-0.00070100	-0.00005000

State=1-A\HF=-6978.0990047\RMSD=7.446e-09\RMSF=3.052e-04\ZeroPoint=0.1342741\Thermal=0.1477212\

triplet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 3

C	-1.22293200	0.28680200	-1.37420400
C	-0.92410000	1.46372400	-0.62721100

C	-0.09239200	1.79635700	0.48190100
C	-0.68434400	-1.03949800	-1.41788500
C	0.68436700	1.04054100	1.41829800
C	0.09240900	-1.79531300	-0.48148400
C	0.92409900	-1.46269100	0.62764700
H	-1.92060000	0.48566100	-2.18953700
H	-1.47164100	2.33184800	-0.99942700
H	-0.18163900	2.84797000	0.75968100
H	-1.08993700	-1.64404500	-2.23073500
H	0.18164000	-2.84693100	-0.75925300
C	1.22293800	-0.28576700	1.37463500
H	1.08995200	1.64508500	2.23115300
H	1.92058500	-0.48463300	2.18998400
H	1.47161300	-2.33082400	0.99988300
Sc	1.20306500	0.28841500	-1.09720600
Sc	-1.20305300	-0.28733300	1.09758400
Br	-3.08871600	-0.81748600	2.64658100
Br	3.08868300	0.81861800	-2.64624400

HF=-6978.0755978\S2=2.006859\S2-1=0.\S2A=2.000024\RMSD=4.060e-09\RMSF=8.549e-06\ZeroPoint=0.1317902\Thermal=0.1464534\

5. The detailed Cartesian coordinates of XSc-C_8H_8-ScX (X = F, Cl, Br) obtained at PBEPBE/ TZVPD level.

singlet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 1

C	-0.00072200	1.34683500	-1.27482200
C	0.00010000	1.85318900	0.05095900
C	0.00087300	1.27498600	1.34673200
C	-0.00166900	0.05106400	-1.85301900
C	0.00166900	-0.05080000	1.85307800
C	-0.00088900	-1.27472400	-1.34667400
C	-0.00010100	-1.85292300	-0.05090000
H	-0.00149500	2.14251800	-2.02751200
H	0.00014000	2.94813000	0.08132500
H	0.00171200	2.02767200	2.14241900
H	-0.00212400	0.08142500	-2.94796100
H	-0.00172700	-2.02741200	-2.14236000
C	0.00073800	-1.34657300	1.27488200
H	0.00212400	-0.08116300	2.94802000
H	0.00151200	-2.14225800	2.02757200
H	-0.00014000	-2.94786600	-0.08126600
Sc	1.62370400	0.00007100	-0.00093800
Sc	-1.62370400	0.00011000	0.00097800
F	-3.52291000	-0.00058100	0.00022700
F	3.52291000	-0.00066200	-0.00050600

State=1-A\HF=-2030.1291603\RMSD=4.868e-09\RMSF=1.799e-04\ZeroPoint=0.134054\Thermal=0.1477516\

triplet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 3

C	0.24584200	0.71361900	1.70129600
C	0.25476100	-0.70240700	1.70624900
C	0.20940600	-1.71505400	0.69369600
C	0.19042900	1.71976200	0.68313000
C	-0.19042900	-1.71976100	-0.68313100
C	-0.20940700	1.71505400	-0.69369600
C	-0.25476300	0.70240800	-1.70624800
H	0.41636300	1.13605400	2.69349000
H	0.42984400	-1.11633700	2.70118700
H	0.30621300	-2.72026200	1.10951600
H	0.27593900	2.72779400	1.09469400
H	-0.30621700	2.72026200	-1.10951500
C	-0.24583900	-0.71361700	-1.70129600
H	-0.27593700	-2.72779300	-1.09469500
H	-0.41635900	-1.13605200	-2.69349100
H	-0.42984700	1.11633900	-2.70118700
Sc	1.69144600	0.00303500	-0.10285100
Sc	-1.69144600	-0.00303500	0.10285100
F	-3.57115400	-0.00592100	0.18795000
F	3.57115400	0.00592000	-0.18795000

State=3-A\S2-1=0.\S2A=2.000016\RMSD=6.425e-10\RMSF=2.089e-05\ZeroPoint=0.1327853\Thermal=0.146969\

singlet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 1

C	0.00020700	-1.36150400	1.26254700
C	0.00004400	-0.06979500	1.85574600
C	-0.00015100	1.26250300	1.36156600
C	0.00052800	-1.85569100	-0.06974700
C	-0.00052800	1.85571000	0.06986200
C	0.00014900	-1.26248400	-1.36145000
C	-0.00004400	0.06981400	-1.85563000
H	0.00049100	-2.16423500	2.00781400
H	0.00006800	-0.11059800	2.95028200
H	-0.00039400	2.00775900	2.16430700
H	0.00061800	-2.95022600	-0.11055100
H	0.00039100	-2.00774000	-2.16419200
C	-0.00020500	1.36152200	-1.26243200
H	-0.00061800	2.95024500	0.11066500
H	-0.00048900	2.16425300	-2.00769900
H	-0.00006800	0.11061600	-2.95016600
Cl	3.92324000	0.00000700	-0.00016300
Cl	-3.92324000	-0.00005800	-0.00015900
Sc	-1.58390300	-0.00029900	0.00007500
Sc	1.58390300	0.00031600	0.00003100

State=1-A\HF=-2750.6076809\RMSD=4.575e-09\RMSF=6.472e-05\ZeroPoint=
0.1344589\Thermal=0.1476585\

triplet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 3

C	0.05738700	-1.31112000	-1.31868800
C	-0.01136900	0.01411900	-1.84015700
C	-0.07944300	1.33098900	-1.30056100
C	0.25466300	-1.86953900	-0.01483100
C	-0.25466900	1.86954300	0.01483300
C	0.07944000	-1.33098400	1.30056300
C	0.01137000	-0.01411400	1.84016000
H	0.11393200	-2.06006400	-2.11139500
H	-0.01968700	0.02099400	-2.93251100
H	-0.15005200	2.09120900	-2.08123300
H	0.38501300	-2.95356600	-0.02403400
H	0.15004800	-2.09120500	2.08123500
C	-0.05738700	1.31112600	1.31869000
H	-0.38502300	2.95356900	0.02403600
H	-0.11393200	2.06006900	2.11139700
H	0.01969000	-0.02098800	2.93251300
Sc	1.66284400	-0.01196600	-0.00367900
Sc	-1.66284200	0.01196700	0.00368300
Cl	3.99845500	0.08896300	-0.00383500
Cl	-3.99845400	-0.08897100	0.00382700

State=3-A\HF=-2750.5860311\S2=2.006443\S2-1=0.\S2A=2.000021\RMSD=2.048e-
09\RMSF=3.339e-05\ZeroPoint=0.1320957\

singlet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 1

C	0.00103100	-1.21838500	1.40209000
C	-0.00002900	0.12976800	1.85330000
C	-0.00100200	1.40181700	1.21886100
C	0.00171500	-1.85282500	0.13004300
C	-0.00171400	1.85302800	-0.12929100
C	0.00099800	-1.40161300	-1.21810800
C	0.00003000	-0.12956600	-1.85254700
H	0.00184400	-1.93727900	2.22859200
H	-0.00000700	0.20616900	2.94601900
H	-0.00187000	2.22831600	1.93775800
H	0.00252600	-2.94554300	0.20644300
H	0.00186700	-2.22811100	-1.93700500
C	-0.00102500	1.21858500	-1.40133800
H	-0.00252500	2.94574500	-0.20569400
H	-0.00183900	1.93747900	-2.22784000
H	0.00000700	-0.20596700	-2.94526400
Sc	-1.57461100	-0.00118900	0.00045000

Sc	1.57461100	0.00138100	0.00026300
Br	-4.07114400	-0.00019200	-0.00051300
Br	4.07114300	-0.00008400	-0.00051600

