Planar Tetracoordinate Carbon in Tungstenacyclobutadiene of Alkyne Metathesis and Expanded Structures

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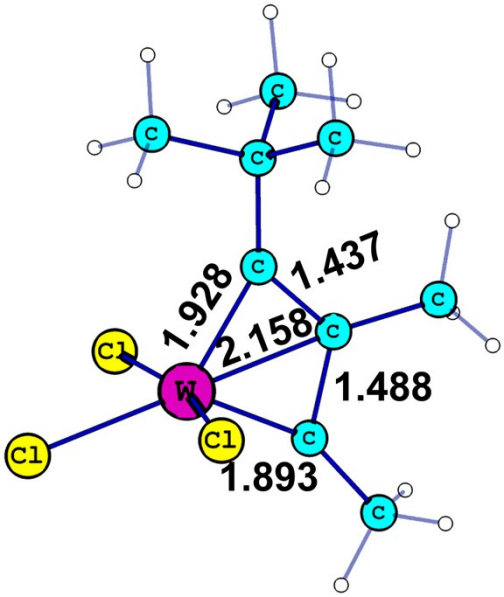
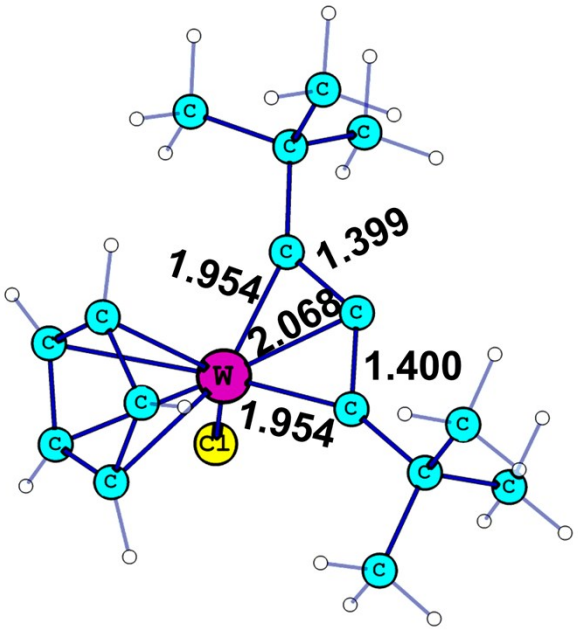
i. **Fig. S1** Optimised Structure of BONXOR and CEGGAW

BONXOR is the metallacycle intermediate of alkyne mtathesis reported by Schrock et al.[1] this crystal showed a single bond like MC_{β} distance of 2.115 Å. This structure was thoroughly analysed by suresh and Frenking computationally to establish the presence of 1,3-MC bond.[2] CEGGAW is the deprotiometallacycle reported by Schrock et al. and has a formal single bond between W and C_{β}.

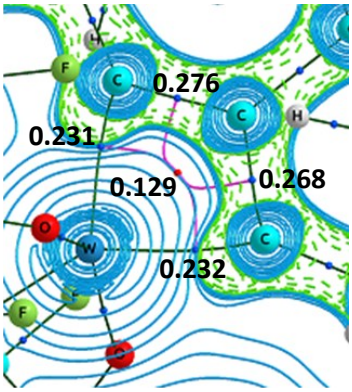


BONXOR

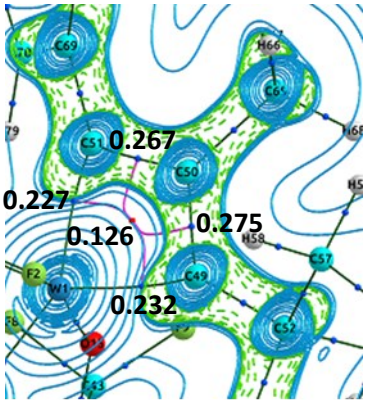


CEGGAW

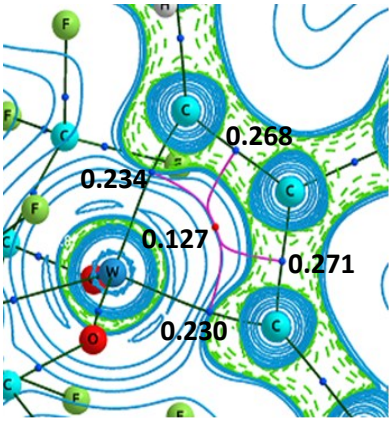
ii. **Fig. S2** Contour of Laplacian of electron density along with the molecular graph of optimized geometries of crystal structures (ρ values are given in au).



