

Testing the Effectiveness of the Isoelectronic Substitution Principle through the Transformation of Aromatic Osmathiophene Derivatives into their Inorganic Analogues

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SUPPORTING INFORMATION

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SI-Cartesian coordinates of the systems

Figure SI1. Lone pairs of **1**

Figure SI2. 2c- 2e of **1**

Figure SI3. 4c – 2e of **1**

Figure SI4. Lone pairs of **7**

Figure SI5. 2c- 2e of **7**

Figure SI6. 4c – 2e of **7**

Figure SI7. Lone pairs of **14**

Figure SI8. 2c- 2e of **14**

Figure SI9. 4c – 2e of **14**

SI- Cartesian coordinates in Å, computed at B3PW91 functional and the def2-TZVP basis set, including pseudo-potentials for Os atom.

System 1

C	-1.018940880	-0.838628930	0.005217463
C	0.295780469	-1.219946229	-0.001902165
Os	1.899647015	0.000000000	0.000000000
S	0.073752880	1.525578400	0.000000000
C	-1.250239484	0.532996759	-0.003315298
H	-1.831579102	-1.557066416	-0.002917382
H	0.522501753	-2.284276372	0.030698001
Cl	3.175228369	-1.765391441	-0.665786222
H	-2.235869123	0.986834172	-0.031596206
P	2.126503496	0.836039854	-2.238868327
H	3.326910028	0.470846135	-2.873329267
H	1.172731961	0.426990036	-3.187344275
H	2.110788588	2.232839004	-2.395078449
P	2.079215115	-0.807238419	2.231962318
H	1.231916028	-0.235888591	3.197002008
H	1.878582926	-2.182307346	2.442714805
H	3.345294170	-0.599595818	2.804739151
Cl	2.937833916	1.888203657	0.846253096

System 2

C	-1.076809645	0.964124953	-0.005126140
B	0.393372205	0.985878098	0.013008362
Os	1.996170968	-0.069386751	0.000000000

S	0.000000000	-1.491473989	0.000000000
C	-1.312733528	-0.389142311	-0.007882222
H	-1.850512055	1.717428313	-0.008961994
H	1.544588614	1.637265469	0.132362529
Cl	4.160082859	0.993621603	-0.053357854
H	-2.307894474	-0.829777250	-0.014650164
P	2.266172012	-0.363309809	2.315383541
H	3.603989924	-0.452531054	2.737702100
H	1.784229996	0.594434857	3.231498242
H	1.723138017	-1.532114549	2.879285476
P	2.178546804	-0.042730742	-2.335943000
H	1.160930879	-0.615829929	-3.125190867
H	2.331139188	1.192009936	-2.995182077
H	3.301155543	-0.733485637	-2.821969072
Cl	2.987374072	-2.250021570	-0.091001422

System 3

B	-2.083937000	-0.081589000	-1.368859000
C	-0.684009000	0.284182000	-1.841665000
Os	0.033391000	0.003749000	-0.121388000
S	-1.683171000	1.303386000	0.792330000
C	-2.787302000	0.797146000	-0.322325000
H	-2.583394000	-1.077732000	-1.824714000
H	-0.219421000	0.501678000	-2.799538000
Cl	1.719604000	-1.569538000	-0.887313000
H	-3.846530000	0.999543000	-0.180658000

P	1.567507000	1.739984000	-0.537339000
H	2.906794000	1.337793000	-0.424536000
H	1.597008000	2.375695000	-1.799835000
H	1.536001000	2.870080000	0.298825000
P	-0.987138000	-1.986000000	0.663504000
H	-2.261641000	-1.949629000	1.267562000
H	-1.152539000	-3.038916000	-0.252263000
H	-0.235429000	-2.622504000	1.666772000
Cl	1.291820000	0.221016000	1.977454000