State=1-A\HF=-6978.0948374\RMSD=2.253e-09\RMSF=1.315e-04\ZeroPoint=0.1341319\Thermal=0.1475675\

triplet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 3

C	-0.03654200	-1.32910100	1.30332200
C	-0.00082100	-0.00875600	1.83970300
C	0.03455500	1.31659100	1.31541000
C	-0.20737500	-1.87659400	-0.00881500
C	0.20737900	1.87659600	0.00881500
C	-0.03455200	-1.31659000	-1.31540900
C	0.00082200	0.00875700	-1.83970300
H	-0.08190300	-2.08829200	2.08694300
H	-0.00156800	-0.01366000	2.93217400
H	0.07860500	2.06845200	2.10615300
H	-0.31154800	-2.96345200	-0.01404900
H	-0.07860100	-2.06845100	-2.10615300
C	0.03654300	1.32910300	-1.30332100
H	0.31155400	2.96345300	0.01404900
H	0.08190200	2.08829300	-2.08694300
H	0.00156700	0.01366100	-2.93217300
Sc	-1.65535100	-0.05132300	-0.00001000
Sc	1.65535100	0.05132300	0.00000900
Br	4.15060700	-0.04089200	0.00011300
Br	-4.15060900	0.04089100	-0.00011300

State=3-A\HF=-6978.071461\S2=2.006826\S2-1=0.\S2A=2.000024\RMSD=2.479e-09\RMSF=1.112e-05\ZeroPoint=0.1316826\Thermal=0.1463371\

6. The detailed Cartesian coordinates of XSc-C_8H_8-ScX (X = F, Cl, Br) obtained at BP86/ TZVP level.

singlet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 1

C	0.04598600	-1.31051300	-1.31841900
C	-0.00178900	-1.86115700	-0.00809100
C	-0.04791800	-1.32205600	1.30681300
C	-0.06364300	0.00818000	-1.85579800
C	0.06363500	-0.00817400	1.85579900
C	0.04791200	1.32206100	-1.30681200
C	0.00178000	1.86116300	0.00809300
H	0.01115800	-2.07815300	-2.09733200
H	-0.00256900	-2.95542800	-0.01273500
H	-0.01473200	-2.09649000	2.07903600
H	-0.01848600	0.01272500	-2.94888100
H	0.01472800	2.09649500	-2.07903400

C	-0.04599400	1.31051900	1.31842000
H	0.01848000	-0.01271900	2.94888300
H	-0.01116400	2.07815900	2.09733400
H	0.00256300	2.95543400	0.01273600
Sc	-1.63714300	0.00125200	-0.00438300
Sc	1.63712600	-0.00124800	0.00438500
F	3.53428900	-0.00024400	-0.00379000
F	-3.53422700	0.00021600	0.00378200

State=1-A\HF=-2031.3031605\RMSD=2.933e-09\RMSF=1.156e-04\ZeroPoint=0.1336631\Thermal=0.1458701\

triplet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 3

C	-1.25489200	0.28060900	-1.34253000
C	-0.92104100	1.46744700	-0.62827800
C	-0.05421700	1.80749300	0.45012300
C	-0.72860900	-1.05103700	-1.37719300
C	0.73659600	1.05518300	1.37766700
C	0.06318100	-1.80304900	-0.45025300
C	0.93055400	-1.46280000	0.62769000
H	-1.97153200	0.47122900	-2.14384600
H	-1.46843700	2.33582300	-1.00101400
H	-0.12246800	2.86451300	0.71472200
H	-1.17800500	-1.66903200	-2.15703500
H	0.13156700	-2.86002300	-0.71499100
C	1.26380900	-0.27609400	1.34235600
H	1.18536600	1.67298900	2.15801700
H	1.98061500	-0.46668200	2.14353300
H	1.47859800	-2.33104600	0.99977400
Sc	1.22920600	0.26227000	-1.19905800
Sc	-1.22052800	-0.25803400	1.19848600
F	-2.56393600	-0.57781800	2.47802400
F	2.57216800	0.58250600	-2.47896300

HF=-2031.2938139\S2=2.007761\S2-1=0.\S2A=2.000028\RMSD=3.211e-09\RMSF=2.607e-05\ZeroPoint=0.1328758\Thermal=0.1462445\

singlet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 1

C	-0.00372000	-1.32228200	-1.30895000
C	0.00094400	-0.00933100	-1.86009900
C	0.00511300	1.30917800	-1.32204900
C	-0.00426700	-1.86087900	0.00933200
C	0.00426700	1.86088100	-0.00932600
C	-0.00511400	-1.30917500	1.32205500
C	-0.00094400	0.00933300	1.86010500
H	-0.00545000	-2.10032500	-2.07951800
H	0.00152800	-0.01489000	-2.95516300

H	0.00771700	2.07919300	-2.10063600
H	-0.00583900	-2.95588700	0.01489300
H	-0.00771700	-2.07919100	2.10064300
C	0.00371900	1.32228400	1.30895600
H	0.00583900	2.95588900	-0.01488700
H	0.00545000	2.10032700	2.07952400
H	-0.00152900	0.01489200	2.95516900
Sc	1.59940100	-0.00410800	0.00079000
Sc	-1.59940200	0.00410900	-0.00078500
Cl	-3.93632800	0.00035600	-0.00008500
Cl	3.93633000	-0.00036100	0.00006900

State=1-A\HF=-2752.0606839\RMSD=2.287e-09\RMSF=7.704e-05\ZeroPoint=0.1344639\Thermal=0.147704\

triplet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 3

C	-1.26646300	0.27716100	-1.33265100
C	-0.92519700	1.46802200	-0.62503100
C	-0.05056400	1.81061700	0.44747900
C	-0.74959700	-1.05817600	-1.36268200
C	0.75788500	1.06258500	1.36318400
C	0.05955700	-1.80602900	-0.44748000
C	0.93443700	-1.46333400	0.62479800
H	-1.99258600	0.46532900	-2.12636300
H	-1.47631700	2.33541000	-0.99561100
H	-0.11469300	2.86887900	0.70917400
H	-1.20119900	-1.67641200	-2.14135200
H	0.12374600	-2.86426100	-0.70927400
C	1.27547500	-0.27248400	1.33255100
H	1.20899600	1.68066500	2.14226500
H	2.00180100	-0.46062600	2.12608800
H	1.48624900	-2.33054200	0.99476700
Sc	1.20069400	0.24980500	-1.17772600
Sc	-1.19186900	-0.24549200	1.17723600
Cl	-2.88636000	-0.64669200	2.73565400
Cl	2.89400100	0.65002200	-2.73779300

HF=-2752.0410176\S2=2.008379\S2-1=0.\S2A=2.000035\RMSD=2.826e-09\RMSF=3.389e-05\ZeroPoint=0.1321546\Thermal=0.1466272\

singlet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 1

C	-0.00319900	-1.34068300	-1.29099400
C	0.00100400	-0.03506200	-1.86081400
C	0.00466500	1.29112300	-1.34054400
C	-0.00083300	-1.86108200	0.03507100
C	0.00083400	1.86108600	-0.03505800
C	-0.00466400	-1.29111900	1.34055700

C	-0.00100400	0.03506600	1.86082600
H	-0.00422900	-2.12943800	-2.05076600
H	0.00157500	-0.05569900	-2.95577900
H	0.00660400	2.05060500	-2.12957800
H	-0.00505300	-2.95602800	0.05571400
H	-0.00660400	-2.05060100	2.12959000
C	0.00319900	1.34068700	1.29100600
H	0.00505300	2.95603300	-0.05570100
H	0.00423000	2.12944200	2.05077900
H	-0.00157500	0.05570300	2.95579100
Sc	1.58953900	-0.00225800	0.00085100
Sc	-1.58953900	0.00226100	-0.00083900
Br	-4.07931800	0.00022800	-0.00005200
Br	4.07931800	-0.00023300	0.00003500

