Electronic Supplementary Material (ESI) for

Dinuclear First-Row Transition Metals-C_8Me_6 Complexes: Metal-Metal and Metal-Ligand Bonds determined by the electron configuration of metal atom

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Table *S*1 Cartesian coordinates for the optimized geometries of dinuclear first-row transition metals-C_8Me_6 complexes(M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu):

metals-C_8Me_6

Atom	X	Y	Z	Atom	X	Y	Z
Sc	-1.36255000	0.00000000	0.00000000	Ti	0.00000000	0.00000000	-1.11316000
Sc	1.36255000	0.00000000	0.00000000	Ti	0.00000000	0.00000000	1.11316000
C	-3.63735100	2.62137000	0.00000000	C	2.16136200	0.00000000	-3.67578800
C	-1.82801300	2.25477300	2.59105700	C	2.04300400	2.59661700	-1.83696800
C	-2.18490900	2.26913200	0.00000000	C	-2.04300300	-2.59661800	-1.83696800
C	-1.36954300	2.12223900	1.17262100	C	-2.16136200	0.00000000	-3.67578800
H	-4.16191700	2.23316400	0.88459600	C	-2.04300400	2.59661700	-1.83696800
H	-3.78794500	3.71582300	0.00000000	C	2.07047400	0.00000000	-2.18433000
H	-4.16191700	2.23316400	-0.88459600	C	1.95314300	1.17760300	-1.38127200
H	-1.29728200	1.57112900	3.27183900	C	-1.95314300	-1.17760300	-1.38127200
H	-1.66786800	3.27146300	2.99111400	C	-2.07047400	0.00000000	-2.18433000
H	-2.90180200	2.04286400	2.69960400	C	-1.95314300	1.17760300	-1.38127200
H	-2.90180200	2.04286400	-2.69960400	H	1.68595200	0.88673000	-4.12004900
C	1.82801300	2.25477300	2.59105700	H	3.20945900	0.00000000	-4.01669000
C	3.63735100	2.62137000	0.00000000	H	1.68595300	-0.88673000	-4.12004900
C	1.82801300	2.25477300	-2.59105700	H	1.35583600	3.25093900	-1.27827200
C	-1.36954300	2.12223900	-1.17262100	H	3.05525700	3.01749200	-1.70451300
C	0.00000000	2.04239200	0.72221600	H	1.79180500	2.70519800	-2.90196400
C	1.36954300	2.12223900	1.17262100	H	-1.79180400	-2.70519800	-2.90196400
C	2.18490900	2.26913200	0.00000000	H	-3.05525600	-3.01749200	-1.70451300
C	1.36954300	2.12223900	-1.17262100	H	-1.35583500	-3.25093900	-1.27827100
C	0.00000000	2.04239200	-0.72221600	H	-1.68595200	0.88673000	-4.12004900
C	-1.82801300	2.25477300	-2.59105700	H	-3.20945900	0.00000000	-4.01669000
H	2.90180200	2.04286500	2.69960400	H	-1.68595300	-0.88673000	-4.12004900
H	1.66786800	3.27146300	2.99111400	H	-1.35583600	3.25093900	-1.27827200
H	1.29728200	1.57112900	3.27183900	H	-1.79180500	2.70519800	-2.90196400
H	4.16191700	2.23316400	-0.88459600	H	-3.05525700	3.01749200	-1.70451300
H	3.78794500	3.71582400	0.00000000	H	1.79180400	-2.70519800	-2.90196400
H	4.16191700	2.23316400	0.88459600	C	1.95314300	-1.17760300	-1.38127200
H	1.29728200	1.57112900	-3.27183900	C	1.92030700	0.72613800	0.00000000
H	1.66786800	3.27146300	-2.99111400	C	1.92030700	-0.72613800	0.00000000
H	2.90180200	2.04286500	-2.69960400	C	2.04300300	-2.59661800	-1.83696800
H	-1.29728200	1.57112900	-3.27183900	H	1.35583500	-3.25093900	-1.27827100
H	-1.66786800	3.27146300	-2.99111400	H	3.05525600	-3.01749200	-1.70451300