System 4

C	-2.239164000	-1.043761000	-1.522738000
C	-0.908176000	-0.862239000	-1.473915000
Os	0.250246000	0.029662000	-0.016910000
S	-2.002467000	0.235908000	0.884612000
B	-3.034422000	-0.553254000	-0.316377000
H	-2.674247000	-1.519672000	-2.400902000
H	-0.281375000	-1.260864000	-2.274025000
Cl	2.027755000	-0.001836000	-1.491125000
H	-4.211320000	-0.630433000	-0.130691000
P	-0.239097000	2.254807000	-0.590581000
H	0.731735000	3.015768000	-1.277476000
H	-1.350360000	2.461104000	-1.428984000
H	-0.547513000	3.129283000	0.467767000
P	0.588333000	-2.203609000	0.589420000
H	-0.559844000	-2.942281000	0.935095000

H	1.164427000	-3.071754000	-0.360079000
H	1.404811000	-2.479710000	1.704914000
Cl	0.805309000	0.631483000	2.166123000

System 5

C	2.269158000	1.431520000	-0.987988000
N	0.996865000	1.190161000	-1.154580000
Os	-0.161121000	-0.019220000	-0.012933000
S	1.917195000	-0.226123000	0.961917000
C	2.894701000	0.749097000	0.068895000
H	2.793661000	2.119135000	-1.646391000
H	0.553257000	1.694314000	-1.920959000
Cl	-1.464978000	-0.122128000	-1.865784000
H	3.954591000	0.812284000	0.295105000
P	0.187697000	-2.376857000	-0.539865000
H	-1.053819000	-3.003469000	-0.731884000
H	0.890762000	-2.635180000	-1.728962000
H	0.832799000	-3.166665000	0.426931000
P	-1.321264000	2.043228000	0.602845000
H	-0.853856000	2.675949000	1.767506000
H	-1.364314000	3.073665000	-0.352148000
H	-2.672347000	1.779006000	0.878184000
Cl	-1.033161000	-0.741445000	1.939713000

System 6

N	-1.968140000	-1.572134000	-1.223102000
C	-0.670475000	-1.231741000	-1.256532000
Os	0.171870000	0.042302000	-0.024799000
S	-2.068740000	0.103555000	0.684203000
C	-2.775315000	-0.969992000	-0.332492000
H	-2.347482000	-2.253810000	-1.879582000
H	-0.108592000	-1.745105000	-2.035018000
Cl	1.747716000	0.344758000	-1.622888000
H	-3.837965000	-1.192735000	-0.312736000
P	-0.245102000	2.422006000	-0.451264000
H	0.956829000	3.133796000	-0.302954000
H	-0.664029000	2.729825000	-1.756006000
H	-1.153536000	3.100570000	0.378804000
P	1.464018000	-1.897322000	0.625737000
H	0.883606000	-2.708985000	1.614167000
H	1.850607000	-2.790046000	-0.387904000
H	2.676185000	-1.474429000	1.193687000
Cl	0.484641000	0.518427000	2.205463000

System 7

C	-2.017498000	-1.758768000	-0.990725000
C	-0.667260000	-1.471385000	-1.048963000
Os	0.144292000	0.028583000	-0.026844000
S	-2.014080000	0.247441000	0.598715000
N	-2.757332000	-0.963307000	-0.227179000

H	-2.507808000	-2.554812000	-1.542974000
H	-0.056806000	-2.079307000	-1.710345000
Cl	1.594336000	0.237222000	-1.759762000
H	-3.771085000	-1.053753000	-0.158697000
P	-0.155483000	2.412897000	-0.512817000
H	1.098124000	3.044272000	-0.462583000
H	-0.636522000	2.670424000	-1.806424000
H	-0.974705000	3.165268000	0.345900000
P	1.556859000	-1.813030000	0.658935000
H	1.032650000	-2.577807000	1.712692000
H	1.924978000	-2.735132000	-0.333660000
H	2.768959000	-1.304642000	1.152563000
Cl	0.568639000	0.611023000	2.165694000

System 8

N	-2.442580000	0.008977000	-1.661318000
B	-1.007955000	0.073710000	-1.682208000
Os	0.248395000	0.018547000	-0.063604000
S	-2.019263000	-0.157478000	0.862880000
C	-3.001916000	-0.103817000	-0.454781000
H	-3.032471000	0.040921000	-2.484002000
H	-0.419831000	0.171129000	-2.715990000
Cl	2.232689000	0.183955000	-1.154049000
H	-4.082017000	-0.159470000	-0.351371000
P	0.262204000	2.383874000	0.151438000
H	0.962089000	3.101350000	-0.834958000