State=1-A\HF=-6980.4125772\RMSD=2.810e-09\RMSF=1.093e-04\ZeroPoint=0.134063\Thermal=0.1475615\

triplet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 3

C	-1.26786200	0.27701200	-1.33182000
C	-0.92644100	1.46857900	-0.62472700
C	-0.05064600	1.81109200	0.44730900
C	-0.75322700	-1.05920500	-1.35976200
C	0.76155100	1.06360300	1.36016200
C	0.05964500	-1.80652700	-0.44741100
C	0.93563100	-1.46392600	0.62442100
H	-1.99424500	0.46472100	-2.12548100
H	-1.47820200	2.33584200	-0.99485700
H	-0.11480900	2.86925300	0.70960200
H	-1.20412100	-1.67722300	-2.13909000
H	0.12381000	-2.86467100	-0.70976200
C	1.27687500	-0.27236000	1.33164000
H	1.21204400	1.68150900	2.13981500
H	2.00338200	-0.46008600	2.12518500
H	1.48800700	-2.33101900	0.99403500
Sc	1.19539400	0.24894200	-1.17340000
Sc	-1.18659300	-0.24455900	1.17305400
Br	-2.99386700	-0.66829600	2.83724500
Br	3.00167200	0.67176600	-2.83892800

HF=-2752.0410176\S2=2.008379\S2-1=0.\S2A=2.000035\RMSD=2.826e-09\RMSF=3.389e-05\ZeroPoint=0.1321546\Thermal=0.1466272\

7. The detailed Cartesian coordinates of XSc-C_8H_8-ScX (X = F, Cl, Br) obtained at MPW91PW91/ TZVP level.

singlet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 1

C	0.00276300	-1.29871300	-1.30969700

C	-0.00043700	-1.84449100	-0.00778900
C	-0.00355500	-1.30986200	1.29855500
C	0.00490000	0.00778800	-1.84389800
C	-0.00493900	-0.00778600	1.84389900
C	0.00351600	1.30986300	-1.29855300
C	0.00039900	1.84449300	0.00779100
H	0.00270800	-2.06261000	-2.08028300
H	-0.00078700	-2.92954100	-0.01231300
H	-0.00384600	-2.08004600	2.06285600
H	0.00621800	0.01231100	-2.92894800
H	0.00380500	2.08004800	-2.06285400
C	-0.00280200	1.29871500	1.30969800
H	-0.00626000	-0.01231000	2.92894900
H	-0.00274800	2.06261100	2.08028500
H	0.00074800	2.92954200	0.01231400
Sc	-1.60789700	0.00037900	-0.00365700
Sc	1.60786000	-0.00037800	0.00365700
F	3.50328400	-0.00009400	0.00038400
F	-3.50307700	0.00008600	-0.00038800

State=1-A\HF=-2031.0672884\RMSD=2.009e-09\RMSF=7.216e-05\ZeroPoint=0.1402169\Thermal=0.1529725\

triplet FSc-C_8H_8-ScF

Charge = 0 Multiplicity = 3

C	-1.25766000	0.20894100	-1.30002600
C	-0.99769600	1.38745700	-0.54759100
C	-0.03242800	1.78658200	0.41078200
C	-0.73021400	-1.09660900	-1.38302200
C	0.86604200	1.06041200	1.22223100
C	0.15683100	-1.81306800	-0.58199300
C	0.84814300	-1.49522100	0.60571700
H	-2.00060400	0.39830900	-2.06372400
H	-1.56608700	2.22899600	-0.92117000
H	-0.04053200	2.84913200	0.61278300
H	-1.11359400	-1.65368500	-2.22896400
H	0.33789900	-2.82691200	-0.91707800
C	1.12088400	-0.32624000	1.36795400
H	1.41147900	1.67459200	1.92590500
H	1.83285500	-0.52507200	2.15811700
H	1.38466300	-2.34596700	1.00499000
Sc	1.25849500	0.31408400	-1.11299800
Sc	-1.32922700	-0.06727400	1.42046000
F	-2.69630300	-0.43733600	2.65042300
F	2.63504900	0.72333000	-2.32556500

State=3-A\HF=-2031.0571035\S2=2.008214\S2-1=0.\S2A=2.000033\RMSD=7.645e-10\RMSF=1.295e-05\ZeroPoint=0.1393432\Thermal=0.1527397\

singlet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 1

C	-0.00546100	-1.32096500	-1.29145500
C	0.00108400	-0.02085300	-1.84723200
C	0.00703900	1.29154400	-1.32086600
C	-0.00566700	-1.84744400	0.02085600
C	0.00566600	1.84744600	-0.02084900
C	-0.00704000	-1.29154200	1.32087200
C	-0.00108500	0.02085500	1.84723900
H	-0.00813400	-2.09675800	-2.05010200
H	0.00173800	-0.03316300	-2.93224600
H	0.01069100	2.04991100	-2.09692800
H	-0.01099100	-2.93244100	0.03316700
H	-0.01069200	-2.04990900	2.09693500
C	0.00546000	1.32096700	1.29146100
H	0.01098900	2.93244300	-0.03316100
H	0.00813200	2.09676000	2.05010800
H	-0.00173900	0.03316500	2.93225200
Sc	1.56730700	-0.00572200	0.00094600
Sc	-1.56730700	0.00572300	-0.00094000
Cl	-3.90108100	0.00065000	-0.00010500
Cl	3.90108400	-0.00065600	0.00008800

State=1-A\HF=-2751.834374\RMSD=7.157e-09\RMSF=8.345e-05\ZeroPoint=0.1401503\
Thermal=0.152797\

triplet ClSc-C_8H_8-ScCl

Charge = 0 Multiplicity = 3

C	-1.19728900	0.29400800	-1.35919800
C	-0.91978600	1.46250700	-0.62563100
C	-0.10282300	1.77395000	0.47724000
C	-0.83215000	-1.06019600	-1.24393600
C	0.84108300	1.06611500	1.24433300
C	0.02337500	-1.79041200	-0.39800700
C	0.93079500	-1.45620200	0.62461400
H	-1.91163900	0.46402900	-2.15422200
H	-1.46276400	2.32247900	-0.99489000
H	-0.15598000	2.82015400	0.74906200
H	-1.32555700	-1.68664900	-1.97527800
H	0.04419800	-2.84477900	-0.64118200
C	1.29311800	-0.26592800	1.28246200
H	1.33158000	1.69169100	1.97839700
H	2.04274100	-0.42684400	2.04629300
H	1.47591100	-2.31549900	0.99222500
Sc	1.31855700	0.33273300	-1.16891600
Sc	-1.31316400	-0.32952500	1.16691200
Cl	-3.02431500	-0.77164800	2.68738500
Cl	3.03210600	0.76446800	-2.69043200

State=3-A\HF=-2751.8184038\S2=2.008568\S2-1=0.\S2A=2.000044\RMSD=5.964e-10\
RMSF=7.915e-05\ZeroPoint=0.1393884\Thermal=0.1530761\

singlet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 1

C	-0.00501600	-1.31932900	-1.29415500
C	0.00099400	-0.01784900	-1.84807200
C	0.00645200	1.29423100	-1.31924600
C	-0.00527000	-1.84825100	0.01785600
C	0.00526900	1.84825500	-0.01784400
C	-0.00645300	-1.29422700	1.31925800
C	-0.00099500	0.01785300	1.84808400
H	-0.00746700	-2.09403400	-2.05396300
H	0.00159200	-0.02846300	-2.93316000
H	0.00980200	2.05386500	-2.09411900
H	-0.01011200	-2.93333100	0.02847200
H	-0.00980200	-2.05386100	2.09413100
C	0.00501500	1.31933200	1.29416700
H	0.01011100	2.93333400	-0.02846000
H	0.00746700	2.09403700	2.05397500
H	-0.00159300	0.02846700	2.93317200
Sc	1.55917600	-0.00510500	0.00086400
Sc	-1.55917500	0.00510900	-0.00085400
Br	-4.04580700	0.00032400	-0.00004800
Br	4.04580800	-0.00032900	0.00003300