C	-1.82801300	-2.25477300	-2.59105700	C	-1.95314300	1.17760300	1.38127200
C	-3.63735100	-2.62137000	0.00000000	C	-1.92030700	-0.72613800	0.00000000
C	-1.82801300	-2.25477300	2.59105700	C	-1.92030700	0.72613800	0.00000000
C	1.36954300	-2.12223900	1.17262100	C	-2.04300400	2.59661700	1.83696800
C	0.00000000	-2.04239200	-0.72221600	H	-1.35583600	3.25093900	1.27827200
C	-1.36954300	-2.12223900	-1.17262100	H	-3.05525700	3.01749200	1.70451300
C	-2.18490900	-2.26913200	0.00000000	C	-2.16136200	0.00000000	3.67578800
C	-1.36954300	-2.12223900	1.17262100	C	-2.04300300	-2.59661800	1.83696800
C	0.00000000	-2.04239200	0.72221600	C	2.04300400	2.59661700	1.83696800
C	1.82801300	-2.25477300	2.59105700	C	2.16136200	0.00000000	3.67578800
H	-2.90180200	-2.04286400	-2.69960400	C	2.04300300	-2.59661800	1.83696800
H	-1.66786800	-3.27146300	-2.99111400	C	-2.07047400	0.00000000	2.18433000
H	-1.29728200	-1.57112900	-3.27183900	C	-1.95314300	-1.17760300	1.38127200
H	-4.16191700	-2.23316400	0.88459600	C	1.95314300	1.17760300	1.38127200
H	-3.78794500	-3.71582300	0.00000000	C	2.07047400	0.00000000	2.18433000
H	-4.16191700	-2.23316400	-0.88459600	C	1.95314300	-1.17760300	1.38127200
H	-1.29728200	-1.57112900	3.27183900	H	-1.68595300	-0.88673000	4.12004900
H	-1.66786800	-3.27146300	2.99111400	H	-3.20945900	0.00000000	4.01669000
H	-2.90180200	-2.04286400	2.69960400	H	-1.68595200	0.88673000	4.12004900
H	1.29728200	-1.57112900	3.27183900	H	-1.35583500	-3.25093900	1.27827100
H	1.66786800	-3.27146300	2.99111400	H	-3.05525600	-3.01749200	1.70451300
C	3.63735100	-2.62137000	0.00000000	H	-1.79180400	-2.70519800	2.90196400
C	1.82801300	-2.25477300	-2.59105700	H	1.79180500	2.70519800	2.90196400
C	2.18490900	-2.26913200	0.00000000	H	3.05525700	3.01749200	1.70451300
C	1.36954300	-2.12223900	-1.17262100	H	1.35583600	3.25093900	1.27827200
H	4.16191700	-2.23316400	-0.88459600	H	1.68595300	-0.88673000	4.12004900
H	3.78794500	-3.71582400	0.00000000	H	3.20945900	0.00000000	4.01669000
H	4.16191700	-2.23316400	0.88459600	H	1.68595200	0.88673000	4.12004900
H	1.29728200	-1.57112900	-3.27183900	H	1.35583500	-3.25093900	1.27827100
H	1.66786800	-3.27146300	-2.99111400	H	1.79180400	-2.70519800	2.90196400
H	2.90180200	-2.04286500	-2.69960400	H	3.05525600	-3.01749200	1.70451300
H	2.90180200	-2.04286500	2.69960400	H	-1.79180500	2.70519800	2.90196400

