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Electronic Supporting Information (ESI)

Synthetic and Structural Studies of Monocyclopentadienyl Cyclometalated Aryl Tantalum(V) Compounds.

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Figure S1. Optimised structures of the isomers of compounds **2-4**.

Figure S2. Optimised structures of compounds **3s** and **3d**.

Figure S3. Optimised structures of compounds **4s** and **4d**.

Table S1. Selected structural data of optimised compounds **2s-4s** and **2d-4d**.

Table S2. Coordinates of the calculated compounds.

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Figure S1. Optimised structures of the isomers of compounds **2**-**4**.

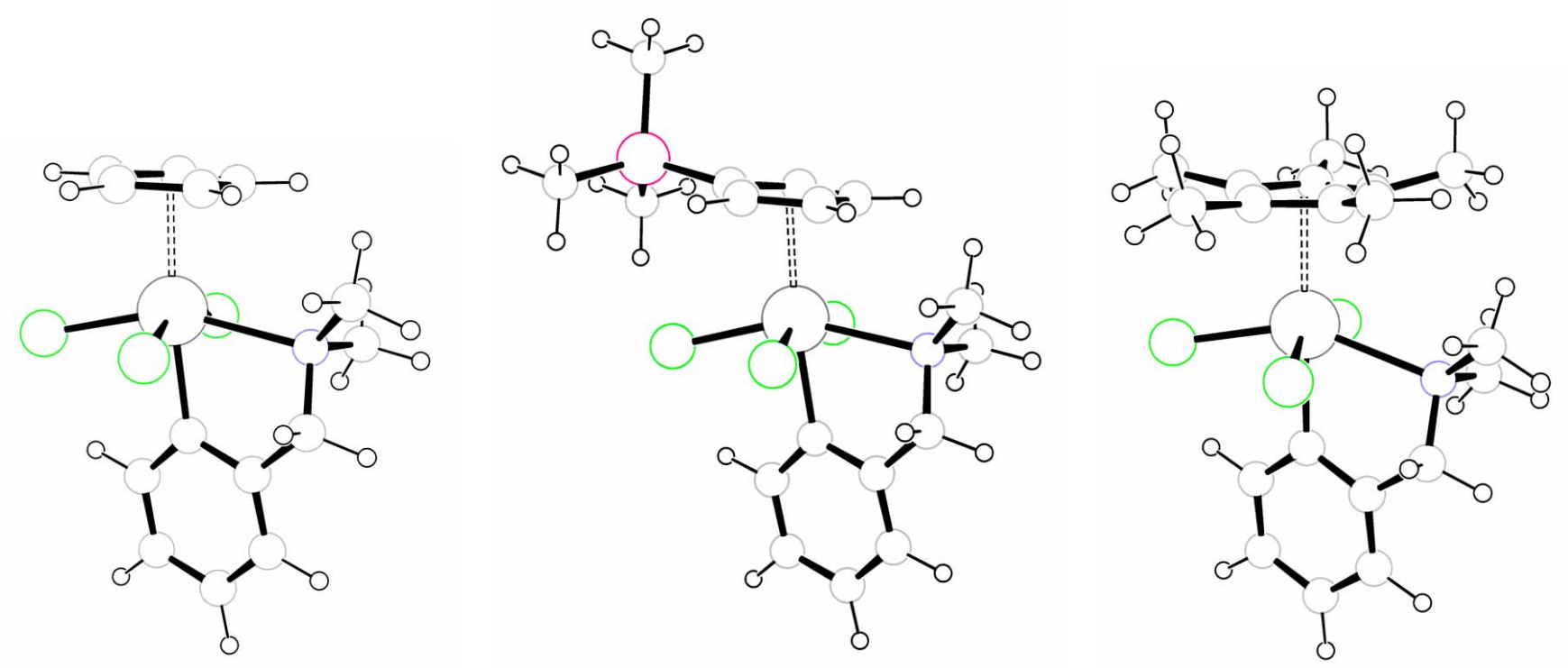

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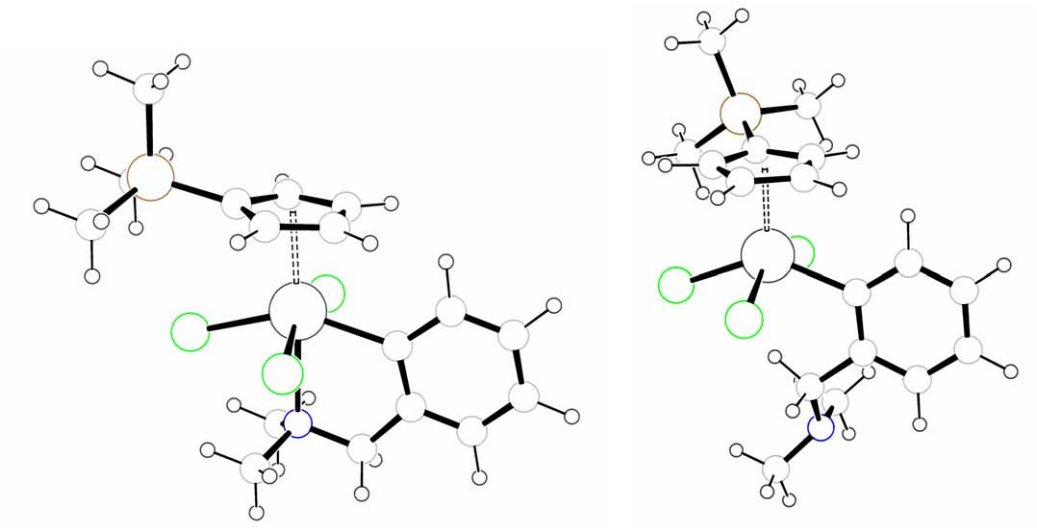
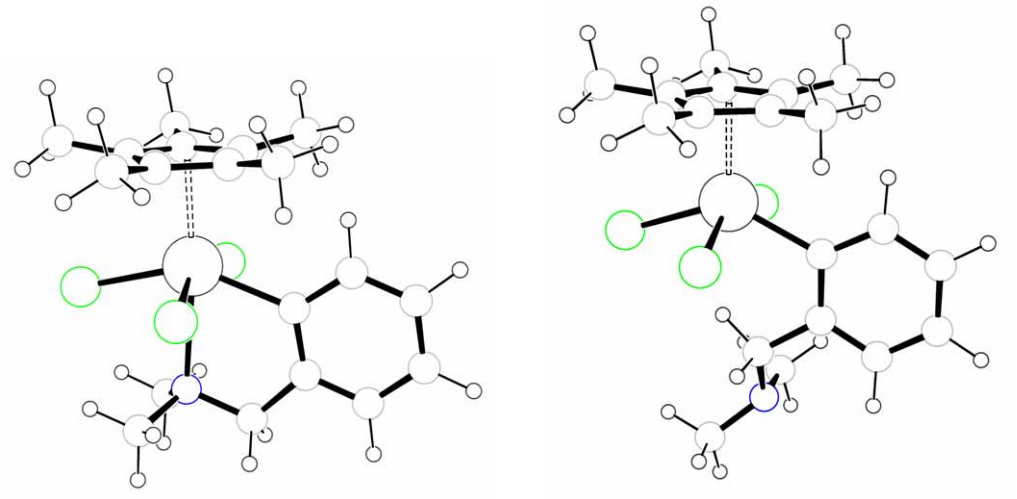
Figure S2. Optimised structures of compounds **3s** and **3d**.



3s **3d**

Figure S3. Optimised structures of compounds **4s** and **4d**.



4s **4d**

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Table S1. Selected structural data of optimised compounds **2s**-**4s** and **2d**-**4d**.

Bond distances (Å) and angles (deg)	**2s**	**2d**	**3s**	**3d**	**4s**	**4d**
Ta-Cl	2.445	2.414 2.417	2.445	2.413 2.420	2.436	2.415 2.418
Ta-Cl (*trans* to C)	2.462	2.406	2.454	2.406	2.449	2.404
Ta-C	2.233	2.207	2.237	2.214	2.242	2.218
Ta-N	2.574	-	2.597	-	2.642	-
Ta-Cp[a]	2.192	2.148	2.207	2.148	2.251	2.186
Cl-Ta-Cl (*trans*)	157.0	148.0	157.3	145.5	154.7	147.0
Cl-Ta-C (*trans*)	149.9	138.5	148.5	138.3	146.5	134.3
N-Ta-Cp	177.4	-	177.8	-	174.4	-

[a]Cp is the centroid of cyclopentadienyl ring.

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Table S2. Coordinates of the calculated compounds.