State=1-A\HF=-6980.0650993\RMSD=4.488e-09\RMSF=8.224e-05\ZeroPoint=0.139731\
Thermal=0.1526576\

triplet BrSc-C_8H_8-ScBr

Charge = 0 Multiplicity = 3

C	-1.26559200	0.26635500	-1.31875900
C	-0.91695600	1.45356600	-0.64132600
C	-0.06269100	1.78807400	0.43593800
C	-0.80172500	-1.06619500	-1.30181600
C	0.83525900	1.06478700	1.25562200
C	0.04281000	-1.79564000	-0.43860100
C	0.93261100	-1.46294600	0.60386400
H	-1.96522100	0.45131500	-2.12452100
H	-1.44386300	2.31795600	-1.02587500
H	-0.07601900	2.84545400	0.66690300
H	-1.23652100	-1.67581000	-2.08397600
H	0.12104600	-2.83864500	-0.71964700
C	1.24968800	-0.28620900	1.32295000
H	1.35938900	1.69764200	1.96043900
H	2.00828200	-0.45019200	2.07743300
H	1.49608700	-2.31865300	0.95441600
Sc	1.19336300	0.29020000	-1.08470300
Sc	-1.26205600	-0.24194500	1.29478300

Br	-3.15094400	-0.76818800	2.85722600
Br	3.03104600	0.77352400	-2.69311900

State=3-A\HF=-6980.0423768\S2=2.012527\S2-1=0.\S2A=2.000074\RMSD=4.242e-09\
RMSF=1.443e-05\ZeroPoint=0.1385876\Thermal=0.1516734\

8. The detailed Cartesian coordinates of $Sc_2C_8H_8X_2$ (X = F, Cl, Br) obtained at PBEPBE/ TZVP level.

singlet Isomer 2 of X = F

Charge = 0 Multiplicity = 1

C	-0.47507200	-0.00030300	-1.84388800
C	-0.52768400	1.32542400	-1.30825100
C	-0.57210600	1.88098800	-0.00024000
C	-0.52770000	-1.32585700	-1.30783200
C	-0.52742300	1.32585400	1.30794100
C	-0.57209100	-1.88099100	0.00036100
C	-0.52738600	-1.32542600	1.30836100
H	-0.49969700	-0.00047600	-2.94384300
H	-0.58400300	2.08891100	-2.09760400
H	-0.66344500	2.97617500	-0.00041400
H	-0.58403200	-2.08959900	-2.09693600
H	-0.66342100	-2.97617900	0.00055500
C	-0.47465900	0.00030100	1.84398500
H	-0.58356300	2.08959700	2.09705900
H	-0.49902700	0.00047500	2.94394600
H	-0.58350200	-2.08891300	2.09772800
Sc	1.29747000	0.00000100	-0.00015900
Sc	-1.97771600	-0.00000700	0.00021400
F	2.45390700	1.49446700	-0.00025200
F	2.45393500	-1.49444400	-0.00022100

State=1-A\HF=-2030.0687531\RMSD=5.831e-09\RMSF=6.127e-
05\ZeroPoint=0.1354966\Thermal=0.147571\

triplet Isomer 2 of X = F

Charge = 0 Multiplicity = 3

C	-0.42963300	-0.00030100	-1.83932700
C	-0.51722400	1.31740800	-1.30560900
C	-0.58369200	1.86750700	-0.00024200
C	-0.51724400	-1.31783700	-1.30518900
C	-0.51696300	1.31783500	1.30528900
C	-0.58366900	-1.86751000	0.00035800
C	-0.51691000	-1.31741000	1.30571000
H	-0.41306400	-0.00047400	-2.93216600
H	-0.54639900	2.07947300	-2.08800000
H	-0.66420800	2.95703000	-0.00041400
H	-0.54643300	-2.08015500	-2.08733400
H	-0.66417200	-2.95703400	0.00054800

C	-0.42921300	0.00030000	1.83940700
H	-0.54597000	2.08015300	2.08744100
H	-0.41240800	0.00047400	2.93224100
H	-0.54588700	-2.07947600	2.08810800
Sc	1.36174100	0.00000100	-0.00016100
Sc	-2.14940100	-0.00001100	0.00023300
F	2.52479800	1.46486400	-0.00025800
F	2.52483600	-1.46483600	-0.00022400

State=3-A\HF=-2030.0739482\S2=2.004202\S2-1=0.\S2A=2.000009\RMSD=4.752e-09\
RMSF=5.700e-05\ZeroPoint=0.1358831\Thermal=0.1489057\

singlet Isomer 2 of X = Cl

Charge = 0 Multiplicity = 1

C	-0.84220000	-0.00031000	-1.84678700
C	-0.89213000	1.32506100	-1.31003900
C	-0.93364200	1.87883400	-0.00026900
C	-0.89211600	-1.32551200	-1.30962300
C	-0.89183400	1.32549200	1.30966900
C	-0.93356400	-1.87885400	0.00032900
C	-0.89174300	-1.32507400	1.31008700
H	-0.85770200	-0.00048500	-2.94504100
H	-0.93312500	2.09018800	-2.09619400
H	-1.00224000	2.97378400	-0.00044800
H	-0.93310900	-2.09089400	-2.09552900
H	-1.00210700	-2.97380700	0.00053000
C	-0.84171500	0.00029700	1.84682000
H	-0.93260400	2.09087300	2.09558400
H	-0.85691200	0.00047000	2.94507700
H	-0.93244700	-2.09020500	2.09625100
Sc	0.88672900	-0.00000300	-0.00021300
Sc	-2.32876600	-0.00004100	0.00020100
Cl	2.36602700	1.84373700	-0.00003600
Cl	2.36613000	-1.84365500	-0.00002800

State=1-A\HF=-2750.5307626\RMSD=5.361e-09\RMSF=5.036e-04\ ZeroPoint=0.1345363\
Thermal=0.1472015\

triplet Isomer 2 of X = Cl

Charge = 0 Multiplicity = 3

C	-0.80947500	-0.00030100	-1.84258500
C	-0.89424700	1.31670100	-1.30733000
C	-0.96076400	1.86509700	-0.00021500
C	-0.89427000	-1.31713100	-1.30690900
C	-0.89399600	1.31712800	1.30706400
C	-0.96074600	-1.86510100	0.00038500
C	-0.89394800	-1.31670400	1.30748500
H	-0.78700600	-0.00047500	-2.93505200
H	-0.91582700	2.08107800	-2.08728900

H	-1.02896600	2.95515000	-0.00038800
H	-0.91586000	-2.08175900	-2.08662100
H	-1.02893600	-2.95515400	0.00057200
C	-0.80906700	0.00030000	1.84272000
H	-0.91541200	2.08175600	2.08678100
H	-0.78637100	0.00047400	2.93518200
H	-0.91533800	-2.08108100	2.08744900
Sc	0.95485800	-0.00000100	-0.00011800
Sc	-2.50639500	-0.00001000	0.00025000
Cl	2.42866600	1.81631700	-0.00022500
Cl	2.42869000	-1.81629800	-0.00019100

State=3-A\HF=-2750.5309774\S2=2.004578\S2-1=0.\S2A=2.000011\RMSD=6.483e-09\
RMSF=3.229e-05\ZeroPoint=0.134545\Thermal=0.148188\

singlet Isomer 2 of X = Br

Charge = 0 Multiplicity = 1

C	-1.40330400	-0.00030900	-1.85145200
C	-1.44658400	1.32273100	-1.31138400
C	-1.48181400	1.87377700	-0.00020200
C	-1.44658900	-1.32317400	-1.31096200
C	-1.44631200	1.32315700	1.31115200
C	-1.48179500	-1.87379200	0.00040100
C	-1.44628000	-1.32274400	1.31157500
H	-1.41434600	-0.00048300	-2.94992600
H	-1.47936400	2.09214800	-2.09424200
H	-1.53451200	2.97011300	-0.00037300
H	-1.47936500	-2.09284700	-2.09356800
H	-1.53447800	-2.97012900	0.00058500
C	-1.40288400	0.00029600	1.85163300
H	-1.47889400	2.09283100	2.09376400
H	-1.41367300	0.00047000	2.95010900
H	-1.47884700	-2.09216300	2.09444000
Sc	0.31070900	-0.00000500	-0.00010100
Sc	-2.89253200	-0.00001600	0.00025500
Br	1.93376900	1.95012200	-0.00013700
Br	1.93380600	-1.95009800	-0.00010900