Atom	X	Y	Z	Atom	X	Y	Z
V	-1.04827600	0.00000000	0.00000000	Cr	-1.05467400	0.00000000	0.00000000
V	1.04827600	0.00000000	0.00000000	Cr	1.05467400	0.00000000	0.00000000
C	-3.68110600	1.97574000	0.00000000	C	-3.68093700	1.80574900	0.00000000
C	-1.83942200	1.92586100	2.59477300	C	-1.83841600	1.82996200	2.60186600
C	-1.83942200	-1.92586100	-2.59477300	C	-2.18802000	1.78592600	0.00000000
C	-3.68110600	-1.97574000	0.00000000	C	-1.38073700	1.67688300	1.19210400
C	-1.83942200	-1.92586100	2.59477300	H	-4.10322500	1.31069300	0.88703300
C	-2.18917800	1.92633300	0.00000000	H	-4.06891200	2.83788900	0.00000000
C	-1.38129600	1.81954500	1.17923000	H	-4.10322500	1.31069300	-0.88703300
C	-1.38129600	-1.81954500	-1.17923000	H	-1.20554300	1.26088800	3.29678300
C	-2.18917800	-1.92633300	0.00000000	H	-1.82185000	2.88202900	2.93572900
C	-1.38129600	-1.81954500	1.17923000	H	-2.86828300	1.46830100	2.73506000
H	-4.11011800	1.48677000	0.88698800	H	-2.86828300	1.46830100	-2.73506000
H	-4.05100500	3.01411300	0.00000000	C	1.83841600	1.82996200	2.60186600
H	-4.11011800	1.48677000	-0.88698800	C	3.68093700	1.80574900	0.00000000
H	-1.23326300	1.30308500	3.26782600	C	1.83841600	1.82996200	-2.60186600
H	-1.77857100	2.96073500	2.97513900	C	-1.38073700	1.67688300	-1.19210400
H	-2.88381700	1.60360500	2.71435700	C	0.00000000	1.75001300	0.72455100
H	-2.88381700	-1.60360500	-2.71435700	C	1.38073700	1.67688300	1.19210400
H	-1.77857100	-2.96073500	-2.97513900	C	2.18802000	1.78592600	0.00000000
H	-1.23326300	-1.30308500	-3.26782600	C	1.38073700	1.67688300	-1.19210400
H	-4.11011800	-1.48677000	0.88698800	C	0.00000000	1.75001300	-0.72455100
H	-4.05100500	-3.01411300	0.00000000	C	-1.83841600	1.82996200	-2.60186600
H	-4.11011800	-1.48677000	-0.88698800	H	2.86828300	1.46830100	2.73506000
H	-1.23326300	-1.30308500	3.26782600	H	1.82185000	2.88202900	2.93572900
H	-2.88381700	-1.60360500	2.71435700	H	1.20554300	1.26088800	3.29678300
H	-1.77857100	-2.96073500	2.97513900	H	4.10322500	1.31069300	-0.88703300
H	-2.88381700	1.60360500	-2.71435700	H	4.06891200	2.83788900	0.00000000
C	-1.38129600	1.81954500	-1.17923000	H	4.10322500	1.31069300	0.88703300
C	0.00000000	1.85417400	0.72164300	H	1.20554300	1.26088800	-3.29678300
C	0.00000000	1.85417400	-0.72164300	H	1.82185000	2.88202900	-2.93572900
C	-1.83942200	1.92586100	-2.59477300	H	2.86828300	1.46830100	-2.73506000
H	-1.23326300	1.30308500	-3.26782600	H	-1.20554300	1.26088800	-3.29678300
H	-1.77857100	2.96073500	-2.97513900	H	-1.82185000	2.88202900	-2.93572900
C	1.38129600	-1.81954500	1.17923000	C	-1.83841600	-1.82996200	-2.60186600
C	0.00000000	-1.85417400	-0.72164300	C	-3.68093700	-1.80574900	0.00000000

C	0.00000000	-1.85417400	0.72164300	C	-1.83841600	-1.82996200	2.60186600
C	1.83942200	-1.92586100	2.59477300	C	1.38073700	-1.67688300	1.19210400
H	1.23326300	-1.30308500	3.26782600	C	0.00000000	-1.75001300	-0.72455100
H	1.77857100	-2.96073500	2.97513900	C	-1.38073700	-1.67688300	-1.19210400
C	3.68110600	-1.97574000	0.00000000	C	-2.18802000	-1.78592600	0.00000000
C	1.83942200	-1.92586100	-2.59477300	C	-1.38073700	-1.67688300	1.19210400
C	1.83942200	1.92586100	2.59477300	C	0.00000000	-1.75001300	0.72455100
C	3.68110600	1.97574000	0.00000000	C	1.83841600	-1.82996200	2.60186600
C	1.83942200	1.92586100	-2.59477300	H	-2.86828300	-1.46830100	-2.73506000
C	2.18917800	-1.92633300	0.00000000	H	-1.82185000	-2.88202900	-2.93572900
C	1.38129600	-1.81954500	-1.17923000	H	-1.20554300	-1.26088800	-3.29678300
C	1.38129600	1.81954500	1.17923000	H	-4.10322500	-1.31069300	0.88703300
C	2.18917800	1.92633300	0.00000000	H	-4.06891200	-2.83788900	0.00000000
C	1.38129600	1.81954500	-1.17923000	H	-4.10322500	-1.31069300	-0.88703300
H	4.11011800	-1.48677000	-0.88698800	H	-1.20554300	-1.26088800	3.29678300
H	4.05100500	-3.01411300	0.00000000	H	-1.82185000	-2.88202900	2.93572900
H	4.11011800	-1.48677000	0.88698800	H	-2.86828300	-1.46830100	2.73506000
H	1.23326300	-1.30308500	-3.26782600	H	1.20554300	-1.26088800	3.29678300
H	1.77857100	-2.96073500	-2.97513900	H	1.82185000	-2.88202900	2.93572900
H	2.88381700	-1.60360500	-2.71435700	C	3.68093700	-1.80574900	0.00000000
H	2.88381700	1.60360500	2.71435700	C	1.83841600	-1.82996200	-2.60186600
H	1.77857100	2.96073500	2.97513900	C	2.18802000	-1.78592600	0.00000000
H	1.23326300	1.30308500	3.26782600	C	1.38073700	-1.67688300	-1.19210400
H	4.11011800	1.48677000	-0.88698800	H	4.10322500	-1.31069300	-0.88703300
H	4.05100500	3.01411300	0.00000000	H	4.06891200	-2.83788900	0.00000000
H	4.11011800	1.48677000	0.88698800	H	4.10322500	-1.31069300	0.88703300
H	1.23326300	1.30308500	-3.26782600	H	1.20554300	-1.26088800	-3.29678300
H	2.88381700	1.60360500	-2.71435700	H	1.82185000	-2.88202900	-2.93572900
H	1.77857100	2.96073500	-2.97513900	H	2.86828300	-1.46830100	-2.73506000
H	2.88381700	-1.60360500	2.71435700	H	2.86828300	-1.46830100	2.73506000