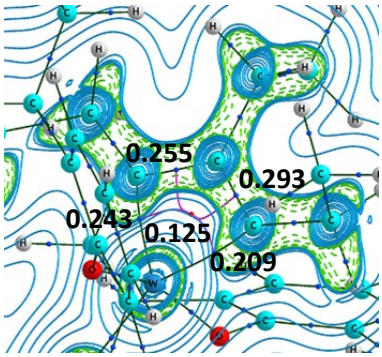
WEMYOE



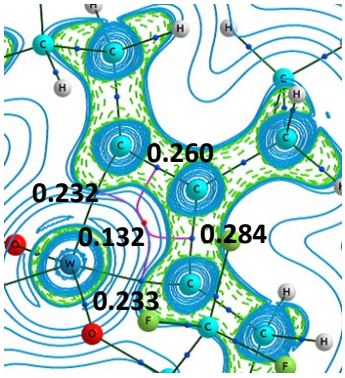
WEMYIY



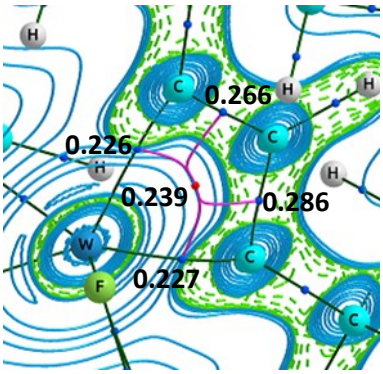
WEMYUK



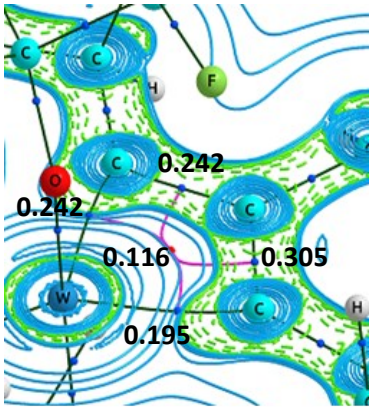
COMRE



CONISH

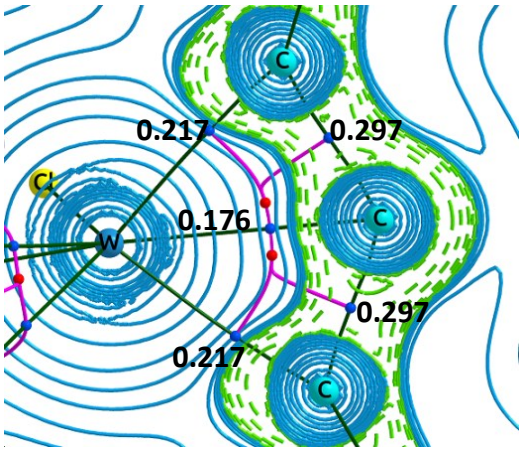


CUYJEL



KISGID

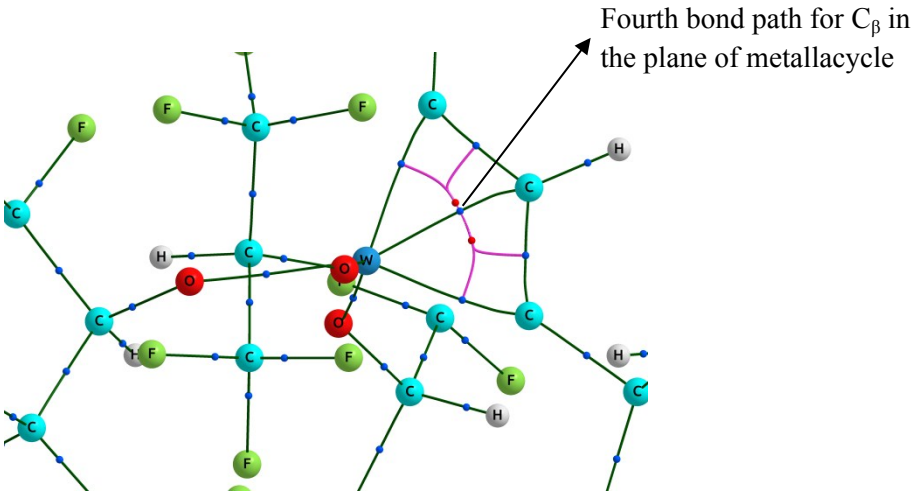
iii. **Fig. S3** Contour of Laplacian of electron density along with the molecular graph of CEGGAW (only tungstenacyclobutane region is shown for clarity and electron densities are in au).



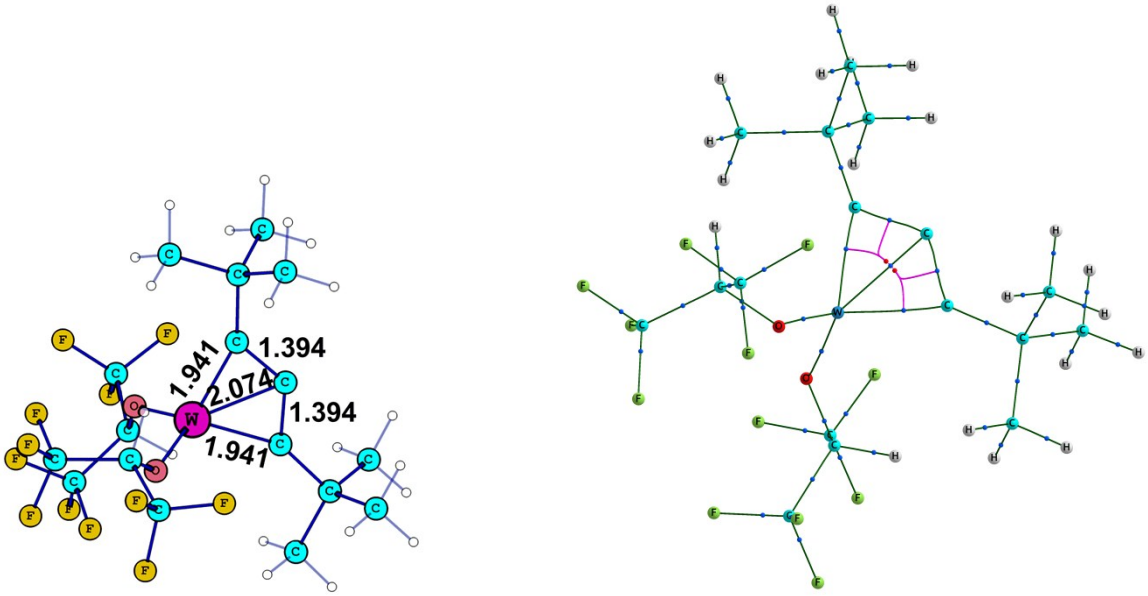
iv. Constrained geometry of CUYJEL

To further establish the catastrophe nature of the RCP in the WCBD models, we decreased the WC_β distance of CUYJEL manually and optimized the geometry after freezing the W and C_β coordinate. Thus obtained geometry is a saddle point in the potential energy surface. At a WC_β distance of 1.990Å, a clear BP along with a BCP was located for CUYJEL as given in Fig. S4.

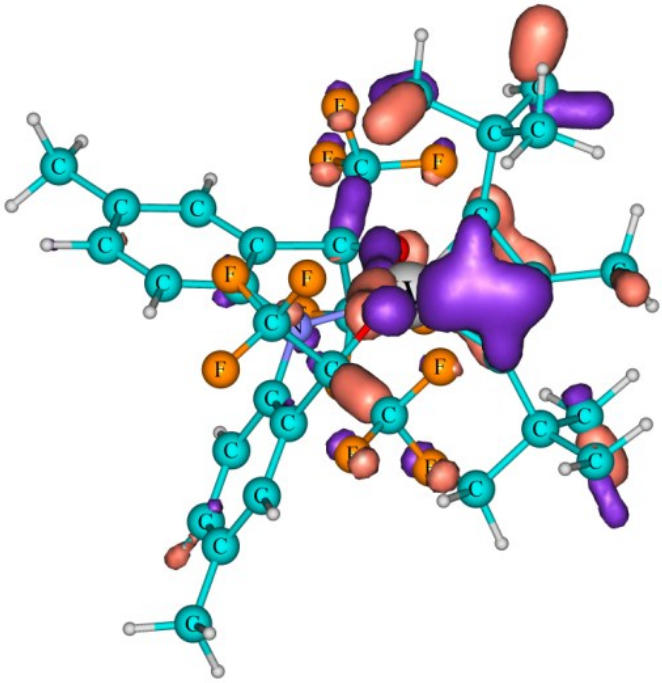
v. **Fig.S4** Molecular graph of the constrained geometry of CUYJEL at WC_β =1.99 Å showing a fourth bond path for the C_β in the QTAIM analysis.



vi. **Fig.S5** Optimized geometry and Molecular graph of the deprotiometallacycle corresponding to CUYJEL showing a clear WC_{β} bond.



vii. **Fig. S6** Molecular orbital (HOMO - 25) showing significant 1,3-WC interaction in WEMYUK due to the overlap of metal d-orbital and p-orbital on C_{β} (isosurface value of 0.05 is used).



viii. **Experimental ^{13}C-NMR values of the WCBD structures**

The experimental ^{13}C-NMR values of the crystal structures and calculated gas phase values for the optimized geometries at BP86/def2-tzvpp level of theory are presented in Table S1 for C_α and C_β atoms. Both theory and experiment agree to the fact that C_α atoms have significantly large chemical shift than the C_β atoms. Though the theory could not reproduce chemical shift values very close to the experiment, the trends in chemical shift difference between C_α and C_β values obtained from theory is in close agreement with experiment.

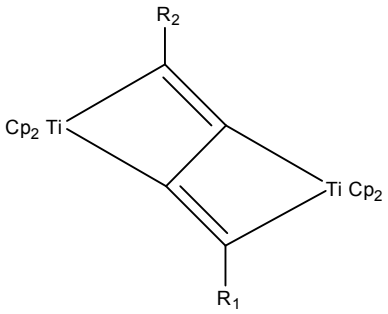
Table S1. Experimental ^{13}C-NMR values of the WCBD

MCBD	^{13}C-NMR		
	δC_α	δC_β	δC_α- δC_β
WEMYIY[3]	242.3	138.2	102.3
WEMYOE[3]	238.6	142.8	102.9
WEMYUK[3]	252.8	139.0	113.8
COMREB[4]	244.9	136.6	108.3
CONISH[5]	242.9	147.3	95.6
CUYJEL[6]	252.7	128.3	124.4
KISGID[7]	242.3	123.9	117.9

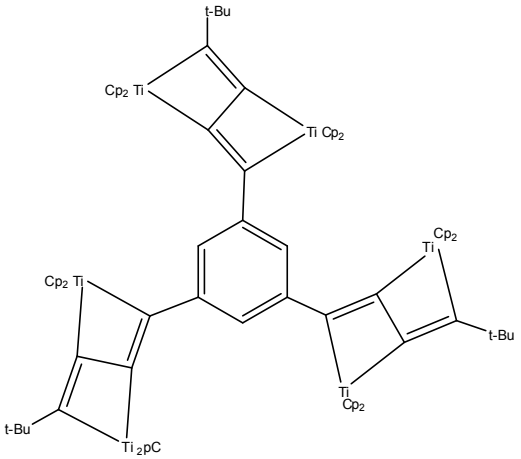
ix. **Complexes with more than one MCBD unit**

Many crystal structures are known containing **4** type moieties (scheme 1). Rosental *et al.* synthesized many such molecules possessing titanium center. These molecules showed significant interaction between Ti and β-carbon center indicated by the short distance (~ 2.3 Å).[8-11]

x. **Fig. S7** Molecular drawings of the crystal structures of the complexes containing **4**-type architecture.