State=1-A\HF=-6978.0224519\RMSD=2.484e-09\RMSF=1.037e-04\ZeroPoint=0.134013\
Thermal=0.1470539\

triplet Isomer 2 of X = Br

Charge = 0 Multiplicity = 3

C	-1.37474400	-0.00030300	-1.84400800
C	-1.45818100	1.31611700	-1.30787300
C	-1.52232100	1.86389600	-0.00017000
C	-1.45820200	-1.31655100	-1.30745300
C	-1.45793400	1.31654400	1.30769700
C	-1.52230300	-1.86390400	0.00042800

C	-1.45788800	-1.31612500	1.30811800
H	-1.35089300	-0.00047700	-2.93638900
H	-1.47608000	2.08160800	-2.08674700
H	-1.58557900	2.95414600	-0.00034300
H	-1.47610900	-2.08229200	-2.08608000
H	-1.58555000	-2.95415600	0.00061300
C	-1.37434700	0.00029700	1.84423300
H	-1.47567300	2.08228400	2.08632800
H	-1.35027500	0.00047000	2.93660900
H	-1.47560400	-2.08161600	2.08699500
Sc	0.38072800	-0.00000200	-0.00006600
Sc	-3.06814200	-0.00001200	0.00029100
Br	1.97094500	1.93548800	-0.00019000
Br	1.97096800	-1.93547300	-0.00013900

State=3-A\HF=-6978.0212783\S2=2.004777\S2-1=0.\S2A=2.000012\RMSD=4.767e-09\
RMSF=3.573e-05\ZeroPoint=0.1339723\Thermal=0.1470691\

singlet Isomer 3 of X = F

Charge = 0 Multiplicity = 1

H	0.82213200	2.01506200	-2.12715100
H	1.26898600	2.98804800	0.00367800
H	0.81960600	2.01079900	2.13205000
H	-0.31657100	-0.06469400	-2.50629800
H	-2.64924200	0.38407100	-2.13647400
H	-0.31923900	-0.06995200	2.50550800
H	-2.65158200	0.37958600	2.13416900
H	-3.68573000	0.61976000	-0.00149500
C	-1.99006800	0.40024400	-1.26600500
C	-2.59310600	0.56409400	-0.00094200
C	-1.99147400	0.39750500	1.26444400
C	-0.50760500	0.34121500	1.50122300
C	0.39405400	1.51285300	1.25797800
C	0.62914500	2.10100500	0.00241900
C	0.39555300	1.51534300	-1.25459000
C	-0.50596600	0.34432800	-1.50133700
Sc	-1.09884800	-1.26640700	-0.00203000
Sc	1.45320800	-0.12201300	0.00073700
F	0.71431200	-2.15498000	-0.00185400
F	3.31756400	-0.30784000	0.00230000

State=1-A\HF=-2030.1090893\RMSD=3.322e-09\RMSF=9.354e-04\ZeroPoint=0.1332764\
Thermal=0.1455315\

triplet Isomer 3 of X = F

Charge = 0 Multiplicity = 3

H	2.03160400	-1.30914200	2.09367100
H	2.86874900	-1.94806600	0.00004900
H	2.03167700	-1.30912900	-2.09359500
H	-0.00004700	-0.43926800	2.69018200

H	-2.03167400	-1.30913300	2.09359600
H	0.00004900	-0.43926800	-2.69018200
H	-2.03160100	-1.30914600	-2.09367200
H	-2.86874700	-1.94806900	-0.00004900
C	-1.31630400	-1.25179900	1.26783500
C	-1.83772300	-1.58685300	-0.00003200
C	-1.31626200	-1.25180400	-1.26788400
C	0.00002900	-0.80965600	-1.66026400
C	1.31630600	-1.25179600	-1.26783500
C	1.83772500	-1.58684900	0.00003200
C	1.31626400	-1.25180100	1.26788400
C	-0.00002700	-0.80965600	1.66026400
Sc	-1.46326100	0.75243000	-0.00002500
Sc	1.46326000	0.75243200	0.00002500
F	-2.78443300	2.06724500	0.00003600
F	2.78442800	2.06724500	-0.00003600

State=3-A\HF=-2030.0955658\S2=2.004561\S2-1=0.\S2A=2.000011\RMSD=9.553e-09\RMSF=7.617e-04\ZeroPoint=0.1351552\Thermal=0.1480398\

singlet Isomer 3 of X = Cl

Charge = 0 Multiplicity = 1

H	-0.37367000	-2.22364700	-2.12412700
H	-0.73612600	-3.23897100	0.00369900
H	-0.37116500	-2.21919500	2.12899100
H	0.63014200	-0.08167300	-2.50186500
H	2.98313400	-0.37825600	-2.13530900
H	0.63271500	-0.07621000	2.50090900
H	2.98536500	-0.37357200	2.13259800
H	4.03841200	-0.57660600	-0.00170600
C	2.32985200	-0.44427200	-1.26284200
C	2.94452100	-0.58281700	-0.00112100
C	2.33118700	-0.44138900	1.26094300
C	0.84842600	-0.47357900	1.49766400
C	0.03693100	-1.70654400	1.25565100
C	-0.15230900	-2.31470700	0.00239500
C	0.03545700	-1.70915700	-1.25234900
C	0.84686600	-0.47686100	-1.49798400
Sc	1.38953700	1.18544600	-0.00224600
Sc	-1.12232700	-0.16385900	0.00079600
Cl	-0.69795800	2.44877700	-0.00278600
Cl	-3.46238400	-0.29520200	0.00355900

State=1-A\HF=-2750.5703112\RMSD=8.545e-09\RMSF=7.244e-04\ZeroPoint=0.1321815\Thermal=0.1451438\

triplet Isomer 3 of X = Cl

Charge = 0 Multiplicity = 3

H	2.03160500	-1.55971700	2.09367100

H	2.86875000	-2.19864000	0.00004900
H	2.03167800	-1.55970400	-2.09359500
H	-0.00004700	-0.68984300	2.69018200
H	-2.03167300	-1.55970800	2.09359600
H	0.00004900	-0.68984300	-2.69018200
H	-2.03160000	-1.55972100	-2.09367200
H	-2.86874600	-2.19864500	-0.00004900
C	-1.31630300	-1.50237400	1.26783500
C	-1.83772200	-1.83742800	-0.00003200
C	-1.31626100	-1.50237900	-1.26788400
C	0.00002900	-1.06023100	-1.66026400
C	1.31630700	-1.50237100	-1.26783500
C	1.83772600	-1.83742400	0.00003200
C	1.31626500	-1.50237600	1.26788400
C	-0.00002700	-1.06023100	1.66026400
Sc	-1.46326100	0.50185500	-0.00002500
Sc	1.46326000	0.50185700	0.00002500
Cl	-2.78443300	1.81666900	0.00003600
Cl	2.78442800	1.81667000	-0.00003600

State=3-A\HF=-2750.5309774\S2=2.004578\S2-1=0.\S2A=2.000011\RMSD=6.483e-09\
RMSF=3.229e-05\ZeroPoint=0.134545\Thermal=0.148188\

singlet Isomer 3 of X = Br

Charge = 0 Multiplicity = 1

H	-0.03623800	-2.47287300	2.12972400
H	0.36144300	-3.48169900	0.00515100
H	-0.02908500	-2.47627900	-2.12189100
H	-1.11107800	-0.36631000	2.50178700
H	-3.45080600	-0.73741500	2.12988000
H	-1.10259500	-0.37099800	-2.50160900
H	-3.44422100	-0.73835900	-2.13690300
H	-4.49556000	-0.97879500	-0.00461300
C	-2.79426300	-0.78574200	1.25870100
C	-3.40210500	-0.94858200	-0.00326800
C	-2.79054900	-0.78726500	-1.26360600
C	-1.30769700	-0.77207200	-1.49793100
C	-0.46007500	-1.97862600	-1.25098400
C	-0.25429300	-2.57857300	0.00351200
C	-0.46294600	-1.97590800	1.25633600
C	-1.31207500	-0.76926700	1.49801300
Sc	-1.91718300	0.87612500	-0.00164900
Sc	0.64405100	-0.39955800	0.00236600
Br	0.18938600	2.38044500	0.00064200
Br	3.14627000	-0.51784400	-0.00124900