H	-0.956572000	3.086181000	0.188807000
H	0.869898000	2.854708000	1.329928000
P	0.550954000	-2.342288000	-0.126923000
H	-0.445495000	-3.162090000	0.432773000
H	0.745828000	-2.958417000	-1.375695000
H	1.688970000	-2.781146000	0.571630000
Cl	0.476235000	-0.155448000	2.252161000

System 9

B	-2.475624000	-0.199873000	-1.568010000
C	-0.927105000	-0.015593000	-1.608889000
Os	0.079169000	-0.007235000	0.031189000
S	-1.675483000	-1.120966000	0.785293000
N	-2.879070000	-0.755881000	-0.342580000
H	-3.250630000	0.103758000	-2.416135000
H	-0.414590000	0.018899000	-2.573899000
Cl	1.749683000	1.681229000	0.384686000
H	-3.823020000	-1.007471000	-0.076460000
P	-1.121613000	1.977615000	0.479637000
H	-0.804477000	3.062321000	-0.347134000
H	-2.524725000	1.905163000	0.412790000
H	-0.859448000	2.472047000	1.766952000
P	1.923564000	-0.589918000	-1.358764000
H	1.812316000	-1.861417000	-1.947684000
H	2.079921000	0.250375000	-2.476286000
H	3.179818000	-0.591492000	-0.747971000

Cl	1.277419000	-1.698772000	1.177027000
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System 10

N	-2.182265000	-1.221508000	-1.307449000
C	-0.901738000	-0.936031000	-1.377345000
Os	0.219405000	0.036511000	-0.027855000
S	-1.992422000	0.154787000	0.964515000
B	-2.966710000	-0.758003000	-0.165088000
H	-2.596300000	-1.749136000	-2.069859000
H	-0.406800000	-1.324481000	-2.267995000
Cl	1.802290000	0.086509000	-1.666834000
H	-4.124391000	-0.982097000	-0.061960000
P	-0.288855000	2.320846000	-0.527978000
H	0.750704000	3.065208000	-1.115032000
H	-1.350291000	2.578236000	-1.412575000
H	-0.640590000	3.108607000	0.580665000
P	0.961221000	-2.128632000	0.646597000
H	0.093201000	-2.883863000	1.455740000
H	1.295191000	-3.058358000	-0.354898000
H	2.130608000	-2.113532000	1.425337000
Cl	0.873415000	0.688875000	2.076697000

System 11

B	2.146080000	1.283933000	-1.546926000
N	0.799157000	0.931570000	-1.477256000
Os	-0.192160000	-0.053831000	-0.015409000

S	1.969210000	0.200374000	0.909485000
C	2.879602000	0.916236000	-0.233847000
H	2.633161000	1.811122000	-2.495448000
H	0.184489000	1.281118000	-2.205113000
Cl	-1.875370000	-0.510314000	-1.491456000
H	3.928478000	1.063763000	0.011078000
P	0.559819000	-2.302581000	-0.374905000
H	-0.435818000	-3.183484000	-0.831553000
H	1.573489000	-2.497164000	-1.331903000
H	1.082128000	-2.986966000	0.737177000
P	-1.225722000	2.071978000	0.357578000
H	-0.489791000	3.057682000	1.039835000
H	-1.630017000	2.770394000	-0.793617000
H	-2.410895000	2.029339000	1.110307000
Cl	-0.768864000	-0.515549000	2.145393000

System 12

C	2.744133000	-0.000040000	-1.484154000
B	1.243960000	0.000608000	-1.482501000
Os	-0.148763000	0.000092000	-0.180185000
S	1.918894000	-0.001961000	0.997626000
N	3.088961000	-0.001415000	-0.211390000
H	3.508825000	0.000427000	-2.250012000
H	0.114743000	-0.000126000	-2.054372000
Cl	-2.397377000	0.001296000	-0.898020000
H	4.063926000	-0.002042000	0.083039000