Atom	X	Y	Z	Atom	X	Y	Z
Mn	1.10078800	0.00000000	0.00000000	Fe	0.00000000	0.00000100	-1.14768400
Mn	-1.10078800	0.00000000	0.00000000	Fe	0.00000000	0.00000100	1.14768900
C	1.38002900	1.65363700	1.18452400	C	0.00000000	1.88374800	-3.69491000
C	3.69078200	1.82704300	0.00000000	C	-2.59325000	1.73963400	-1.84173800
C	1.83777500	1.78478400	-2.59628900	C	0.00000000	1.72106000	-2.21341000
C	1.83777500	-1.78478400	2.59628900	C	-1.17950300	1.64592200	-1.37848200
C	3.69078200	-1.82704300	0.00000000	H	-0.88489700	1.42257600	-4.15619000
C	1.83777500	-1.78478400	-2.59628900	H	0.00000000	2.94642200	-3.99191200
C	2.20126200	1.74130300	0.00000000	H	0.88489700	1.42257600	-4.15619000
C	1.38002900	1.65363700	-1.18452400	H	-3.27622100	1.17385900	-1.19221800
C	1.38002900	-1.65363700	1.18452400	H	-2.95634700	2.78154200	-1.85702300
C	2.20126200	-1.74130300	0.00000000	H	-2.71438400	1.34197800	-2.85945700
C	1.38002900	-1.65363700	-1.18452400	H	2.71438400	1.34197800	-2.85945700
H	4.12945500	1.34281500	-0.88480600	C	-2.59325100	1.73964000	1.84173100
H	4.03924900	2.87323300	0.00000000	C	0.00000000	1.88376900	3.69490200
H	4.12945500	1.34281500	0.88480600	C	2.59325100	1.73964000	1.84173100
H	1.21030800	1.20249000	-3.28588500	C	1.17950300	1.64592200	-1.37848200
H	1.80867200	2.83191400	-2.94346800	C	-0.72225900	1.71207000	-0.00000400
H	2.87143800	1.43295700	-2.72539600	C	-1.17950300	1.64592500	1.37847500
H	2.87143800	-1.43295700	2.72539600	C	0.00000000	1.72107000	2.21340300
H	1.21030800	-1.20249000	3.28588500	C	1.17950300	1.64592500	1.37847500
H	1.80867200	-2.83191400	2.94346800	C	0.72225900	1.71207000	-0.00000400
H	4.12945500	-1.34281500	-0.88480600	C	2.59325100	1.73963500	-1.84173800
H	4.03924900	-2.87323300	0.00000000	H	-2.71438200	1.34199500	2.85945400
H	4.12945500	-1.34281500	0.88480600	H	-2.95635100	2.78154700	1.85700300
H	1.21030800	-1.20249000	-3.28588500	H	-3.27622000	1.17385400	1.19221800
H	2.87143800	-1.43295700	-2.72539600	H	0.88489700	1.42260200	4.15618600
H	1.80867200	-2.83191400	-2.94346800	H	0.00000000	2.94644600	3.99189500
H	2.87143800	1.43295700	2.72539600	H	-0.88489700	1.42260200	4.15618600
C	0.00000000	1.71276300	-0.72304200	H	3.27622000	1.17385500	1.19221800
C	0.00000000	1.71276300	0.72304200	H	2.95635100	2.78154700	1.85700300
C	1.83777500	1.78478400	2.59628900	H	2.71438200	1.34199500	2.85945400
H	1.21030800	1.20249000	3.28588500	H	3.27622100	1.17385900	-1.19221800
H	1.80867200	2.83191400	2.94346800	H	2.95634700	2.78154300	-1.85702300
C	0.00000000	-1.71276300	0.72304200	C	2.59325100	-1.73963500	-1.84173900
C	0.00000000	-1.71276300	-0.72304200	C	0.00000000	-1.88374800	-3.69491000