State=1-A\HF=-6978.0616654\RMSD=8.278e-09\RMSF=6.923e-
04\ZeroPoint=0.1315884\Thermal=0.1449939\

triplet Isomer 3 of X = Br

Charge = 0 Multiplicity = 3

H	2.02911700	2.13823900	-2.09226900
H	2.87035200	2.79332500	0.00095500
H	2.02774900	2.13814700	2.09360300
H	0.00089100	1.24050900	-2.66424200
H	-2.02775000	2.13814900	-2.09360200
H	-0.00089200	1.24050900	2.66424100
H	-2.02911800	2.13824100	2.09226900
H	-2.87035200	2.79332800	-0.00095500
C	-1.31634000	2.08869200	-1.26421700
C	-1.84044800	2.42992400	-0.00061200
C	-1.31716300	2.08875200	1.26335400
C	-0.00054800	1.63161300	1.64143900
C	1.31633900	2.08869100	1.26421700
C	1.84044700	2.42992200	0.00061300
C	1.31716200	2.08875100	-1.26335400
C	0.00054600	1.63161300	-1.64143900
Sc	-1.45364800	0.09740500	-0.00035400
Sc	1.45364600	0.09740300	0.00035500
Br	-3.16288400	-1.70827500	0.00025700
Br	3.16288700	-1.70827200	-0.00025800

State=3-A\HF=-6978.0212783\S2=2.004777\S2-1=0.\S2A=2.000012\RMSD=4.767e-09\
RMSF=3.573e-05\ZeroPoint=0.1339723\Thermal=0.1470691\

9. The detailed Cartesian coordinates of X[Sc-C_8H_8-Sc]$_2$X (X = F, Cl, Br) obtained at PBEPBE/ TZVP level.

singlet F[Sc-C_8H_8-Sc]$_2$F

Charge = 0 Multiplicity = 1

C	-1.04455900	3.27599300	1.45566100
C	-1.70089500	3.11251400	0.20465700
C	-1.27525900	3.03286600	-1.14967500
C	0.30878800	3.41993900	1.87005400
C	-0.01775700	3.07099900	-1.81271000
C	1.56701500	3.46515500	1.20709000
C	1.99296800	3.39020800	-0.14883700
H	-1.74642300	3.30630900	2.29816300
H	-2.79152400	3.05869500	0.30588900
H	-2.11290000	2.90975300	-1.84650800
H	0.40448300	3.53369600	2.95719200
H	2.40299800	3.61446500	1.90212600
C	1.33553800	3.22010500	-1.39963000
H	-0.11495800	2.98209900	-2.90178400
H	2.03509000	3.22070100	-2.24486100
H	3.08111100	3.48353000	-0.25436200
Sc	0.27621100	1.62370800	0.16534800
Sc	0.01775700	4.82623800	-0.10975100
F	-0.16480700	6.71312200	-0.30478400
C	1.04455900	-3.27599300	1.45566100

C	1.70089500	-3.11251400	0.20465700
C	1.27525900	-3.03286600	-1.14967500
C	-0.30878800	-3.41993900	1.87005400
C	0.01775700	-3.07099900	-1.81271000
C	-1.56701500	-3.46515500	1.20709000
C	-1.99296800	-3.39020800	-0.14883700
H	1.74642300	-3.30630900	2.29816300
H	2.79152400	-3.05869500	0.30588900
H	2.11290000	-2.90975300	-1.84650800
H	-0.40448300	-3.53369600	2.95719200
H	-2.40299800	-3.61446500	1.90212600
C	-1.33553800	-3.22010500	-1.39963000
H	0.11495800	-2.98209900	-2.90178400
H	-2.03509000	-3.22070100	-2.24486100
H	-3.08111100	-3.48353000	-0.25436200
Sc	-0.27621100	-1.62370800	0.16534800
Sc	-0.01775700	-4.82623800	-0.10975100
F	0.16480700	-6.71312200	-0.30478400

State=1-A\HF=-3860.4101534\

triplet F[Sc-C_8H_8-Sc]$_2$F

Charge = 0 Multiplicity = 3

C	-1.12925400	3.26480400	1.45182800
C	-1.77682100	3.10440000	0.19418900
C	-1.34429000	2.99534600	-1.15768000
C	0.22249000	3.37896000	1.88020000
C	-0.08255900	2.99714400	-1.81439500
C	1.48422800	3.38178700	1.22367300
C	1.91660200	3.27488900	-0.12955900
H	-1.84144700	3.34209500	2.28050600
H	-2.86780900	3.08247500	0.28561100
H	-2.18184500	2.90902900	-1.85784300
H	0.30940600	3.53723200	2.96117600
H	2.31909500	3.53796500	1.91617400
C	1.26921300	3.11364000	-1.38769600
H	-0.17567400	2.92531500	-2.90360500
H	1.97652500	3.11176100	-2.22467500
H	3.00485700	3.35452800	-0.22737100
Sc	0.14874400	1.48500700	0.18729300
Sc	-0.01566100	4.77541800	-0.12623400
F	-0.14874400	6.65390100	-0.34172900
C	1.12925400	-3.26480400	1.45182800
C	1.77682100	-3.10440000	0.19418900
C	1.34429000	-2.99534600	-1.15768000
C	-0.22249000	-3.37896000	1.88020000
C	0.08255900	-2.99714400	-1.81439500
C	-1.48422800	-3.38178700	1.22367300
C	-1.91660200	-3.27488900	-0.12955900

H	1.84144700	-3.34209500	2.28050600
H	2.86780900	-3.08247500	0.28561100
H	2.18184500	-2.90902900	-1.85784300
H	-0.30940600	-3.53723200	2.96117600
H	-2.31909500	-3.53796500	1.91617400
C	-1.26921300	-3.11364000	-1.38769600
H	0.17567400	-2.92531500	-2.90360500
H	-1.97652500	-3.11176100	-2.22467500
H	-3.00485700	-3.35452800	-0.22737100
Sc	-0.14874400	-1.48500700	0.18729300
Sc	0.01566100	-4.77541800	-0.12623400
F	0.14874400	-6.65390100	-0.34172900

State=3-B\HF=-3860.3987068\S2=2.022695\S2-1=0.\S2A=2.00011\

singlet Cl[Sc-C_8H_8-Sc]$_2$Cl

Charge = 0 Multiplicity = 1

C	-1.08381700	3.27074700	1.46996200
C	-1.73675800	3.11935500	0.21456700
C	-1.30664100	3.04770100	-1.13979800
C	0.26909100	3.40844800	1.89032300
C	-0.04622500	3.09005500	-1.79887600
C	1.53027400	3.45508900	1.23156600
C	1.96072300	3.38671100	-0.12405700
H	-1.78807400	3.29401000	2.30991600
H	-2.82685600	3.06018600	0.31235300
H	-2.14177500	2.92998600	-1.83972700
H	0.36149200	3.51016200	2.97825600
H	2.36436600	3.59186300	1.93040900
C	1.30664100	3.23210600	-1.37944100
H	-0.13959100	3.00733400	-2.88818000
H	2.00920200	3.23402700	-2.22131800
H	3.04915000	3.47401200	-0.22489800
Sc	0.23447700	1.64703200	0.16924900
Sc	-0.00927400	4.82039700	-0.07796500
C	1.08381700	-3.27074700	1.46996200
C	1.73675800	-3.11935500	0.21456700
C	1.30664100	-3.04770100	-1.13979800
C	-0.26909100	-3.40844800	1.89032300
C	0.04622500	-3.09005500	-1.79887600
C	-1.53027400	-3.45508900	1.23156600
C	-1.96072300	-3.38671100	-0.12405700
H	1.78807400	-3.29401000	2.30991600
H	2.82685600	-3.06018600	0.31235300
H	2.14177500	-2.92998600	-1.83972700
H	-0.36149200	-3.51016200	2.97825600
H	-2.36436600	-3.59186300	1.93040900
C	-1.30664100	-3.23210600	-1.37944100
H	0.13959100	-3.00733400	-2.88818000