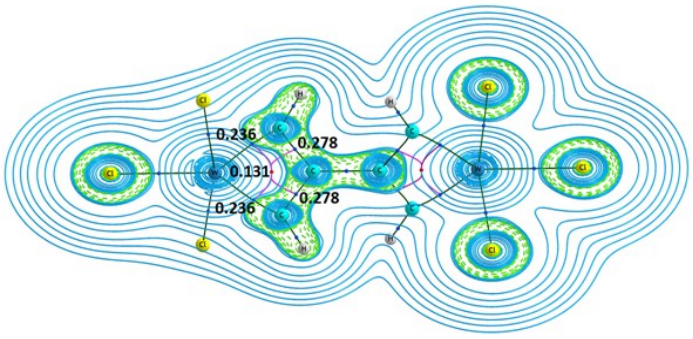


R_1, R_2=H, t-Bu, Ph

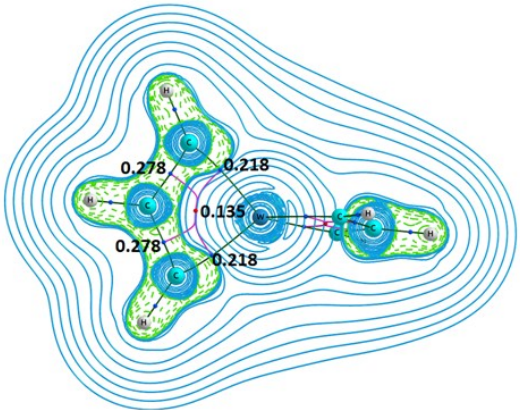


WOFGED

xi. **Fig. S8** Contour of Laplacian of electron density along with molecular graph of dimetallacycles **1** - **4**. Electron density at the critical points is given in au.



1



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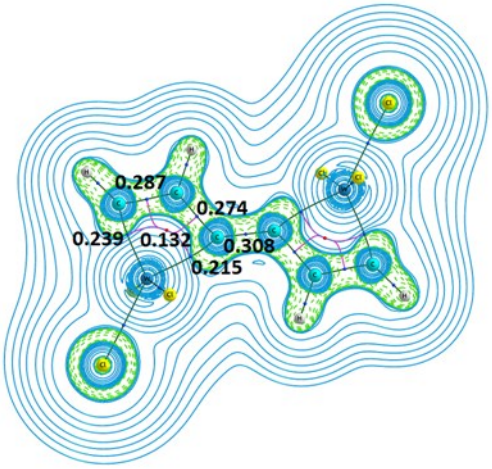

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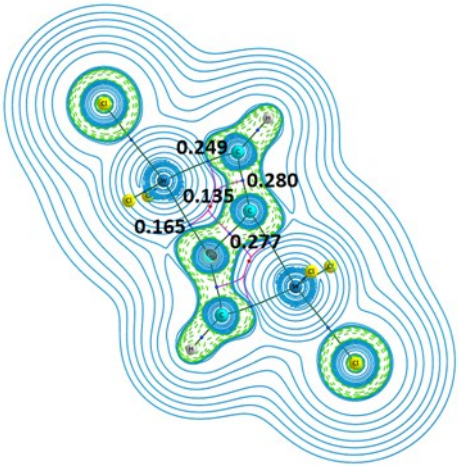

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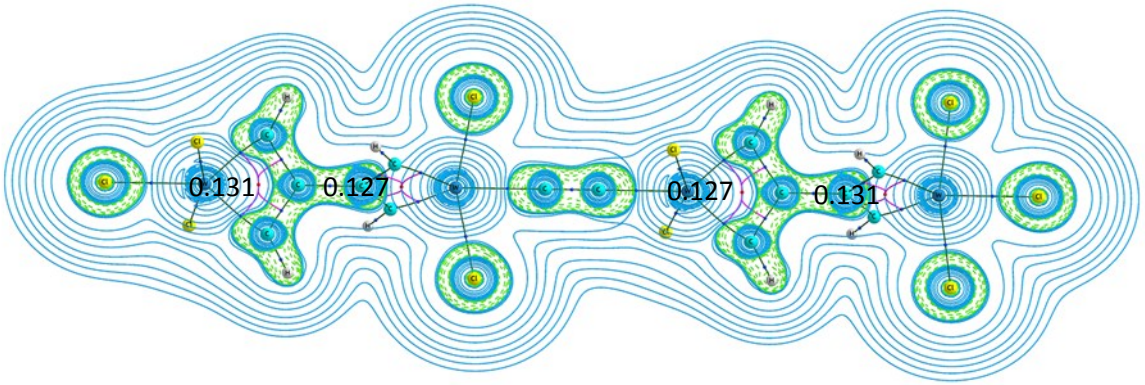
xii. **Fig. S9** Contour of Laplacian of electron density along with molecular graph of extended WCBD systems **5 - 10**. Electron density at the critical points is given in au.



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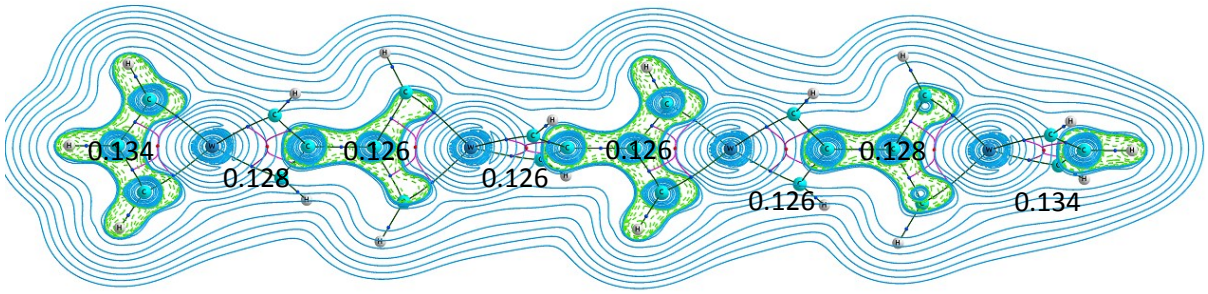