C	-1.83777500	-1.78478400	-2.59628900	C	-2.59325100	-1.73963500	-1.84173800
H	-1.21030800	-1.20249000	-3.28588500	C	-1.17950300	-1.64592400	1.37847500
H	-1.80867200	-2.83191400	-2.94346800	C	0.72225900	-1.71206900	-0.00000400
C	-1.38002900	-1.65363700	-1.18452400	C	1.17950400	-1.64592100	-1.37848200
C	-3.69078200	-1.82704300	0.00000000	C	0.00000000	-1.72105900	-2.21341000
C	-1.83777500	-1.78478400	2.59628900	C	-1.17950400	-1.64592100	-1.37848200
C	-1.83777500	1.78478400	-2.59628900	C	-0.72225900	-1.71206900	-0.00000400
C	-3.69078200	1.82704300	0.00000000	C	-2.59325100	-1.73964000	1.84173100
C	-1.83777500	1.78478400	2.59628900	H	2.71438500	-1.34197900	-2.85945700
C	-2.20126200	-1.74130300	0.00000000	H	2.95634700	-2.78154400	-1.85702300
C	-1.38002900	-1.65363700	1.18452400	H	3.27622200	-1.17386000	-1.19221800
C	-1.38002900	1.65363700	-1.18452400	H	-0.88489700	-1.42257600	-4.15619100
C	-2.20126200	1.74130300	0.00000000	H	0.00000000	-2.94642300	-3.99191100
C	-1.38002900	1.65363700	1.18452400	H	0.88489700	-1.42257600	-4.15619100
H	-4.12945500	-1.34281500	0.88480600	H	-3.27622200	-1.17386000	-1.19221800
H	-4.03924900	-2.87323300	0.00000000	H	-2.95634700	-2.78154400	-1.85702300
H	-4.12945500	-1.34281500	-0.88480600	H	-2.71438500	-1.34197900	-2.85945700
H	-1.21030800	-1.20249000	3.28588500	H	-3.27622100	-1.17385500	1.19221800
H	-1.80867200	-2.83191400	2.94346800	H	-2.95635000	-2.78154800	1.85700300
H	-2.87143800	-1.43295700	2.72539600	C	0.00000000	-1.88376900	3.69490200
H	-2.87143800	1.43295700	-2.72539600	C	2.59325100	-1.73964000	1.84173100
H	-1.21030800	1.20249000	-3.28588500	C	0.00000000	-1.72106900	2.21340300
H	-1.80867200	2.83191400	-2.94346800	C	1.17950300	-1.64592400	1.37847500
H	-4.12945500	1.34281500	0.88480600	H	0.88489700	-1.42260200	4.15618600
H	-4.03924900	2.87323300	0.00000000	H	0.00000000	-2.94644700	3.99189400
H	-4.12945500	1.34281500	-0.88480600	H	-0.88489700	-1.42260200	4.15618600
H	-1.21030800	1.20249000	3.28588500	H	3.27622100	-1.17385500	1.19221800
H	-2.87143800	1.43295700	2.72539600	H	2.95635000	-2.78154800	1.85700300
H	-1.80867200	2.83191400	2.94346800	H	2.71438300	-1.34199600	2.85945400
H	-2.87143800	-1.43295700	-2.72539600	H	-2.71438300	-1.34199500	2.85945400