2

C	2.728300	-1.395400	-0.513100
H	3.615800	-0.812800	-0.709200
C	2.260000	-1.794900	0.764900
H	2.731200	-1.575100	1.711100
C	1.026500	-2.476700	0.587200
H	0.417900	-2.877800	1.382700
C	0.723000	-2.480300	-0.801400
H	-0.150400	-2.904300	-1.271400
C	1.786300	-1.824400	-1.476600
H	1.838400	-1.638900	-2.537200
C	-0.077900	3.253700	-0.445800
H	0.738500	3.567500	0.200500
H	-0.818300	4.061500	-0.516500
H	0.315000	3.030400	-1.435300
C	-1.144500	2.401800	1.514100
H	-0.259200	2.549100	2.130300
H	-1.746900	1.605000	1.944700
H	-1.731600	3.329500	1.484200
C	-1.966900	1.768700	-0.665300
H	-2.712400	2.548900	-0.458200
H	-1.699800	1.837400	-1.722700
C	-3.877100	0.181500	-0.367100
H	-4.548500	1.009800	-0.582300
C	-2.495600	0.400900	-0.354000
C	-1.572000	-0.636300	-0.077900
C	-2.144500	-1.895500	0.208700
H	-1.517700	-2.739900	0.471500
C	-3.520100	-2.123100	0.198400
H	-3.903700	-3.112900	0.431000
C	-4.398000	-1.081700	-0.100000
H	-5.471500	-1.247000	-0.109400
Cl	0.248700	-0.147500	2.418000
Cl	2.366400	1.525400	0.426700
Cl	0.437800	0.635800	-2.340000
N	-0.732900	2.043900	0.128200
Ta	0.605100	-0.122800	-0.009900

3

Ta	0.130800	-0.024500	0.147300
Cl	-0.002900	0.655500	-2.205900
Cl	0.869600	-0.025700	2.496400
Cl	-1.246100	1.888900	0.819700
Si	-3.926100	-0.226800	-0.295300
C	-2.229700	-1.058100	-0.031500
C	-1.615700	-1.425600	1.205900
H	-1.940500	-1.109100	2.186800
C	-0.486800	-2.249900	0.949600
H	0.166400	-2.665500	1.701000
C	-0.356800	-2.374900	-0.459400
H	0.400400	-2.923200	-0.997200
C	-1.421500	-1.646100	-1.047500
H	-1.575200	-1.536800	-2.110200
C	-5.055000	-1.642700	-0.860800
H	-4.712600	-2.084600	-1.802900
H	-6.075100	-1.274700	-1.020900
H	-5.104600	-2.443500	-0.115300
C	-4.557100	0.452000	1.345500
H	-3.900900	1.235100	1.733100
H	-4.635200	-0.337300	2.101500

H	-5.558400	0.878400	1.215900
C	-3.848100	1.080900	-1.648500
H	-3.461800	0.666400	-2.585500
H	-3.200400	1.911200	-1.358200
H	-4.851200	1.475200	-1.848400
N	1.764700	1.939600	-0.050400
C	1.201300	3.216300	-0.572200
H	0.614000	3.025700	-1.467900
H	2.025900	3.901000	-0.811200
H	0.564700	3.670200	0.183800
C	2.448200	2.269100	1.230600
H	1.707900	2.561700	1.973200
H	3.148100	3.098500	1.060800
H	2.994500	1.403400	1.598000
C	2.192500	-0.832400	-0.208100
C	2.643800	-2.136700	0.095200
H	1.970400	-2.866600	0.529800
C	3.958300	-2.552200	-0.111200
H	4.247900	-3.567900	0.144700
C	4.898100	-1.664400	-0.634500
H	5.925100	-1.977200	-0.799600
C	4.503600	-0.360500	-0.919100
H	5.228900	0.353900	-1.302400
C	3.182500	0.048700	-0.705800
C	2.794700	1.462300	-1.018300
H	3.662700	2.135900	-0.986800
H	2.361200	1.527300	-2.019200