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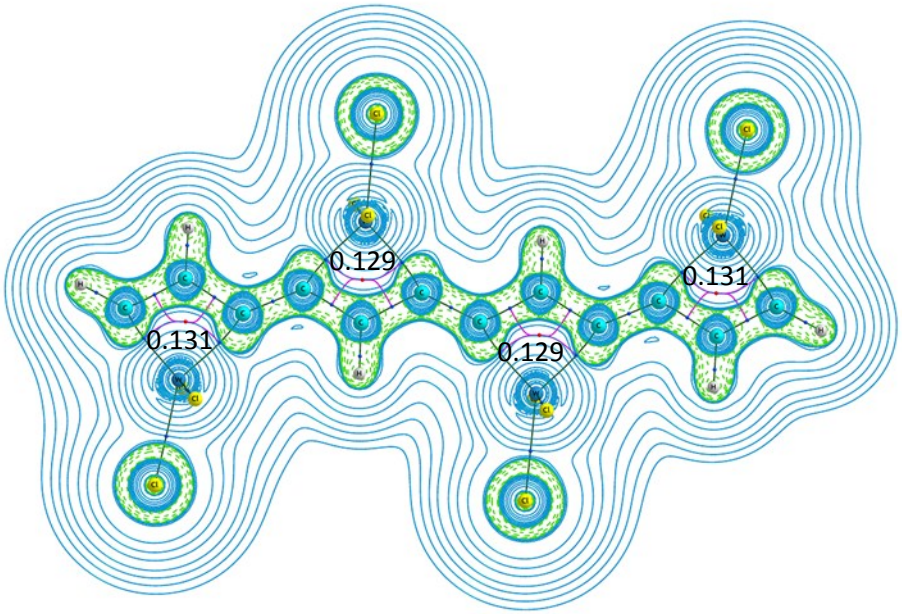

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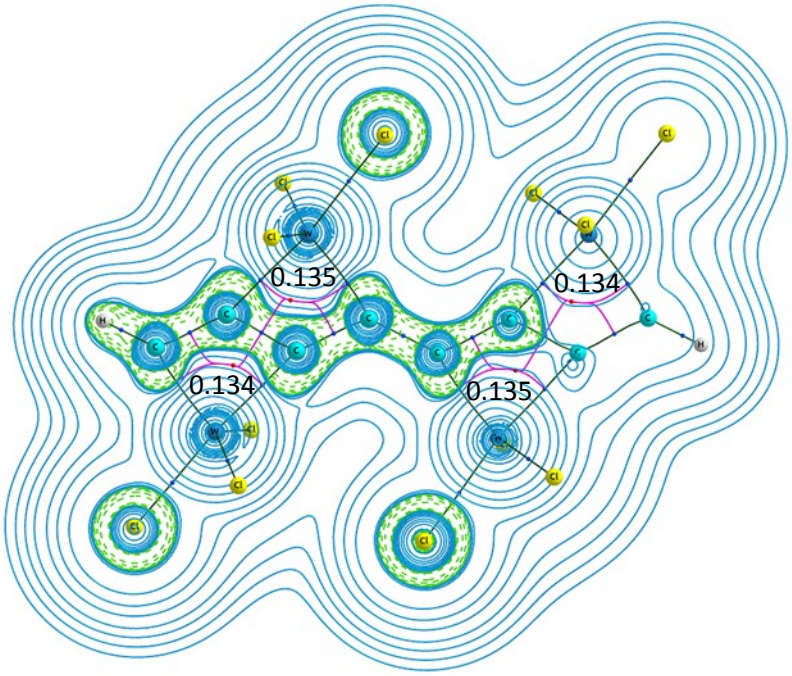

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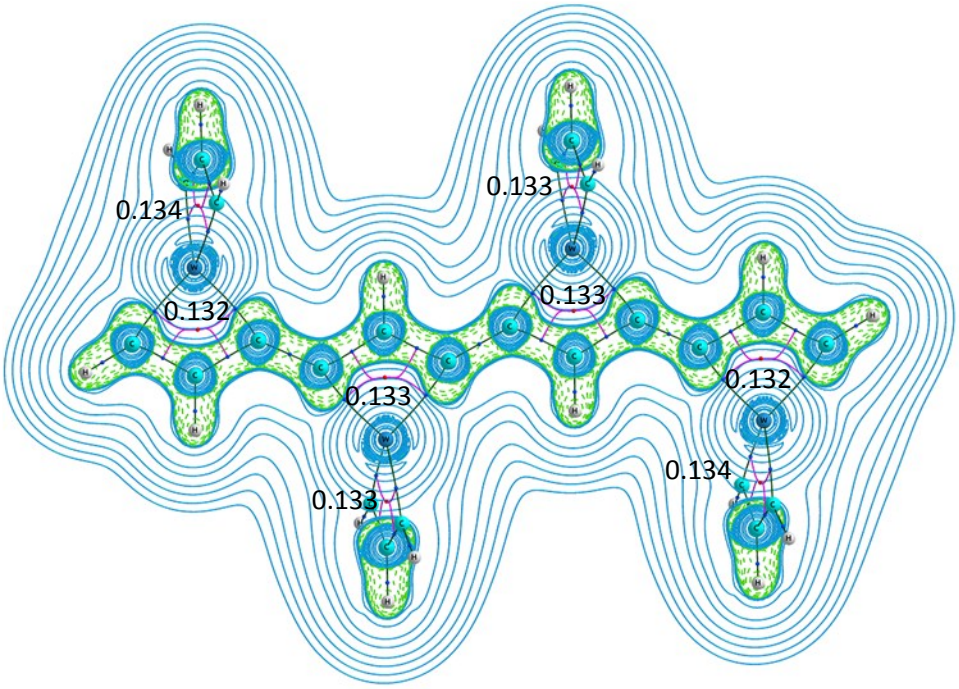