Atom	X	Y	Z	Atom	X	Y	Z
Co	-0.02916500	-0.02113400	-1.22312900	Ni	0.00000000	0.00000000	-1.25615700
Co	0.02916500	0.02113400	1.22312900	Ni	0.00000000	0.00000000	1.25616500
C	3.09332200	-0.09579900	-1.61512200	C	0.00000000	1.91516200	-3.67143200
C	1.87889000	0.63683300	-1.15464800	C	-2.59095800	1.80808700	-1.84580000
H	3.25015000	-1.02901000	-1.05273800	C	0.00000000	1.74070600	-2.19151200
H	4.01000900	0.50626400	-1.49103700	C	-1.18618100	1.72817900	-1.35193200
H	3.02722400	-0.36855000	-2.67757400	H	-0.88577900	1.45894900	-4.13632700
C	-0.40898600	-1.81457000	-0.24777100	H	0.00000000	2.98100100	-3.95520700
C	-1.58461900	-0.97616200	-0.23468300	H	0.88577900	1.45894900	-4.13632700
C	-3.10541900	0.13460300	-2.06248400	H	-3.29528800	1.31259200	-1.16329400
H	-3.44685800	0.86326500	-1.31493700	H	-2.93506000	2.85067000	-1.95742100
H	-3.96484300	-0.52067200	-2.28315800	H	-2.70642100	1.32895400	-2.82898800
C	-1.01622600	-1.36605100	-3.92553800	H	2.70642100	1.32895400	-2.82898800
C	1.10708500	-2.87535600	-2.10792200	C	-2.59095900	1.80808000	1.84579500
C	-1.12390100	2.91190100	-1.56481000	C	0.00000000	1.91516600	3.67143300
C	1.16005000	1.68220300	-3.45047300	C	2.59095900	1.80808000	1.84579500
C	-1.92607100	-0.64400300	-1.58870000	C	1.18618100	1.72817900	-1.35193200
C	-0.96017800	-1.31056400	-2.43784300	C	-0.73885600	1.79945700	0.00000000
C	-0.00318600	-2.01496000	-1.60986400	C	-1.18618000	1.72818100	1.35193200
C	-0.02875700	1.99689300	-1.13318200	C	0.00000000	1.74070500	2.19151300
C	1.00223200	1.43809100	-1.98874900	C	1.18618000	1.72818100	1.35193200
H	-0.01563500	-1.48015200	-4.36676000	C	0.73885600	1.79945700	0.00000000
H	-1.45802900	-0.45333000	-4.35067900	C	2.59095800	1.80808700	-1.84580000
H	-1.62407700	-2.21399800	-4.28414200	H	-2.70641700	1.32896700	2.82899300
H	1.92036900	-2.96681100	-1.37540000	H	-2.93507700	2.85066100	1.95739100
H	1.54843100	-2.48393200	-3.03627700	H	-3.29528200	1.31256400	1.16329800
H	0.76102800	-3.89959900	-2.32723200	H	0.88577900	1.45895400	4.13632900
H	-1.36883800	2.78475900	-2.62856400	H	0.00000000	2.98100700	3.95520400
H	-0.85642100	3.97266000	-1.41799600	H	-0.88577900	1.45895400	4.13632900
H	-2.05138500	2.73855700	-0.99788000	H	3.29528200	1.31256400	1.16329800
H	1.63399200	0.82817300	-3.95588800	H	2.93507700	2.85066100	1.95739100
H	1.78537700	2.56763200	-3.65697700	H	2.70641700	1.32896700	2.82899300
H	0.19029400	1.85027300	-3.94093200	H	3.29528800	1.31259200	-1.16329400
H	-2.88768900	0.69372700	-2.98450200	H	2.93506000	2.85067000	-1.95742100
C	1.01622600	1.36605100	3.92553800	C	2.59095800	-1.80808700	-1.84580000
C	-1.10708500	2.87535600	2.10792200	C	0.00000000	-1.91516200	-3.67143200

C	1.12390100	-2.91190100	1.56481000	C	-2.59095800	-1.80808700	-1.84580000
C	-1.16005000	-1.68220300	3.45047300	C	-1.18618000	-1.72818100	1.35193200
C	1.92607100	0.64400300	1.58870000	C	0.73885600	-1.79945700	0.00000000
C	0.96017800	1.31056400	2.43784300	C	1.18618100	-1.72817900	-1.35193200
C	0.00318600	2.01496000	1.60986400	C	0.00000000	-1.74070600	-2.19151200
C	0.02875700	-1.99689300	1.13318200	C	-1.18618100	-1.72817900	-1.35193200
C	-1.00223200	-1.43809100	1.98874900	C	-0.73885600	-1.79945700	0.00000000
H	0.01563500	1.48015200	4.36676000	C	-2.59095900	-1.80808000	1.84579500
H	1.45802900	0.45333000	4.35067900	H	2.70642100	-1.32895400	-2.82898800
H	1.62407700	2.21399800	4.28414200	H	2.93506000	-2.85067000	-1.95742100
H	-1.92036900	2.96681100	1.37540000	H	3.29528800	-1.31259200	-1.16329400
H	-1.54843100	2.48393200	3.03627700	H	-0.88577900	-1.45894900	-4.13632700
H	-0.76102800	3.89959900	2.32723200	H	0.00000000	-2.98100100	-3.95520700
H	1.36883800	-2.78475900	2.62856400	H	0.88577900	-1.45894900	-4.13632700
H	0.85642100	-3.97266000	1.41799600	H	-3.29528800	-1.31259200	-1.16329400
H	2.05138500	-2.73855700	0.99788000	H	-2.93506000	-2.85067000	-1.95742100
H	-1.63399200	-0.82817300	3.95588800	H	-2.70642100	-1.32895400	-2.82898800
H	-1.78537700	-2.56763200	3.65697700	H	-3.29528200	-1.31256400	1.16329800
H	-0.19029400	-1.85027300	3.94093200	H	-2.93507700	-2.85066100	1.95739100
H	2.88768900	-0.69372700	2.98450200	C	0.00000000	-1.91516600	3.67143300
C	0.40898600	1.81457000	0.24777100	C	2.59095900	-1.80808000	1.84579500
C	1.58461900	0.97616200	0.23468300	C	0.00000000	-1.74070500	2.19151300
C	3.10541900	-0.13460300	2.06248400	C	1.18618000	-1.72818100	1.35193200
H	3.44685800	-0.86326500	1.31493700	H	0.88577900	-1.45895400	4.13632900
H	3.96484300	0.52067200	2.28315800	H	0.00000000	-2.98100700	3.95520400
C	-3.09332200	0.09579900	1.61512200	H	-0.88577900	-1.45895400	4.13632900
C	-1.87889000	-0.63683300	1.15464800	H	3.29528200	-1.31256400	1.16329800
H	-3.25015000	1.02901000	1.05273800	H	2.93507700	-2.85066100	1.95739100
H	-4.01000900	-0.50626400	1.49103700	H	2.70641700	-1.32896700	2.82899300
H	-3.02722400	0.36855000	2.67757400	H	-2.70641700	-1.32896700	2.82899300