P	-0.517713000	-2.354900000	-0.043778000
H	-1.659211000	-2.652793000	0.713533000
H	-0.767839000	-3.035846000	-1.247227000
H	0.459406000	-3.172479000	0.552794000
P	-0.514319000	2.355316000	-0.042700000
H	0.462076000	3.170204000	0.558696000
H	-0.758582000	3.038445000	-1.246132000
H	-1.658184000	2.654334000	0.710591000
Cl	-0.660759000	0.000184000	2.133634000

System 13

C	2.636192000	0.303408000	-1.168228000
N	1.367093000	0.403379000	-1.352349000
Os	-0.201508000	0.024564000	0.001635000
S	1.725941000	-0.558275000	1.234603000
B	3.111223000	-0.186984000	0.229940000
H	3.289759000	0.572294000	-1.998241000
H	1.073996000	0.744554000	-2.265349000
Cl	-1.429750000	0.338943000	-1.900810000
H	4.225228000	-0.342150000	0.599961000
P	-0.403653000	-2.317176000	-0.388104000
H	-1.601814000	-2.728093000	-0.997952000
H	0.554958000	-2.932249000	-1.214268000
H	-0.354878000	-3.135225000	0.753247000
P	-0.173804000	2.370239000	0.466418000
H	1.073947000	2.974225000	0.713989000

H	-0.691669000	3.214259000	-0.534156000
H	-0.907809000	2.778884000	1.593987000
Cl	-1.584558000	-0.255773000	1.760943000

System 14

N	2.797974000	0.206962000	-1.442798000
B	1.440760000	0.160393000	-1.209403000
Os	-0.145142000	0.016039000	-0.166914000
S	1.991244000	-0.119365000	1.126669000
B	3.297640000	0.045190000	-0.085427000
H	3.328181000	0.315484000	-2.290345000
H	0.261188000	0.191067000	-1.870783000
Cl	-2.350026000	0.152665000	-1.135009000
H	4.458647000	0.025959000	0.179071000
P	-0.341493000	-2.322382000	-0.215056000
H	-1.657447000	-2.792748000	-0.068102000
H	0.057552000	-3.072942000	-1.341668000
H	0.321024000	-3.041423000	0.796735000
P	-0.392102000	2.316679000	0.206831000
H	0.625220000	3.029129000	0.874693000
H	-0.611164000	3.179377000	-0.885506000
H	-1.500047000	2.639530000	1.007935000
Cl	-1.084454000	-0.280530000	2.014646000

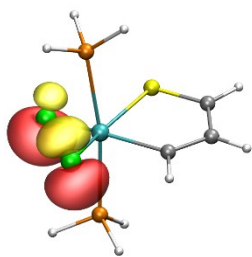
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B	2.593441000	-1.136834000	-0.825646000
N	1.185355000	-1.205794000	-0.949483000
Os	-0.117913000	-0.021796000	-0.031199000
S	1.787523000	0.821864000	0.721182000
N	2.969078000	-0.065404000	0.055011000
H	3.370967000	-1.827316000	-1.388758000
H	0.798642000	-1.899312000	-1.582375000
Cl	-1.383221000	-0.285847000	-1.902410000
H	3.922009000	0.246539000	0.234953000
P	-0.899505000	-2.210360000	0.720222000
H	-2.254795000	-2.153758000	1.081393000
H	-0.803601000	-3.257925000	-0.210712000
H	-0.229637000	-2.663686000	1.868192000
P	-0.566758000	2.322047000	-0.557572000
H	-0.134753000	3.274318000	0.380512000
H	-0.038481000	2.732077000	-1.793104000
H	-1.953052000	2.507865000	-0.671615000
Cl	-1.109165000	0.547914000	1.953205000

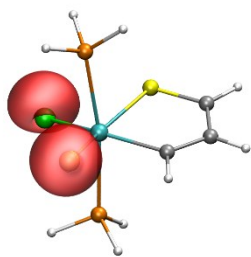
System 16

N	2.690229000	0.001430000	-1.243333000
B	1.330741000	0.000942000	-1.513798000
Os	-0.170493000	-0.000073000	-0.038712000
N	1.752017000	0.000349000	0.903211000
B	2.937259000	0.001072000	0.197500000