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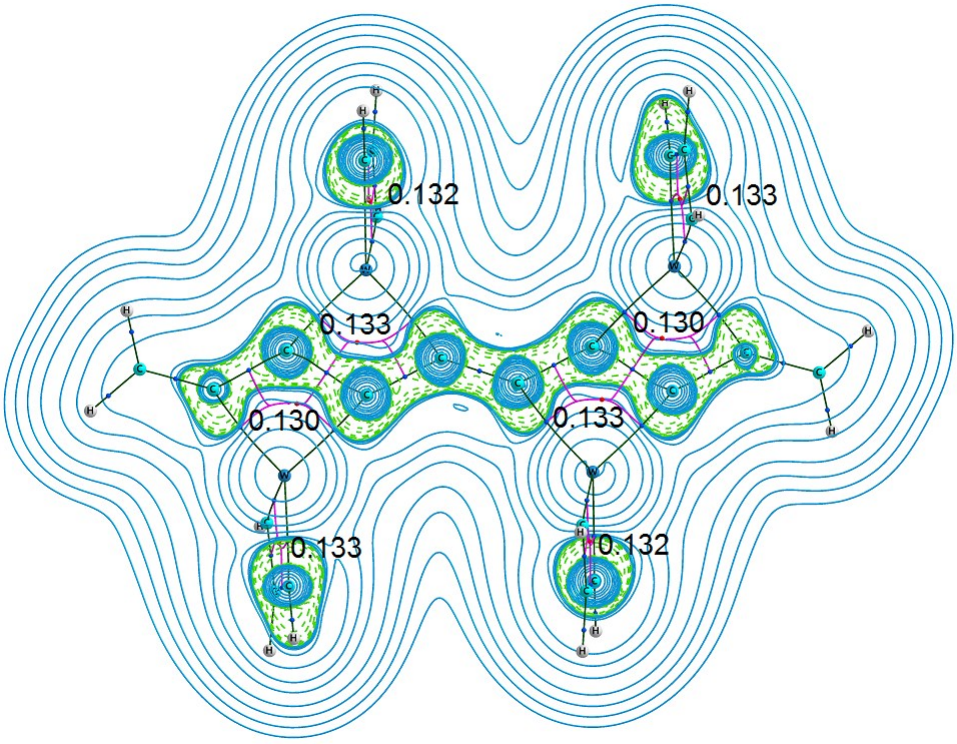
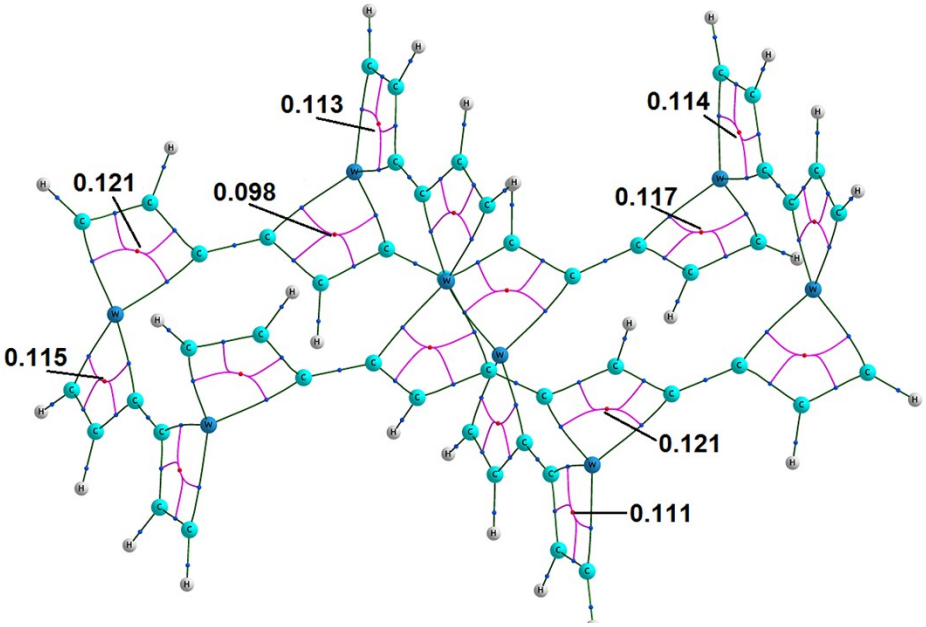
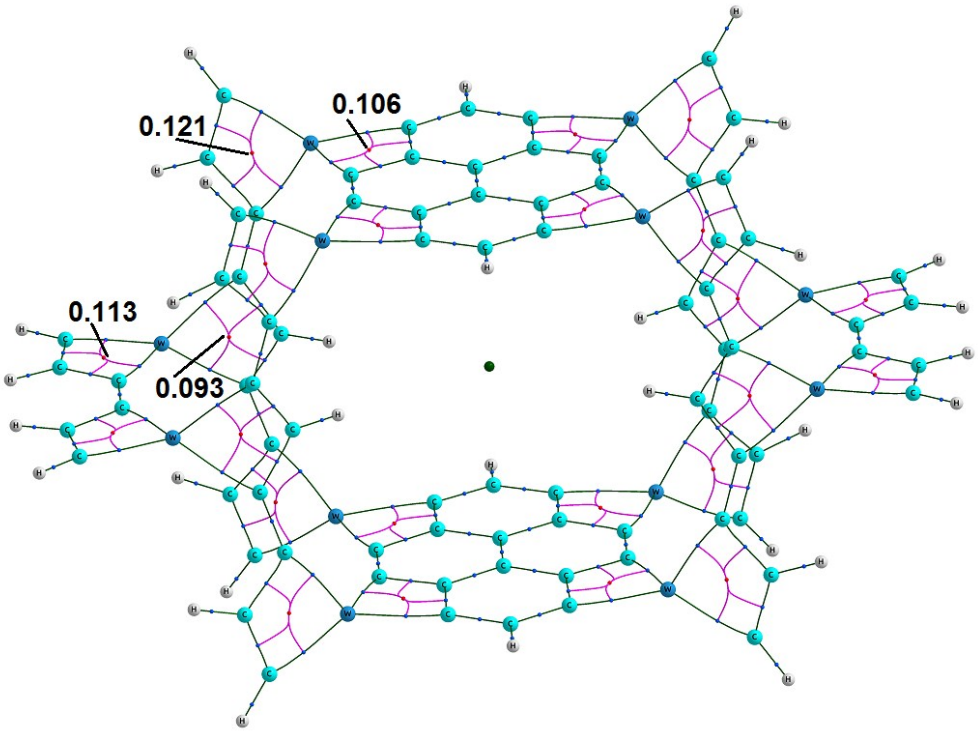


10

xiii. **Fig. S10** QTAIM topography of the 3-dimensional metal carbon networks (a) **11** and (b) **12**.



(a)



(b)

xiv. Eigenvalues at the catastrophe RCP of dimetallacycles **1** – **4**

Eigenvalue at the catastrophe RCP is analyzed to understand the intensity of 1,3-WC interaction in dimetallacycles. Among the three one value is negative and other two are positive. Among the two positive values, one (eigenvalue 2) is close to zero compared to other (eigenvalue 3). Recently we have discussed the analysis of eigenvalue to understand the strength of 1,3-MC interaction. Larger the eigenvalue 3 and smaller the eigenvalue 2 greater is the interaction.

Table S2. Eigenvalue at the catastrophe RCP of dimetallacycles in au

MCBD	ρ at WC_β RCP	Eigenvalue 1	Eigenvalue 2	Eigenvalue 3
1	0.131	-0.1150	0.0798	0.4380
2	0.135	-0.1254	0.0523	0.4445
3	0.132	-0.1186	0.0679	0.4390
4	0.135	-0.1306	0.0561	0.3934

xv. Cartesian coordinates of optimized geometries of the models studied are given below. All geometries are characterized by zero imaginary frequencies in the vibrational frequency analysis.

1

W	0.000005000	2.908168000	-0.000105000
C	0.889792000	1.452651000	0.887424000
C	-0.000005000	0.739268000	-0.001051000
C	-0.889667000	1.453283000	-0.888933000
C	0.889667000	-1.453283000	-0.888933000
C	0.000005000	-0.739268000	-0.001051000
C	-0.889792000	-1.452651000	0.887424000
H	-1.580338000	-0.978371000	1.577404000
H	1.581163000	-0.980170000	-1.578756000
W	-0.000005000	-2.908168000	-0.000105000
H	1.580338000	0.978371000	1.577404000
H	-1.581163000	0.980170000	-1.578756000
Cl	-1.660830000	-3.176008000	-1.663511000
Cl	0.000776000	-5.224162000	0.001070000
Cl	1.660987000	-3.173498000	1.663880000
Cl	-0.000776000	5.224162000	0.001070000
Cl	-1.660987000	3.173498000	1.663880000
Cl	1.660830000	3.176008000	-1.663511000

2

C	-0.108257000	0.463832000	-2.098502000
C	0.640690000	1.358877000	-1.255847000
C	-0.789526000	-0.718471000	-1.641677000
W	-0.000086000	0.000227000	0.000055000
C	-0.979709000	0.366540000	1.655211000
C	0.108710000	-0.465085000	2.098202000
C	1.129244000	-1.008681000	1.241889000
H	1.941338000	-1.632226000	1.595218000
H	0.163636000	-0.699964000	3.162972000
H	1.145431000	2.245276000	-1.620120000
H	-0.163709000	0.700109000	-3.162937000
H	-1.737596000	0.766702000	2.317508000
H	-1.349693000	-1.378756000	-2.292357000

3

C	1.042543000	2.997918000	0.000000000
C	1.152705000	1.572900000	0.000000000
H	2.139771000	1.104266000	0.000000000
C	-0.006423000	0.694853000	0.000000000
C	0.006423000	-0.694853000	0.000000000
C	-1.152705000	-1.572900000	0.000000000
H	-2.139771000	-1.104266000	0.000000000
C	-1.042543000	-2.997918000	0.000000000
H	1.871468000	3.697487000	0.000000000
W	-0.808391000	2.493838000	0.000000000
W	0.808391000	-2.493838000	0.000000000
H	-1.871468000	-3.697487000	0.000000000
Cl	-1.152705000	2.417504000	2.327063000
Cl	-2.746744000	3.767552000	0.000000000
Cl	-1.152705000	2.417504000	-2.327063000
Cl	1.152705000	-2.417504000	-2.327063000
Cl	1.152705000	-2.417504000	2.327063000
Cl	2.746744000	-3.767552000	0.000000000