4

C	2.686200	0.247000	0.432000
C	2.381800	0.728300	-0.879700
C	1.499000	1.850800	-0.747000
C	1.210100	2.020800	0.643300
C	1.965500	1.042600	1.365000
C	3.726100	-0.771300	0.791500
H	4.653400	-0.257100	1.076900
H	3.411100	-1.391400	1.633900
H	3.946200	-1.434400	-0.044600
C	3.049000	0.285200	-2.147900
H	4.022700	0.782500	-2.249400
H	3.215800	-0.793900	-2.150400
H	2.444200	0.530300	-3.021500
C	1.164300	2.785700	-1.873400
H	2.091300	3.109200	-2.360500
H	0.542900	2.304000	-2.633200
H	0.651700	3.682600	-1.520000
C	0.527600	3.176900	1.322400
H	1.233900	3.659400	2.008000
H	0.192500	3.932500	0.611700
H	-0.341400	2.860900	1.904700
C	2.170700	1.050800	2.847500
H	2.968300	1.767800	3.088000
H	1.270100	1.352900	3.383900
H	2.472200	0.072400	3.222900
C	-1.436300	-3.320800	0.538600
H	-0.793600	-3.881000	-0.136900
H	-2.381500	-3.864500	0.673700
H	-0.937400	-3.213400	1.499600
C	-2.294200	-2.210600	-1.392200
H	-1.528300	-2.627800	-2.044400
H	-2.646400	-1.272400	-1.815000
H	-3.135100	-2.914100	-1.315200
C	-2.758200	-1.323500	0.805700
H	-3.719100	-1.840900	0.670600
H	-2.461800	-1.448600	1.849600
C	-4.121500	0.748000	0.499700
H	-4.990100	0.169500	0.807100

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C	-2.866500	0.130200	0.453700
C	-1.698400	0.828400	0.059900
C	-1.907000	2.162800	-0.347200
H	-1.082100	2.739700	-0.737300
C	-3.153400	2.787100	-0.307700
H	-3.250400	3.818900	-0.636000
C	-4.271700	2.083700	0.137300
H	-5.248700	2.557500	0.173900
N	-1.721000	-1.980500	-0.039600
Cl	-0.229500	-0.192300	-2.443900
Cl	1.337300	-2.412300	-0.542600
Cl	-0.044900	-0.936000	2.290400
Ta	0.248500	-0.276200	-0.041600

Isomer of 2

C	3.098500	-0.967100	0.183600
H	3.330900	-2.021400	0.204500
C	2.956700	-0.172900	-0.980600
H	3.071600	-0.509600	-2.000500
C	2.576200	1.129900	-0.577200
H	2.419200	1.965200	-1.239500
C	2.445500	1.128800	0.840500
H	2.210900	1.972900	1.471600
C	2.787400	-0.171500	1.303600
H	2.759600	-0.503700	2.329300
C	0.234400	3.217100	-0.362400
H	1.143400	3.414400	0.206300
H	-0.391100	4.118500	-0.325000
H	0.482700	3.005600	-1.402700
C	-0.822400	2.391000	1.634700
H	0.088200	2.394400	2.234000
H	-1.501700	1.642700	2.036600
H	-1.293400	3.381400	1.688400
C	-1.806300	1.974800	-0.532900
H	-2.437200	2.831300	-0.256100
H	-1.569400	2.062100	-1.596300
C	-3.875600	0.593800	-0.237800
H	-4.463400	1.499600	-0.372100
C	-2.478500	0.665400	-0.263000
C	-1.666400	-0.471600	-0.082400
C	-2.341100	-1.689800	0.126300
H	-1.774700	-2.598400	0.288500
C	-3.733600	-1.772700	0.136400
H	-4.210300	-2.736300	0.296500
C	-4.511900	-0.629500	-0.046600
H	-5.596500	-0.688000	-0.030500
Cl	0.178700	0.316600	-2.383500
Cl	0.620600	-2.545600	-0.555700
Cl	0.012600	-0.614200	2.327500
N	-0.509200	2.067500	0.213400
Ta	0.552200	-0.229100	-0.020300

Isomer of 3

C	-2.543600	-0.643300	0.067600
C	-1.971400	-1.318400	-1.052100
C	-1.025800	-2.269900	-0.600300
H	-0.481900	-2.953900	-1.230300
C	-0.949800	-2.158200	0.817400
H	-0.373300	-2.771300	1.493500
C	-1.885100	-1.163300	1.211400
H	-2.042300	-0.837700	2.228900
H	-2.200500	-1.123800	-2.091000
Si	-4.034100	0.539800	0.080400
C	-4.334400	1.213900	-1.654900