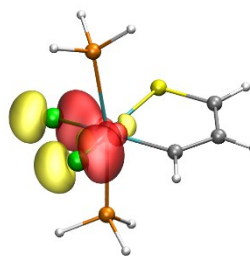
H	3.405973000	0.001899000	-1.950643000
H	0.825106000	0.001008000	-2.603393000
Cl	-1.989165000	-0.000680000	-1.461355000
H	4.036499000	0.001374000	0.674498000
P	-0.096945000	-2.331124000	0.012395000
H	-0.744761000	-3.079354000	-0.992895000
H	1.176567000	-2.932976000	-0.020789000
H	-0.623483000	-2.967537000	1.156218000
P	-0.099050000	2.331002000	0.012873000
H	1.174070000	2.933831000	-0.017647000
H	-0.745401000	3.078803000	-0.993670000
H	-0.628428000	2.966965000	1.155634000
Cl	-0.725138000	-0.000450000	2.238319000
H	1.728658000	0.000049000	1.909748000



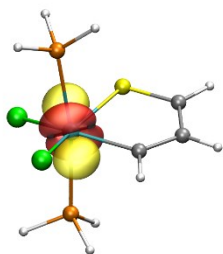
2x1c-2e Cl lone pairs
ON = 1.97|e|



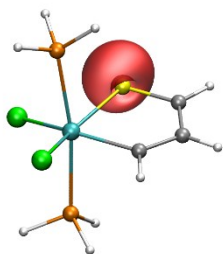
2x1c-2e Cl lone pairs
ON = 1.96|e|



2x2c-2e delocalized Cl lone pairs
ON = 1.89-1.99|e|

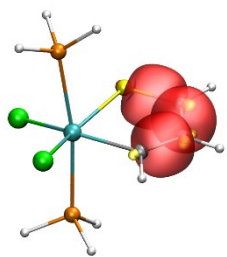


1c-2e Os lone pair
ON = 1.94|e|

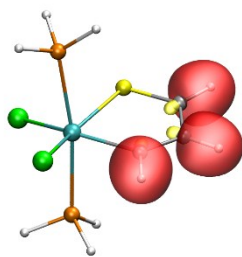


1c-2e S lone pair
ON = 1.94|e|

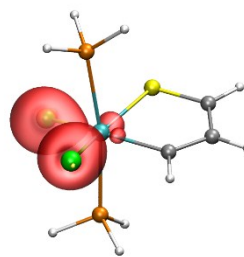
Figure SI 1. Lone pairs of system 1. ON stands for occupation number



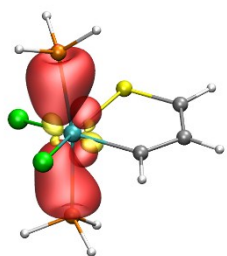
3x2c-2e C-C and S-C σ bonds
ON = 1.98|e|