4

C	1.051833000	-0.000841000	-1.638101000
C	-0.040570000	-0.001823000	-0.717184000
C	0.040577000	-0.001562000	0.717678000
C	-1.051777000	-0.000565000	1.638381000
H	0.985031000	-0.002009000	-2.721341000
W	2.012873000	-0.000316000	-0.004022000
W	-2.012684000	-0.000319000	0.004108000
H	-0.985606000	0.000134000	2.721650000
Cl	2.223531000	-2.201425000	0.698403000
Cl	4.258411000	0.002823000	-0.543390000
Cl	2.217459000	2.201445000	0.699151000
Cl	-4.258439000	0.002207000	0.542454000
Cl	-2.223118000	-2.201620000	-0.698134000
Cl	-2.218659000	2.201133000	-0.699148000

5

W	0.000000000	0.000000000	8.521135000
C	0.000000000	-1.256990000	7.067824000
C	0.000000000	0.000000000	6.352824000
C	0.000000000	1.256990000	7.067824000
C	1.259208000	0.000000000	4.159613000
C	0.000000000	0.000000000	4.874568000
C	-1.259208000	0.000000000	4.159613000

6

C	0.000000000	0.000000000	-5.069594000
C	-0.853703000	0.949449000	-4.404541000
C	0.853703000	-0.949449000	-4.404541000
W	0.000000000	0.000000000	-2.919569000
C	-0.943436000	-0.851542000	-1.430475000
C	0.000000000	0.000000000	-0.745393000
C	0.943436000	0.851542000	-1.430475000

H	-2.233590000	0.000000000	4.638677000	H	1.647238000	1.489138000	-0.908910000
H	2.233590000	0.000000000	4.638677000	H	-1.492522000	1.650143000	-4.928395000
W	0.000000000	0.000000000	2.693575000	H	-1.647238000	-1.489138000	-0.908910000
H	0.000000000	-2.233599000	6.594838000	H	1.492522000	-1.650143000	-4.928395000
H	0.000000000	2.233599000	6.594838000	C	0.000000000	0.000000000	0.745393000
Cl	0.000000000	2.307388000	2.266850000	C	-0.943436000	0.851542000	1.430475000
C	0.000000000	0.000000000	0.622636000	C	0.943436000	-0.851542000	1.430475000
Cl	0.000000000	-2.307388000	2.266850000	W	0.000000000	0.000000000	2.919569000
Cl	0.000000000	0.000000000	10.838957000	C	-0.853703000	-0.949449000	4.404541000
Cl	-2.352201000	0.000000000	8.788711000	C	0.000000000	0.000000000	5.069594000
Cl	2.352201000	0.000000000	8.788711000	C	0.853703000	0.949449000	4.404541000
Cl	0.000000000	0.000000000	-10.838957000	H	1.492522000	1.650143000	4.928395000
W	0.000000000	0.000000000	-8.521135000	H	0.000000000	0.000000000	6.161487000
C	1.256990000	0.000000000	-7.067824000	H	-1.647238000	1.489138000	0.908910000
C	0.000000000	0.000000000	-6.352824000	H	-1.492522000	-1.650143000	4.928395000
C	-1.256990000	0.000000000	-7.067824000	H	1.647238000	-1.489138000	0.908910000
C	0.000000000	-1.259208000	-4.159613000	H	0.000000000	0.000000000	-6.161487000
C	0.000000000	0.000000000	-4.874568000				
C	0.000000000	1.259208000	-4.159613000				
H	0.000000000	2.233590000	-4.638677000				
H	0.000000000	-2.233590000	-4.638677000				
W	0.000000000	0.000000000	-2.693575000				
H	2.233599000	0.000000000	-6.594838000				
H	-2.233599000	0.000000000	-6.594838000				
Cl	-2.307388000	0.000000000	-2.266850000				
Cl	2.307388000	0.000000000	-2.266850000				
Cl	0.000000000	2.352201000	-8.788711000				
Cl	0.000000000	-2.352201000	-8.788711000				
C	0.000000000	0.000000000	-0.622636000				

7				**8**			
C	6.848430000	-1.374483000	0.000339000	C	-4.151232000	1.694707000	-0.156722000
C	5.465123000	-1.739615000	0.000207000	C	-2.731373000	1.702089000	-0.064701000
H	5.186430000	-2.796466000	0.000337000	C	-1.868419000	0.575868000	0.074973000
C	4.396433000	-0.758929000	0.000060000	C	-0.429526000	0.555107000	0.145544000
C	3.029173000	-1.018553000	0.000044000	H	-4.812098000	2.555728000	-0.144356000
C	1.953157000	-0.061055000	0.000055000	W	-3.827897000	-0.178830000	-0.141668000
H	2.204030000	1.002365000	-0.000048000	W	-0.771600000	2.450789000	0.145745000
C	0.550209000	-0.430248000	0.000131000	Cl	-3.853868000	-0.812670000	2.081910000
H	7.684884000	-2.065068000	0.000504000	Cl	-5.884237000	-1.188338000	-0.414146000
W	6.024389000	0.356786000	0.000063000	Cl	-3.226355000	-0.866060000	-2.270196000
W	1.430993000	-2.171700000	0.000208000	Cl	1.244359000	3.546743000	0.401349000
Cl	5.869066000	0.688013000	2.321418000	Cl	-1.391223000	3.113944000	2.277613000
Cl	6.972998000	2.469551000	-0.000095000	Cl	-0.798044000	3.054429000	-2.084966000
Cl	5.869526000	0.687469000	-2.321404000	C	0.429669000	-0.555257000	0.145442000
Cl	1.467573000	-2.426665000	-2.333359000	C	1.868447000	-0.576030000	0.074099000
Cl	1.467963000	-2.426474000	2.333784000	C	2.731565000	-1.702095000	-0.065747000
Cl	0.746443000	-4.383586000	0.000358000	C	4.151611000	-1.694217000	-0.157293000
C	-0.550265000	0.430185000	-0.000048000	W	0.772111000	-2.450953000	0.145440000
C	-1.953251000	0.061071000	-0.000122000	W	3.828003000	0.179152000	-0.141869000
H	-2.204124000	-1.002346000	-0.000237000	H	4.812481000	-2.555249000	-0.144951000
C	-3.029203000	1.018638000	-0.000080000	Cl	1.392878000	-3.114949000	2.276707000
C	-4.396465000	0.758977000	-0.000230000	Cl	-1.244857000	-3.544781000	0.403107000
C	-5.465163000	1.739644000	-0.000223000	Cl	0.796726000	-3.056790000	-2.084561000