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H	-5.222000	1.856700	-1.661300
H	-3.486400	1.803500	-2.012200
H	-4.514000	0.405400	-2.372400
C	-3.780000	1.901700	1.359100
H	-4.667400	2.542600	1.413700
H	-3.615500	1.484000	2.358300
H	-2.919300	2.528200	1.112500
C	-5.512100	-0.530100	0.597500
H	-6.427400	0.072400	0.627600
H	-5.680700	-1.354700	-0.103400
H	-5.368700	-0.963400	1.593300
C	1.963800	-3.157400	-0.144100
H	1.195200	-3.698600	0.407700
H	2.913500	-3.693100	-0.016300
H	1.713900	-3.134600	-1.204900
C	2.433400	-1.831300	1.811900
H	1.579100	-2.199000	2.380600
H	2.686900	-0.835800	2.169800
H	3.285800	-2.506300	1.965300
C	3.274300	-1.167900	-0.354900
H	4.194000	-1.654800	-0.000400
H	3.156100	-1.405100	-1.415600
C	4.534800	0.983400	-0.097100
H	5.460800	0.414900	-0.155900
C	3.307200	0.314600	-0.158900
C	2.077600	0.995200	-0.075500
C	2.150700	2.393400	0.078200
H	1.241000	2.973900	0.168800
C	3.369700	3.070100	0.124500
H	3.376800	4.150900	0.239600
C	4.572300	2.368400	0.035600
H	5.523900	2.890600	0.080500
Cl	0.876200	-0.625700	-2.376900
Cl	-0.831500	1.855300	-0.824400
Cl	0.325300	0.581400	2.245500
N	2.102000	-1.767500	0.360100
Ta	0.165200	-0.164000	-0.070800

Isomer of 4

C	2.577200	-1.103000	0.205400
C	2.501200	-0.370400	-1.021000
C	2.327500	1.010200	-0.699400
C	2.225000	1.119100	0.724700
C	2.397300	-0.191400	1.274500
C	2.983400	-2.536500	0.360500
H	4.055200	-2.585100	0.595000
H	2.439700	-3.027500	1.171100
H	2.812300	-3.108500	-0.551300
C	2.778200	-0.922700	-2.387200
H	3.860600	-0.962400	-2.567400
H	2.381500	-1.934900	-2.494500
H	2.325600	-0.305700	-3.164700
C	2.505200	2.120800	-1.693200
H	3.525900	2.087300	-2.093200
H	1.819600	2.016500	-2.539000
H	2.361400	3.106500	-1.248300
C	2.369400	2.363300	1.560500
H	3.353800	2.357300	2.045000
H	2.317500	3.277200	0.967300
H	1.628400	2.428500	2.361900
C	2.628600	-0.498200	2.721600
H	3.704100	-0.429800	2.937200
H	2.107500	0.200200	3.377600
H	2.297200	-1.505000	2.981600
C	-0.378400	3.224600	-0.375600
H	0.497800	3.481100	0.213200
H	-1.057800	4.088000	-0.372200

H	-0.089400	3.007000	-1.402400
C	-1.396400	2.356900	1.623300
H	-0.489300	2.398200	2.224100
H	-2.046800	1.581800	2.022700
H	-1.907600	3.327600	1.674200
C	-2.358900	1.905100	-0.539700
H	-3.014300	2.742800	-0.260900
H	-2.129300	2.001100	-1.603100
C	-4.383000	0.474300	-0.203700
H	-4.993800	1.363500	-0.348700
C	-2.987500	0.579200	-0.256300
C	-2.138600	-0.528800	-0.069700
C	-2.784200	-1.753000	0.192300
H	-2.195400	-2.643800	0.372400
C	-4.173300	-1.871800	0.237000
H	-4.620000	-2.842000	0.439700
C	-4.986300	-0.756500	0.032800
H	-6.068700	-0.841800	0.071000
N	-1.065000	2.045400	0.204800
Cl	-0.313900	0.400500	-2.380500
Cl	0.069500	-2.514200	-0.679100
Cl	-0.416900	-0.583000	2.295100
Ta	0.103900	-0.212000	-0.046100