H	-2.00920200	-3.23402700	-2.22131800
H	-3.04915000	-3.47401200	-0.22489800
Sc	-0.23447700	-1.64703200	0.16924900
Sc	0.00927400	-4.82039700	-0.07796500
Cl	-0.18781400	7.15015500	-0.26230800
Cl	0.18781400	-7.15015500	-0.26230800

State=1-A\HF=-4580.8866947\

triplet Cl[Sc-C_8H_8-Sc]$_2$Cl

Charge = 0 Multiplicity = 3

C	-1.03850000	3.19108600	1.54076300
C	-1.83063000	3.19218900	0.35840300
C	-1.54754300	3.19166200	-1.03561300
C	0.35869000	3.19217300	1.82029900
C	-0.35900200	3.19268700	-1.82024800
C	1.54722800	3.19148800	1.03567100
C	1.83030500	3.19237300	-0.35834000
H	-1.64523500	3.21893100	2.45179400
H	-2.90439900	3.22314800	0.57142800
H	-2.45347200	3.22507300	-1.64988100
H	0.56805100	3.21182900	2.89473700
H	2.45315300	3.22486900	1.64994100
C	1.03818200	3.19158400	-1.54070200
H	-0.56836800	3.21257900	-2.89468100
H	1.64491900	3.21968400	-2.45172400
H	2.90406700	3.22347400	-0.57136600
Sc	-0.00010400	1.50985700	-0.00024600
Sc	-0.00010400	4.79097000	0.00019800
C	1.03850000	-3.19108600	1.54076300
C	1.83063000	-3.19218900	0.35840300
C	1.54754300	-3.19166200	-1.03561300
C	-0.35869000	-3.19217300	1.82029900
C	0.35900200	-3.19268700	-1.82024800
C	-1.54722800	-3.19148800	1.03567100
C	-1.83030500	-3.19237300	-0.35834000
H	1.64523500	-3.21893100	2.45179400
H	2.90439900	-3.22314800	0.57142800
H	2.45347200	-3.22507300	-1.64988100
H	-0.56805100	-3.21182900	2.89473700
H	-2.45315300	-3.22486900	1.64994100
C	-1.03818200	-3.19158400	-1.54070200
H	0.56836800	-3.21257900	-2.89468100
H	-1.64491900	-3.21968400	-2.45172400
H	-2.90406700	-3.22347400	-0.57136600
Sc	0.00010400	-1.50985700	-0.00024600
Sc	0.00010400	-4.79097000	0.00019800
Cl	0.00322800	7.12777600	-0.00003800
Cl	-0.00322800	-7.12777600	-0.00003800

State=3-A\HF=-4580.8722148\S2=2.024765\S2-1=0.\S2A=2.000107\

singlet Br[Sc-C_8H_8-Sc]$_2$Br

Charge = 0 Multiplicity = 1

C	-1.02562500	3.28502800	1.50789500
C	-1.67562800	3.14334500	0.24963900
C	-1.24069100	3.06192100	-1.10277900
C	0.32782400	3.40052900	1.93414900
C	0.02323800	3.08313500	-1.75677100
C	1.59262600	3.42667200	1.28057400
C	2.02781100	3.34917000	-0.07327400
H	-1.73300100	3.31996700	2.34470800
H	-2.76685000	3.10074400	0.34280200
H	-2.07459500	2.95771400	-1.80620000
H	0.41721700	3.50128600	3.02236900
H	2.42584500	3.55010300	1.98285000
C	1.37667000	3.20360500	-1.33156200
H	-0.06689000	3.00036100	-2.84626800
H	2.08283000	3.19334700	-2.17033200
H	3.11796500	3.41794200	-0.16938900
Sc	0.27129800	1.64061800	0.21409400
Sc	0.08105100	4.80992100	-0.03730900
C	1.02562500	-3.28502800	1.50789500
C	1.67562800	-3.14334500	0.24963900
C	1.24069100	-3.06192100	-1.10277900
C	-0.32782400	-3.40052900	1.93414900
C	-0.02323800	-3.08313500	-1.75677100
C	-1.59262600	-3.42667200	1.28057400
C	-2.02781100	-3.34917000	-0.07327400
H	1.73300100	-3.31996700	2.34470800
H	2.76685000	-3.10074400	0.34280200
H	2.07459500	-2.95771400	-1.80620000
H	-0.41721700	-3.50128600	3.02236900
H	-2.42584500	-3.55010300	1.98285000
C	-1.37667000	-3.20360500	-1.33156200
H	0.06689000	-3.00036100	-2.84626800
H	-2.08283000	-3.19334700	-2.17033200
H	-3.11796500	-3.41794200	-0.16938900
Sc	-0.27129800	-1.64061800	0.21409400
Sc	-0.08105100	-4.80992100	-0.03730900
Br	0.08105100	-7.29355500	-0.24743600
Br	-0.08105100	7.29355500	-0.24743600

State=1-A\HF=-8808.3808757\

triplet Br[Sc-C_8H_8-Sc]$_2$Br

Charge = 0 Multiplicity = 3

C	-1.12925400	3.26480400	1.45182800

C	-1.77682100	3.10440000	0.19418900
C	-1.34429000	2.99534600	-1.15768000
C	0.22249000	3.37896000	1.88020000
C	-0.08255900	2.99714400	-1.81439500
C	1.48422800	3.38178700	1.22367300
C	1.91660200	3.27488900	-0.12955900
H	-1.84144700	3.34209500	2.28050600
H	-2.86780900	3.08247500	0.28561100
H	-2.18184500	2.90902900	-1.85784300
H	0.30940600	3.53723200	2.96117600
H	2.31909500	3.53796500	1.91617400
C	1.26921300	3.11364000	-1.38769600
H	-0.17567400	2.92531500	-2.90360500
H	1.97652500	3.11176100	-2.22467500
H	3.00485700	3.35452800	-0.22737100
Sc	0.14874400	1.48500700	0.18729300
Sc	-0.01566100	4.77541800	-0.12623400
F	-0.14874400	6.65390100	-0.34172900
C	1.12925400	-3.26480400	1.45182800
C	1.77682100	-3.10440000	0.19418900
C	1.34429000	-2.99534600	-1.15768000
C	-0.22249000	-3.37896000	1.88020000
C	0.08255900	-2.99714400	-1.81439500
C	-1.48422800	-3.38178700	1.22367300
C	-1.91660200	-3.27488900	-0.12955900
H	1.84144700	-3.34209500	2.28050600
H	2.86780900	-3.08247500	0.28561100
H	2.18184500	-2.90902900	-1.85784300
H	-0.30940600	-3.53723200	2.96117600
H	-2.31909500	-3.53796500	1.91617400
C	-1.26921300	-3.11364000	-1.38769600
H	0.17567400	-2.92531500	-2.90360500
H	-1.97652500	-3.11176100	-2.22467500
H	-3.00485700	-3.35452800	-0.22737100
Sc	-0.14874400	-1.48500700	0.18729300
Sc	0.01566100	-4.77541800	-0.12623400
F	0.14874400	-6.65390100	-0.34172900