H	-5.186479000	2.796497000	-0.000156000	Cl	5.882836000	1.191606000	-0.413173000
C	-6.848478000	1.374502000	-0.000330000	Cl	3.852480000	0.810719000	2.082445000
W	-1.430959000	2.171678000	0.000112000	Cl	3.226330000	0.865368000	-2.270810000
W	-6.024432000	-0.356745000	-0.000372000				
Cl	-1.467532000	2.426227000	2.333717000				
Cl	-0.746669000	4.383640000	0.000334000				
Cl	-1.467465000	2.426689000	-2.333463000				
Cl	-5.869041000	-0.687716000	-2.321754000				
Cl	-5.869249000	-0.687954000	2.320994000				
Cl	-6.973456000	-2.469325000	-0.000517000				
H	-7.684942000	2.065074000	-0.000347000				
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C	0.354313000	7.047245000	0.000000000	C	3.287973000	3.334411000	1.993785000
C	-0.341729000	5.775665000	0.000000000	C	2.790891000	4.415482000	1.182587000
H	-1.432772000	5.791077000	0.000000000	C	0.679238000	-0.067957000	-0.025261000
C	0.294641000	4.481218000	0.000000000	C	1.769504000	0.804545000	-0.147041000
C	-0.316067000	3.220365000	0.000000000	C	3.234727000	0.359208000	-0.379794000
C	0.343860000	1.927822000	0.000000000	C	4.262843000	1.248675000	-0.774181000
H	1.434038000	1.929706000	0.000000000	W	2.323322000	-1.239871000	0.468831000
C	-0.312382000	0.627435000	0.000000000	C	2.377000000	4.234132000	-0.191721000
H	-0.167369000	7.997299000	0.000000000	W	2.918569000	2.441275000	0.307759000
W	1.816947000	5.762361000	0.000000000	C	2.594361000	-2.103182000	2.192088000
C	0.312382000	-0.627435000	0.000000000	C	2.759872000	-3.203321000	1.276914000
C	-0.343860000	-1.927822000	0.000000000	H	2.973523000	-4.196937000	1.681252000
H	-1.434038000	-1.929706000	0.000000000	C	2.647437000	-3.052481000	-0.154539000
C	0.316067000	-3.220365000	0.000000000	H	2.747369000	-2.197225000	3.263104000
C	-0.294641000	-4.481218000	0.000000000	C	-4.262843000	-1.248675000	0.774181000
C	0.341729000	-5.775665000	0.000000000	C	-3.234727000	-0.359208000	0.379794000
H	1.432772000	-5.791077000	0.000000000	C	-1.769504000	-0.804545000	0.147041000
C	-0.354313000	-7.047245000	0.000000000	C	-0.679238000	0.067957000	0.025261000
W	1.808743000	-1.919690000	0.000000000	W	-2.918569000	-2.441275000	-0.307759000
W	-1.816947000	-5.762361000	0.000000000	C	-2.594361000	2.103182000	-2.192088000
H	0.167369000	-7.997299000	0.000000000	C	-2.759872000	3.203321000	-1.276914000
C	3.299976000	-1.929933000	1.276581000	C	-2.647437000	3.052481000	0.154539000
C	3.966185000	-1.929246000	0.000000000	W	-2.323322000	1.239871000	-0.468831000
H	5.058212000	-1.919878000	0.000000000	C	-2.377000000	-4.234132000	0.191721000
C	3.299976000	-1.929933000	-1.276581000	C	-2.790891000	-4.415482000	-1.182587000
H	3.827533000	-1.913130000	-2.222853000	C	-3.287973000	-3.334411000	-1.993785000
C	-3.299976000	-5.611967000	1.276811000	H	-2.730524000	-5.418258000	-1.615215000
C	-3.964955000	-5.583922000	0.000000000	H	-2.973523000	4.196937000	-1.681252000
H	-5.056805000	-5.605799000	0.000000000	H	2.730524000	5.418258000	1.615215000
C	-3.299976000	-5.611967000	-1.276811000	H	-2.749893000	3.887506000	0.840925000
H	-3.830432000	-5.697492000	-2.218067000	H	3.540663000	3.451166000	3.043767000
H	-3.830432000	-5.697492000	2.218067000	H	-2.014404000	-5.056876000	0.801411000
C	-3.299976000	1.929933000	1.276581000	H	2.749893000	-3.887506000	-0.840925000
C	-3.966185000	1.929246000	0.000000000	H	2.014404000	5.056876000	-0.801411000
H	-5.058212000	1.919878000	0.000000000	H	-2.747369000	2.197225000	-3.263104000
C	-3.299976000	1.929933000	-1.276581000	H	-3.540663000	-3.451166000	-3.043767000
W	-1.808743000	1.919690000	0.000000000	C	-5.468850000	-1.165314000	1.365938000
H	-3.827533000	1.913130000	-2.222853000	H	-6.132605000	-2.030113000	1.413693000
H	-3.827533000	1.913130000	2.222853000	C	5.468850000	1.165314000	-1.365938000
C	3.299976000	5.611967000	-1.276811000	H	5.828433000	0.232233000	-1.810510000
C	3.964955000	5.583922000	0.000000000	H	-5.828433000	-0.232233000	1.810510000
H	5.056805000	5.605799000	0.000000000	H	6.132605000	2.030113000	-1.413693000

C	3.299976000	5.611967000	1.276811000
H	3.830432000	5.697492000	2.218067000
H	3.830432000	5.697492000	-2.218067000
H	3.827533000	-1.913130000	2.222853000

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C	-6.735776000	-2.777238000	-1.583688000
C	-5.334915000	-2.894566000	-1.700985000
H	-4.831214000	-3.171278000	-2.642934000
C	-4.382514000	-2.723828000	-0.567106000
C	-2.998013000	-2.768484000	-0.676773000
C	-2.000091000	-2.526551000	0.319717000
H	-2.247909000	-1.995326000	1.263929000
C	-0.633810000	-2.673186000	-0.107570000
H	-7.458249000	-2.979478000	-2.374905000
W	-6.155184000	-2.428344000	0.282435000
C	0.532870000	-2.592404000	0.657574000
C	1.899655000	-2.718282000	0.180197000
H	2.014704000	-3.070916000	-0.860631000
C	3.093131000	-2.593332000	0.999252000
C	4.421667000	-2.639228000	0.588088000
C	5.594165000	-2.911715000	1.463506000
H	5.334117000	-3.206016000	2.494742000
C	6.925870000	-2.868841000	1.010962000
W	1.608034000	-2.417009000	2.339002000
W	5.949102000	-2.430050000	-0.670557000
H	7.808650000	-3.097333000	1.608108000
C	1.308685000	-3.064336000	4.209331000
C	1.276122000	-1.667752000	4.427020000
H	1.116304000	-1.252251000	5.437816000
C	1.466361000	-0.692746000	3.326519000
C	6.160174000	-3.069056000	-2.543269000
C	6.254978000	-1.665825000	-2.739832000
H	6.389541000	-1.248164000	-3.754046000
C	6.156255000	-0.695667000	-1.632645000
H	6.229451000	-3.806400000	-3.343597000
C	-0.913233000	-3.069683000	-3.787597000
C	-0.932490000	-1.668384000	-4.027293000
H	-0.659451000	-1.262743000	-5.018857000
C	-1.277728000	-0.701873000	-2.963980000
W	-1.426028000	-2.409565000	-1.972681000
H	-0.666096000	-3.796662000	-4.564102000
C	-6.398716000	-0.686459000	1.223487000
C	-6.794060000	-1.662889000	2.267441000
H	-7.213510000	-1.241134000	3.195961000
C	-6.741533000	-3.066478000	2.079827000
H	-7.055419000	-3.791911000	2.830568000
H	1.168785000	-3.804418000	4.998474000
C	6.935419000	2.850956000	1.023393000
C	5.601906000	2.899877000	1.470754000
H	5.339732000	3.189831000	2.502596000
C	4.431100000	2.637391000	0.590336000
C	3.101611000	2.592260000	0.998002000
C	1.909884000	2.717067000	0.176590000
H	2.026314000	3.067144000	-0.864988000
C	0.542462000	2.591104000	0.651922000