2d

C	-3.330300	-0.242500	-0.174600
H	-3.800500	-1.213200	-0.115600
C	-3.021800	0.602900	0.922300
H	-3.224300	0.392300	1.961400
C	-2.343500	1.749700	0.421800
H	-1.953500	2.557100	1.023400
C	-2.233900	1.610400	-0.988100
H	-1.740100	2.288700	-1.668000
C	-2.841300	0.376900	-1.354300
H	-2.878700	-0.038200	-2.350200
C	3.766200	-2.559000	0.645300
H	4.761200	-2.879100	0.319300
H	3.045900	-3.345800	0.358400
H	3.772500	-2.483200	1.737000
C	3.547800	-1.286300	-1.399400
H	4.566800	-1.558100	-1.693900
H	3.322500	-0.297900	-1.804700
H	2.851000	-2.009300	-1.854700
C	2.250200	-0.674100	0.582800
H	1.334100	-1.221300	0.222700
H	2.233600	-0.831900	1.668000
C	3.192000	1.642300	0.332900
H	4.168800	1.200100	0.502800
C	2.075000	0.804700	0.299200
C	0.772500	1.322900	0.074900
C	0.674500	2.717800	-0.103500
H	-0.285000	3.191100	-0.280400
C	1.790500	3.555600	-0.074100
H	1.665500	4.624900	-0.222400
C	3.057000	3.017800	0.143100
H	3.932200	3.661000	0.168300
Cl	-0.472700	-0.269900	2.391900
Cl	-1.125200	-2.551200	0.125000
Cl	-0.016000	-0.543500	-2.220900
N	3.460500	-1.260100	0.058800
Ta	-0.858700	-0.162400	0.008400

2s

C	-2.646700	-0.984900	0.000000

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C	-1.561100	-2.028200	0.000000
C	-0.188800	-1.696500	0.000000
Cl	-0.235300	2.838200	0.000000
Cl	-0.051800	0.269200	2.396000
Cl	-0.051800	0.269200	-2.396000
N	-2.176500	0.440900	0.000000
Ta	0.397300	0.458500	0.000000
H	-3.288500	-1.137500	-0.874700
H	-3.288500	-1.137500	0.874700
C	-2.771300	1.127100	-1.189800
H	-3.864500	1.124000	-1.095400
H	-2.414700	2.154600	-1.230400
H	-2.483300	0.613200	-2.101600
C	-2.771300	1.127100	1.189800
H	-3.864500	1.124000	1.095400
H	-2.483300	0.613200	2.101600
H	-2.414700	2.154600	1.230400
C	0.694400	-2.802200	0.000000
C	-2.000700	-3.358800	0.000000
H	-3.069400	-3.565400	0.000000
C	-1.098000	-4.415900	0.000000
H	-1.451900	-5.442900	0.000000
C	0.265100	-4.127900	0.000000
H	0.997700	-4.930600	0.000000
H	1.766900	-2.656200	0.000000
C	2.594900	1.779200	0.000000
C	2.583800	0.948900	1.144600
C	2.583800	0.948900	-1.144600
H	2.547400	2.857100	0.000000
C	2.583800	-0.405500	0.710500
H	2.538300	1.283400	2.169300
C	2.583800	-0.405500	-0.710500
H	2.538300	1.283400	-2.169300
H	2.560600	-1.266200	1.360600
H	2.560600	-1.266200	-1.360600

FMO CpTaCl$_3$

C	-0.468200	1.161000	1.728700
H	-0.730800	0.600000	2.612800
C	0.848100	1.465100	1.295900
H	1.762200	1.181600	1.795500
C	0.755100	2.149400	0.054500
H	1.594400	2.488600	-0.532600
C	-0.620400	2.250100	-0.289300
H	-1.033700	2.700500	-1.178000
C	-1.371000	1.651300	0.757000
H	-2.443200	1.542300	0.779100
Cl	2.436200	-0.309700	-0.658500
Cl	0.270400	-1.821800	1.408100
Cl	-2.369100	-0.750200	-0.604400
Ta	0.003500	-0.158700	-0.373000

FMO 2-{(dimethylamino)methyl}phenyl

C	3.328900	-0.063200	-0.602700
H	4.055900	-0.743900	-0.166000
H	3.591600	0.969700	-0.338300
H	3.337300	-0.177000	-1.684500
C	2.074300	-0.296700	1.416300
H	2.699900	-1.110300	1.779200
H	1.087300	-0.381600	1.865600
H	2.522500	0.666200	1.695800
C	1.043100	0.705400	-0.522700
H	1.286300	1.639700	0.002200
H	1.223900	0.866800	-1.588100

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C	-1.327800	1.272400	0.038100
H	-1.013200	2.307700	0.149600
C	-0.381600	0.297800	-0.296500
C	-0.729700	-1.065800	-0.452800
C	-2.088700	-1.373600	-0.220800
H	-2.440300	-2.397400	-0.277500
C	-3.038300	-0.408900	0.113400
H	-4.069800	-0.705300	0.284300
C	-2.662100	0.928100	0.236600
H	-3.392900	1.687900	0.498100
N	1.971900	-0.370900	-0.067700