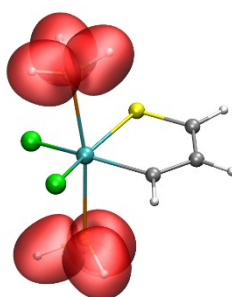
3x2c-2e C-H σ bonds
ON = 1.95-1.97 |e|



2x2c-2e Os-Cl σ bonds
ON = 1.99|e|

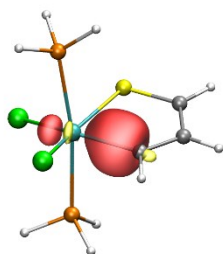


2x2c-2e Os-P σ bonds
ON = 1.91-1.94|e|

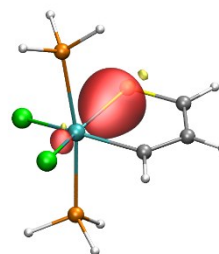


6x2c-2e P-H σ bonds
ON = 1.98-1.99 |e|

Figure SI 2. 2c-2e bonding elements of system 1. ON stands for occupation number

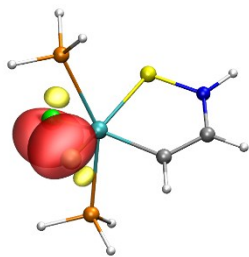


3c-2e σ bond
ON = 1.89

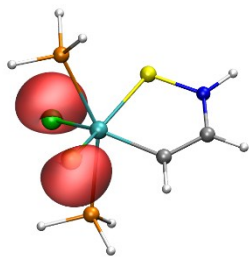


3c-2e σ bond
ON = 1.93

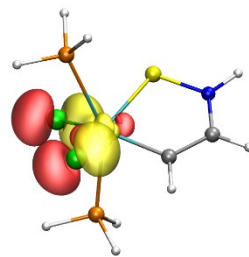
Figure SI 3. Delocalized Os-C and Os-S σ bonds in system 1. ON stands for occupation number



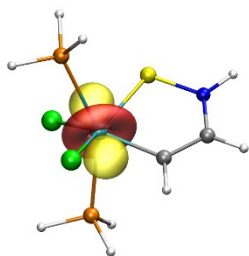
2x1c-2e Cl lone pairs
ON = 1.96|e|



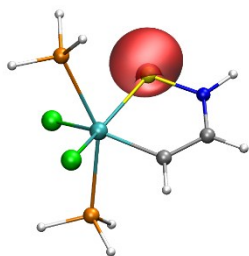
2x1c-2e Cl lone pairs
ON = 1.96|e|



2x2c-2e delocalized Cl lone pairs
ON = 1.89-1.98 |e|

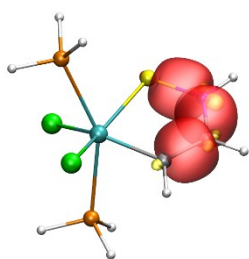


1c-2e Os lone pair
ON = 1.93|e|

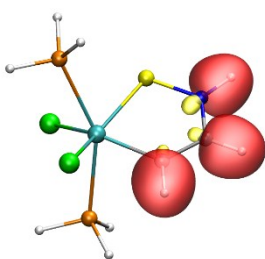


1c-2e S lone pair
ON = 1.94|e|

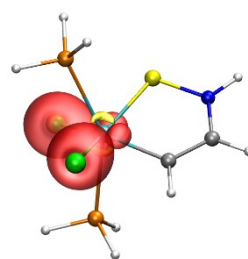
Figure SI 4. Lone pairs of system 7. ON stands for occupation number



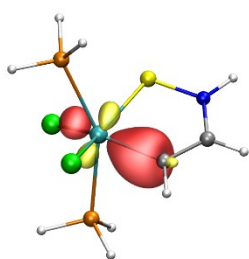
3x2c-2e C-C, C-N and S-N σ bonds
ON = 1.98-1.99 |e|



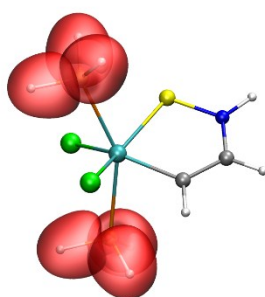
3x2c-2e C-H and N-H σ bonds
ON = 1.96-1.98 |e|