State=3-A\HF=-8808.3657719\S2=2.025337\S2-1=0.\S2A=2.000123\

10. The detailed Cartesian coordinates of XSc-C_8H_8-ScX (X = F, Cl, Br) obtained at CAM-B3LYP/ TZVP level.

singlet FSc-C_8H_8-ScF

Title Card Required\\0,1\C,3.4317404484,1

.5125658341,-1.304151713\C,3.4272434472,0.2166522968,-1.8624573989\C,3

.4207880093,-1.0945506615,-1.3413140217\C,3.4285998056,2.0339732159,0.0069176032\C,3.4136678652,-1.652987858,-0.0455226224\C,3.4219139425,1.4755014765,1.3027022278\C,3.4152733155,0.1643139074,1.8237778849\H,3.438637307,2.2893628731,-2.0595097836\H,3.4339707112,0.2320235664,-2.9458495242\H,3.4211917493,-1.849704543,-2.1183364134\H,3.4319596388,3.1173623546,0.0222761012\H,3.4219722606,2.2306400887,2.0797277415\C,3.4111379297,-1.131588506,1.2655535441\H,3.4081608597,-2.7363686306,-0.060870741\H,3.4050018529,-1.9083838101,2.0209027709\H,3.4110887729,0.1489450875,2.9071795705\Sc,5.0308158556,0.1839637996,-0.0145503876\Sc,1.8126612546,0.1968719686,-0.0245557031\F,-0.08629348,0.200524333,-0.026764757\F,6.929764234,0.1777443268,-0.0050200082\\Version=EM64L-G09RevA.01\HF=-2030.9181294\

triplet FSc-C_8H_8-ScF

Title Card Required\\0,3\C,-1.16778403
31,0.3122447505,-1.4052713195\C,-0.8966957137,1.475145732,-0.6609250877\C,-0.0259518174,1.7965402918,0.4135414029\C,-0.6725647869,-1.0190527721,-1.385800173\C,0.672565059,1.0201018622,1.3862162932\C,0.0259506742,-1.7954913278,-0.4131247561\C,0.8966963401,-1.4740964486,0.6613405841\H,-1.8260409988,0.4979662144,-2.2421019012\H,-1.3963550591,2.3474223267,-1.058259077\H,-0.0693526117,2.8457570875,0.6700088764\H,-1.0924517381,-1.6231058828,-2.1777513492\H,0.0693513975,-2.8447082866,-0.6695915138\C,1.1677848572,-0.3111953539,1.4056863215\H,1.0924521659,1.6241554434,2.1781669731\H,1.8260426266,-0.496916276,2.2425164473\H,1.3963549635,-2.346373133,1.058675155\Sc,1.2247368567,0.4045461314,-1.1179725753\Sc,-1.2247378215,-0.40349692,1.1183896387\F,-2.5338564692,-0.8889206966,2.3770735017\F,2.5338561088,0.8899712577,-2.3766544411\\Version=EM64L-G09RevA.01\HF=-2030.9059809\S2=2.023092\S2-1=0.\S2A=2.000133

singlet ClSc-C_8H_8-ScCl

Title Card Required\\0,1\C,-0.0001420501
,1.254113984,-1.3569544989\C,-0.0000560701,1.8462528762,-0.0726623899\C,0.0000783219,1.3570527492,1.2540415375\C,-0.0007784344,-0.0726002671,-1.8461397394\C,0.0007785582,0.0727487482,1.8461631862\C,-0.0000825594,-1.3569041819,-1.254018067\C,0.0000561808,-1.8461042868,0.072685845\H,-0.000712376,1.9894568796,-2.15219739\H,-0.0000778192,2.928550363,-0.1151726629\H,0.000589701,2.1522713833,1.9894107494\H,-0.0007106017,-0.1151075556,-2.9284378255\H,-0.0005969223,-2.1521231595,-1.9893864577\C,0.0001456513,-1.2539654384,1.3569779041\H,0.0007107858,0.1152547855,2.9284613952\H,0.0007211979,-1.9893091166,2.1522197918\H,0.0000779919,-2.9284014269,0.1151956252\Cl,-3.9198035148,-0.0001966107,0.0000520062\Cl,3.9198027237,-0.0001865253,-0.0001122824\Sc,1.5849592592,0.0000891041,-0.0003567169\Sc,-1.5849600238,0.0000396956,0.00037699\\Version=EM64L-G09RevA.01\HF=-2751.65852\

triplet ClSc-C_8H_8-ScCl

Title Card Required\\0,3\C,-1.2120994
07,0.287881931,-1.3626204803\C,-0.9209086783,1.4541593804,-0.619324450
2\C,-0.1025994674,1.7818202892,0.4842536547\C,-0.6720557288,-1.0256741
009,-1.4041487753\C,0.6720731876,1.0267240406,1.404552596\C,0.10260079
93,-1.7807741084,-0.4838364267\C,0.9209002623,-1.4531177628,0.61974646
59\H,-1.9012940314,0.4823952965,-2.1725526542\H,-1.4668092723,2.312983
482,-0.986264845\H,-0.1966120693,2.8204428019,0.7691688159\H,-1.078327
565,-1.6250854741,-2.2072124106\H,0.1966102038,-2.8193983598,-0.768747
3322\C,1.2120935556,-0.2868402777,1.3630442897\H,1.0783479067,1.626136
9381,2.2076134206\H,1.9012795905,-0.4813542623,2.1729833343\H,1.466790
6822,-2.3119455628,0.9866935108\Sc,1.2222771329,0.2908304277,-1.103211
1711\Sc,-1.2222666648,-0.2897682062,1.1036205119\Cl,2.9791730832,0.757
7527456,-2.5769786831\Cl,-2.9791765198,-0.7566712179,2.5773806289\\Ver
sion=EM64L-G09RevA.01\HF=-2751.6361124\S2=2.025478\S2-1=0.\S2A=2.00013
4

singlet BrSc-C_8H_8-ScBr

Title Card Required\\0,1\C,-0.0011791516
,1.3503957883,-1.2627564621\C,0.0000360614,1.8480374479,0.0615935547\C
,0.000984681,1.2633301251,1.3500340454\C,-0.002352554,0.0619505403,-1.
8474531596\C,0.0023494281,-0.0610250367,1.8476666363\C,-0.0010019672,-
1.262403073,-1.3498206862\C,-0.0000396827,-1.8471063925,-0.0613808723\
H,-0.0024285717,2.1411881163,-2.0029670839\H,-0.0001038971,2.930617077
5,0.0974149245\H,0.0023180394,2.003530327,2.1408362951\H,-0.0029807599
,0.0977692944,-2.9300322096\H,-0.0023343834,-2.0026040841,-2.140619988
2\C,0.0011879572,-1.3494690371,1.2629687477\H,0.00297521,-0.0968443454
,2.9302459793\H,0.002435141,-2.1402632635,2.0031757488\H,0.0000985596,
-2.9296845232,-0.0972026693\Sc,1.5750860796,0.0004958461,-0.0014350407
\Sc,-1.575084646,0.0003828246,0.0016372064\Br,4.0624283402,-0.00054556
34,-0.0003254914\Br,-4.062426884,-0.0006530686,0.0000495252\\Version=E
M64L-G09RevA.01\HF=-6979.773704

triplet BrSc-C_8H_8-ScBr

Title Card Required\\0,3\C,-1.2058111
965,0.2925386032,-1.3696861667\C,-0.9210277687,1.4584299265,-0.6245970
423\C,-0.103464758,1.7819932242,0.4810967279\C,-0.6805361034,-1.026093
5584,-1.3922002212\C,0.6805282452,1.0271431427,1.3926243767\C,0.103470
3806,-1.7809405312,-0.4806826037\C,0.9210292339,-1.4573767636,0.625015
8722\H,-1.89018305,0.4823364626,-2.1851151718\H,-1.4640274501,2.318765
688,-0.9934923089\H,-0.1936394815,2.8202274667,0.7696061631\H,-1.09296
99175,-1.6285944514,-2.1904342115\H,0.1936445959,-2.8191746594,-0.7691
920306\C,1.2058175206,-0.2914839536,1.3700979331\H,1.0929553365,1.6296
420437,2.1908635531\H,1.8901914316,-0.4812813742,2.185525596\H,1.46403

26704,-2.3177114745,0.9939081022\Sc,1.2177709402,0.3006595255,-1.09373
97533\Sc,-1.2177775409,-0.2996129249,1.0941520337\Br,-3.0887925073,-0.
8152117473,2.6657759685\Br,3.088789419,0.8162453555,-2.6653628165\\Ver
sion=EM64L-G09RevA.01\HF=-6979.749722\S2=2.027535\S2-1=0.\S2A=2.000155