Atom	X	Y	Z
Cu	0.00000000	0.00000000	-1.49819400
Cu	0.00000000	0.00000000	1.49819700
C	0.00000000	2.12796800	-3.67925700
C	-2.58468100	1.93891700	-1.83083900
C	0.00000000	1.92589000	-2.20010200
C	-1.17267500	1.84795700	-1.35831600
H	-0.88398100	1.68128300	-4.15788300
H	0.00000000	3.19779300	-3.95043600
H	0.88398100	1.68128300	-4.15788300
H	-3.26408600	1.32065800	-1.22638900
H	-2.96771900	2.97211200	-1.77400800
H	-2.69470600	1.61533100	-2.87578900
H	2.69470600	1.61533100	-2.87578900
C	-2.58468200	1.93891900	1.83083800
C	0.00000000	2.12797200	3.67925600
C	2.58468200	1.93891900	1.83083800
C	1.17267500	1.84795700	-1.35831600
C	-0.71572300	1.92810700	0.00000000
C	-1.17267500	1.84795800	1.35831500
C	0.00000000	1.92589100	2.20010100
C	1.17267500	1.84795800	1.35831500
C	0.71572300	1.92810700	0.00000000
C	2.58468100	1.93891700	-1.83083900
H	-2.69470600	1.61533500	2.87579000
H	-2.96772100	2.97211300	1.77400400
H	-3.26408600	1.32065700	1.22639000
H	0.88398100	1.68128800	4.15788300
H	0.00000000	3.19779900	3.95043300
H	-0.88398100	1.68128800	4.15788300
H	3.26408600	1.32065700	1.22639000
H	2.96772100	2.97211300	1.77400400
H	2.69470600	1.61533500	2.87579000
H	3.26408600	1.32065800	-1.22638900
H	2.96771900	2.97211200	-1.77400800
C	2.58468100	-1.93891700	-1.83083900
C	0.00000000	-2.12796800	-3.67925700

C	-2.58468100	-1.93891700	-1.83083900
C	-1.17267500	-1.84795800	1.35831500
C	0.71572300	-1.92810700	0.00000000
C	1.17267500	-1.84795700	-1.35831600
C	0.00000000	-1.92589000	-2.20010200
C	-1.17267500	-1.84795700	-1.35831600
C	-0.71572300	-1.92810700	0.00000000
C	-2.58468200	-1.93891900	1.83083800
H	2.69470600	-1.61533100	-2.87578900
H	2.96771900	-2.97211200	-1.77400800
H	3.26408600	-1.32065800	-1.22638900
H	-0.88398100	-1.68128300	-4.15788300
H	0.00000000	-3.19779300	-3.95043600
H	0.88398100	-1.68128300	-4.15788300
H	-3.26408600	-1.32065800	-1.22638900
H	-2.96771900	-2.97211200	-1.77400800
H	-2.69470600	-1.61533100	-2.87578900
H	-3.26408600	-1.32065700	1.22639000
H	-2.96772100	-2.97211300	1.77400400
C	0.00000000	-2.12797200	3.67925600
C	2.58468200	-1.93891900	1.83083800
C	0.00000000	-1.92589100	2.20010100
C	1.17267500	-1.84795800	1.35831500
H	0.88398100	-1.68128800	4.15788300
H	0.00000000	-3.19779900	3.95043300
H	-0.88398100	-1.68128800	4.15788300
H	3.26408600	-1.32065700	1.22639000
H	2.96772100	-2.97211300	1.77400400
H	2.69470600	-1.61533500	2.87579000
H	-2.69470600	-1.61533500	2.87579000