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C	-4.885979000	-5.015721000	-3.092711000
C	-5.300207000	-3.670312000	-3.138396000
H	-6.316243000	-3.347728000	-3.432746000
C	-4.406345000	-2.514370000	-2.819786000
C	-4.823556000	-1.186932000	-2.776045000
C	-4.077453000	0.000465000	-2.494460000
H	-3.135905000	0.000913000	-1.905323000
C	-4.824725000	1.187256000	-2.775827000
H	-5.497166000	-5.875663000	-3.368747000
W	-3.223165000	-4.070791000	-2.539334000
C	-4.408450000	2.514927000	-2.819917000
C	-5.302242000	3.670660000	-3.138888000
H	-6.318182000	3.348308000	-3.433759000
C	-4.887885000	5.016107000	-3.093341000
W	-3.225114000	4.071276000	-2.539499000
C	-1.221839000	4.087965000	-2.924522000
C	-1.228422000	4.059349000	-1.455486000
C	-2.504621000	4.093181000	-0.695450000
C	-8.395876000	0.000840000	-3.042797000
C	-8.574521000	0.000774000	-1.630483000
H	-9.589396000	0.002285000	-1.189253000
C	-7.428885000	-0.000459000	-0.701586000
W	-6.488930000	-0.000563000	-2.453173000
H	-9.239212000	0.001864000	-3.737320000
C	-2.502133000	-4.094828000	-0.695359000
C	-1.226215000	-4.061603000	-1.455492000
C	-1.219896000	-4.089035000	-2.924602000
C	0.001875000	-4.105848000	-3.617053000
C	0.000125000	4.106041000	-3.616669000
C	-4.891048000	5.014139000	3.088698000
C	-5.304346000	3.668430000	3.135019000
H	-6.320362000	3.345330000	3.428935000
C	-4.409364000	2.513062000	2.817779000
C	-4.825100000	1.185123000	2.774871000
C	-4.077870000	-0.001822000	2.493989000
H	-3.136216000	-0.001437000	1.905014000
C	-4.824063000	-1.189261000	2.775337000
C	-4.407139000	-2.516784000	2.818454000
C	-5.300845000	-3.672889000	3.136615000
H	-6.316818000	-3.350724000	3.431574000
C	-4.886414000	-5.018256000	3.090207000
W	-6.489226000	-0.002497000	2.452587000
W	-3.223754000	-4.072892000	2.536932000
H	-5.497428000	-5.878280000	3.366369000
C	-7.429066000	-0.001305000	0.701027000
C	-8.574756000	-0.000235000	1.629890000
H	-9.589661000	0.004076000	1.188759000
C	-8.396166000	-0.001282000	3.042224000
H	-9.239499000	0.000148000	3.736752000

H	7.816907000	3.072482000	1.625117000
W	5.962581000	2.424313000	-0.663108000
C	-0.624086000	2.670358000	-0.113966000
C	-1.989552000	2.522783000	0.315051000
H	-2.236978000	1.990564000	1.258844000
C	-2.986965000	2.768745000	-0.680531000
C	-4.371433000	2.727555000	-0.569622000
C	-5.324272000	2.902473000	-1.702602000
H	-4.819738000	3.176807000	-2.644942000
C	-6.725193000	2.790497000	-1.583900000
W	-1.416455000	2.408738000	-1.979456000
W	-6.144136000	2.437357000	0.281594000
H	-7.447902000	2.995149000	-2.374268000
C	-1.275118000	0.698009000	-2.966413000
C	-0.924921000	1.659546000	-4.032514000
H	-0.652734000	1.249690000	-5.022680000
C	-0.900100000	3.061256000	-3.796668000
H	-0.649723000	3.784801000	-4.575377000
C	-6.395566000	0.696733000	1.223097000
C	-6.784454000	1.675059000	2.267708000
H	-7.202155000	1.255157000	3.197892000
C	-6.725854000	3.078215000	2.079519000
H	-7.033646000	3.805461000	2.831016000
C	1.467923000	0.692548000	3.325201000
C	1.274431000	1.669705000	4.423377000
H	1.105346000	1.255926000	5.433375000
C	1.310087000	3.065816000	4.203645000
W	1.613746000	2.415128000	2.335247000
H	1.166468000	3.807538000	4.990580000
C	6.178574000	3.068725000	-2.533348000
C	6.268275000	1.665628000	-2.733364000
H	6.422539000	1.252064000	-3.746263000
C	6.157500000	0.691721000	-1.630205000
H	6.260842000	3.808108000	-3.330559000

C	-2.502421000	-4.094154000	0.693194000
C	-1.226611000	-4.059757000	1.453887000
C	0.001186000	-4.051769000	0.722293000
C	-1.220729000	-4.088745000	2.922946000
C	0.000849000	-4.106738000	3.615734000
C	-2.505172000	4.093316000	0.693077000
C	-1.229598000	4.059985000	1.454012000
C	-1.224194000	4.088321000	2.923031000
W	-3.227259000	4.070106000	2.536599000
C	4.887512000	5.016458000	-3.089775000
C	5.301738000	3.671040000	-3.135793000
H	6.317943000	3.348598000	-3.429722000
C	4.407751000	2.515058000	-2.817885000
C	4.824825000	1.187562000	-2.774300000
C	4.078580000	0.000156000	-2.493114000
H	3.136776000	-0.000284000	-1.904383000
C	4.825941000	-1.186690000	-2.774061000
H	5.498894000	5.876448000	-3.365219000
W	3.224546000	4.071379000	-2.537053000
C	4.409777000	-2.514400000	-2.818042000
C	5.303958000	-3.670082000	-3.136327000
H	6.320015000	-3.347539000	-3.430604000
C	4.889768000	-5.015564000	-3.090922000
W	3.226542000	-4.070908000	-2.538176000
C	1.223468000	-4.087992000	-2.924263000
C	1.229255000	-4.059671000	-1.455196000
C	0.001457000	-4.051678000	-0.723644000
C	2.505030000	-4.093463000	-0.694502000
C	8.397174000	-0.000382000	-3.039854000
C	8.575277000	-0.000587000	-1.627467000
H	9.589995000	-0.002599000	-1.185881000
C	7.429270000	0.000681000	-0.699015000
W	6.490008000	0.001128000	-2.450931000
H	9.240766000	-0.001466000	-3.734068000
C	2.502531000	4.094474000	-0.693519000
C	1.226975000	4.061045000	-1.454473000
C	-0.001040000	4.051407000	-0.723212000
C	1.221495000	4.088973000	-2.923521000
C	4.889402000	-5.014445000	3.090788000
C	5.302747000	-3.668747000	3.137059000
H	6.318630000	-3.345664000	3.431438000
C	4.407987000	-2.513362000	2.819229000
C	4.823859000	-1.185472000	2.776280000
C	4.076732000	0.001500000	2.495210000
H	3.135369000	0.001233000	1.905777000
C	4.822780000	1.188840000	2.777268000
C	4.405751000	2.516311000	2.820698000
C	5.299177000	3.672376000	3.139735000
H	6.315009000	3.350211000	3.435172000
C	4.884658000	5.017724000	3.093543000
W	6.488145000	0.002165000	2.454796000
W	3.222337000	4.072405000	2.539135000
H	5.495450000	5.877684000	3.370396000
C	7.428750000	0.001276000	0.703598000
C	8.574028000	-0.000267000	1.632940000
H	9.589119000	-0.004893000	1.192240000

	C	8.394837000	0.000468000	3.045202000
	H	9.237890000	-0.001306000	3.740067000
	C	2.501991000	4.093770000	0.695028000
	C	1.225784000	4.059254000	1.455028000
	C	-0.001596000	4.051330000	0.722733000
	C	1.219109000	4.088076000	2.924082000
	C	-0.002853000	4.106030000	3.616207000
	C	2.504782000	-4.093881000	0.694032000
	C	1.228822000	-4.060811000	1.454211000
	C	1.222592000	-4.089079000	2.923260000
	W	3.225872000	-4.070407000	2.537979000
	H	-0.003317000	4.126849000	4.712187000
	H	0.000691000	-4.127495000	4.711717000
	H	0.000574000	4.126352000	-4.712659000
	H	0.002033000	-4.125678000	-4.713055000
	H	5.501074000	-5.875329000	-3.367261000
	H	5.501271000	-5.874048000	3.366382000
	H	-5.498936000	5.875877000	-3.370228000
	H	-5.503117000	5.873761000	3.363788000

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