2x2c-2e Os-Cl σ bonds
ON = 1.99|e|

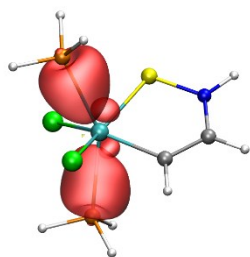


2c-2e Os-C σ bond
ON = 1.93|e|

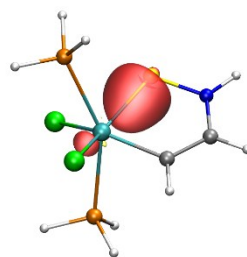


6x2c-2e P-H σ bonds
ON = 1.97-1.99 |e|

Figure SI 5. 2c-2e bonding elements of system 7. ON stands for occupation number

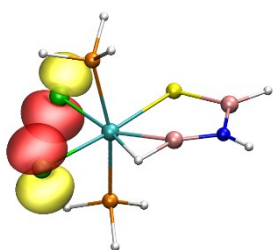


2x3c-2e σ bonds
ON = 1.84-1.91 |e|

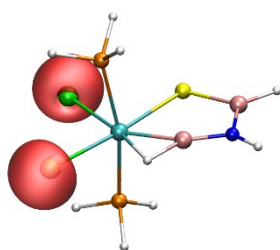


3c-2e σ bond
ON = 1.93|e|

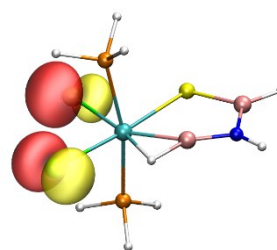
Figure SI 6. Delocalized Os-P and Os-S σ bonds in system 7. ON stands for occupation number



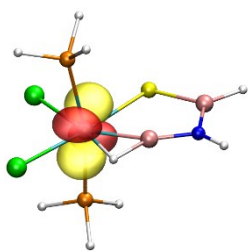
2x1c-2e Cl lone pairs
ON = 1.96|e|



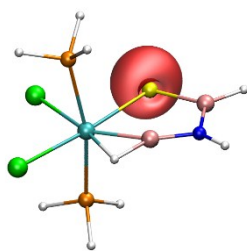
2x1c-2e Cl lone pairs
ON = 1.96|e|



2x1c-2e Cl lone pairs
ON = 1.95|e|

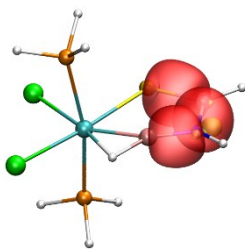


1c-2e Os lone pair
ON = 1.93|e|

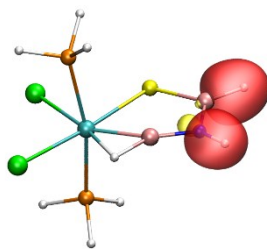


1c-2e S lone pair
ON = 1.93|e|

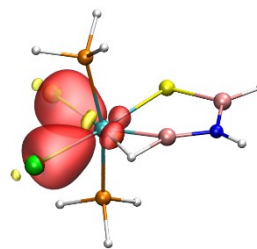
Figure SI 7. Lone pairs of system 14. ON stands for occupation number



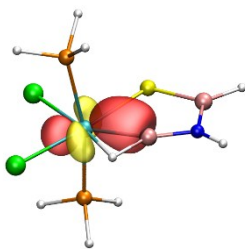
3x2c-2e B-N and S-B σ bonds
ON = 1.94-1.99 |e|



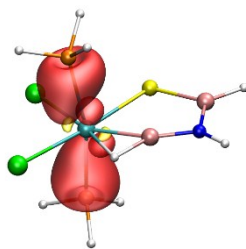
2x2c-2e N-H and B-H σ bonds
ON = 1.98|e|



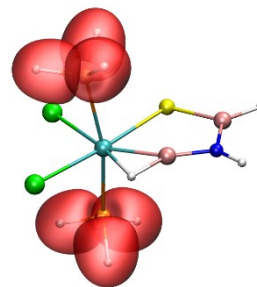
2x2c-2e Os-Cl σ bonds
ON = 1.96-1.98 |e|



2c-2e Os-B σ bond
ON = 1.98|e|

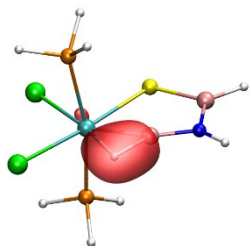


2x2c-2e Os-P σ bond
ON = 1.86-1.99 |e|

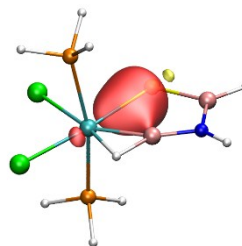


6x2c-2e P-H σ bonds
ON = 1.98-1.99 |e|

Figure SI 8. 2c-2e bonding elements of system 14. ON stands for occupation number



3c-2e σ bond
ON = 1.88|e|



3c-2e σ bond
ON = 1.85|e|

Figure SI 9. Delocalized B-H-Os and Os-S σ bonds in system 14. ON stands for occupation number