Table *S*2 BCP numbers in the molecular graph between metal atom and Pn*

Compounds	**BCP numbers in total molecular graph**	**BCP numbers in σ molecular graph**	**BCP numbers in π molecular graph**
$(C_8Me_6)_2Sc_2$	1	2	2
$(C_8Me_6)_2Ti_2$	2	4	4
$(C_8Me_6)_2V_2$	2	4	4
$(C_8Me_6)_2Cr_2$	1	3	5
$(C_8Me_6)_2Mn_2$	1	3	5
$(C_8Me_6)_2Fe_2$	1	3	3
$(C_8Me_6)_2Co_2$	1	3	1
$(C_8Me_6)_2Ni_2$	1	3	1
$(C_8Me_6)_2Cu_2$	1	3	1

Table *S*3 σ and π electron density topological properties at the BCPs of M-C in $Pn^*_2M_2$ ($Pn^*_2=C_8Me_6$; M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu) (all values in a.u.)

	ρ_σ	ρ_π	$\rho_\sigma : \rho_\pi$
Sc_1-C_1	0.0266	0.0174	1.53
Ti_1-C_1	0.0346	0.0234	1.48
V_1-C_1	0.0444	0.0234	1.90
Cr_1-C_2	0.0671	0.0250	2.68
Mn_1-C_2	0.0727	0.0261	2.79
Fe_1-C_2	0.0728	0.0352	2.07
Co_1-C_2	0.0789	0.0277	2.85
Ni_1-C_2	0.0734	0.0344	2.13
Cu_1-C_2	0.0625	0.0197	3.17

Table *S*4 ELF basin populations ($N(\Omega_i)$), volume $V(\Omega_i)$, variance ($\sigma^2(\Omega_i)$), relative fluctuations ($\lambda_F(\Omega_i)$) of V(Sc, C) in $Pn^*_2M_2$ ($Pn^*_2=C_8Me_6$; M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu) (all values in a.u.)

Compounds	**Ω**	**N(Ω_i)**	***V*(Ω_i)**	**$\sigma^2(\Omega_i)$**	**$\lambda_F(\Omega_i)$**
$(C_8Me_6)_2Sc_2$	V(Sc1, C1/3)	0.91	41.23	0.70	0.84
	V(Sc1, C2)	0.41	21.26	0.36	0.60
	V(Sc1,Sc2,C4/5)	0.24	7.88	0.22	0.47
$(C_8Me_6)_2Ti_2$	V (Ti1, C1/3)	0.90	41.45	0.70	0.83
	V(Ti1,Ti2,C4/5)	0.49	8.86	0.42	0.65
$(C_8Me_6)_2V_2$	V(V1, C1/3)	0.93	39.02	0.72	0.85
	V(V1, V2, C4/5)	0.40	5.88	0.35	0.59
$(C_8Me_6)_2Cr_2$	V (Cr1, C1/3)	1.03	35.75	0.78	0.88
	V (Cr1, C2)	0.44	14.73	0.39	0.62
	V(Cr1,Cr2,C4/5)	0.40	5.77	0.36	0.40
$(C_8Me_6)_2Mn_2$	V(Mn1, C1/3)	1.17	54.26	0.86	0.93
	V(Mn1, C2)	0.68	26.95	0.56	0.75
	V(Mn1,Mn2,C4/5)	0.34	5.10	0.31	0.55
$(C_8Me_6)_2Fe_2$	V(Fe1, C1/3)	0.91	30.46	0.70	0.84
	V(Fe1, C2)	0.69	26.59	0.57	0.75
	V(Fe1, Fe2, C4/5)	0.27	4.61	0.25	0.50
$(C_8Me_6)_2Co_2$	V(Co1, C1/3)	0.92	29.97	0.71	0.85
	V(Co1, C2)	0.81	28.75	0.65	0.81
$(C_8Me_6)_2Ni_2$	V(Ni1, C1/3)	0.75	32.09	0.62	0.79
	V(Ni1, C2)	0.77	29.92	0.63	0.79
$(C_8Me_6)_2Cu_2$	V(Cu1, C1/3)	0.65	30.66	0.55	0.74
	V(Cu1, C2)	0.61	23.43	0.52	0.72