

Supplementary Information for:
Are Metallacyclopentadienes Always Non-Aromatic?

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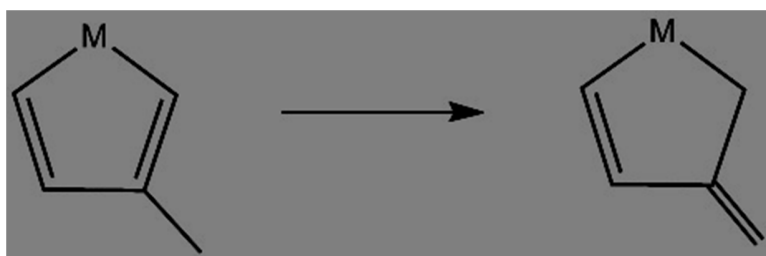


Figure S1. Isomeration reaction for the calculation of ISE.

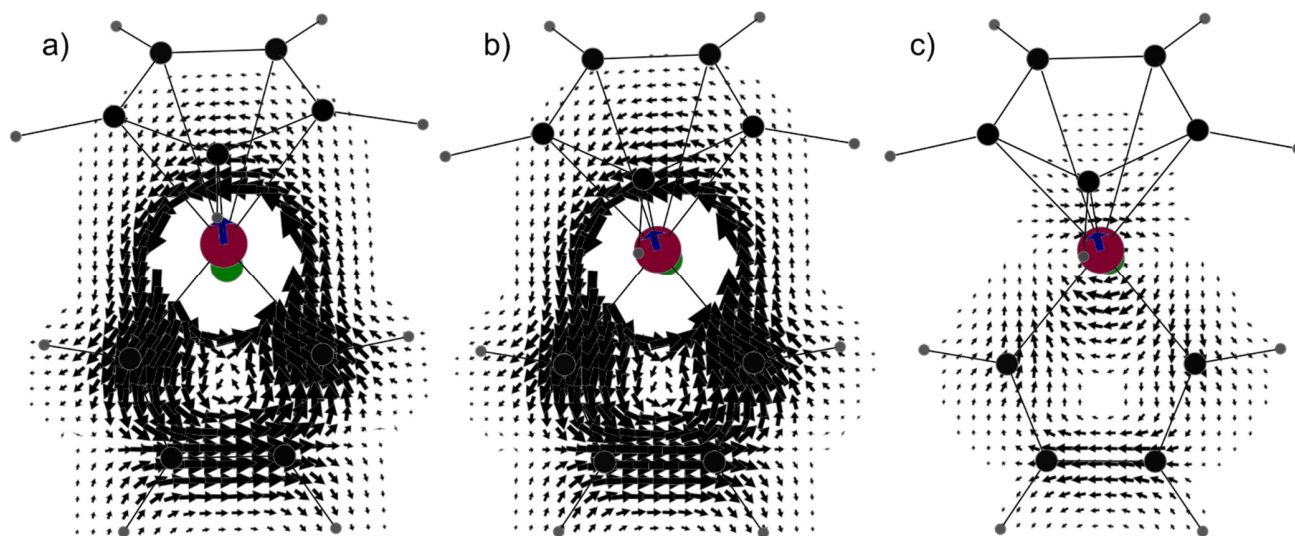


Figure S2. Maps of contributions to $j(r)$ of a) HOMO-1 of complex **6** and its b) rotational and c) translational part.

Table S1. XYZ coordinates of the studied metallacyclopentadienes.

1. Energy: -1391.28233578

Ti	0.0009060000	-0.0771670000	0.0001000000
C	-0.0454740000	1.5253970000	1.3834600000
C	-0.0391650000	2.7004960000	0.7344740000
H	-0.0670180000	3.6552100000	1.2573440000
C	-0.0079550000	2.7006710000	-0.7346650000
H	0.0028140000	3.6556470000	-1.2576820000
C	0.0200720000	1.5257890000	-1.3834440000
C	-1.4984980000	-1.9154730000	0.3821970000
H	-1.1016570000	-2.8513980000	0.7417790000
C	-1.6074500000	-1.5261270000	-0.9738900000
H	-1.3263790000	-2.1201950000	-1.8290450000
C	-2.1581310000	-0.2254650000	-1.0076080000
C	-2.3585660000	0.1960110000	0.3219320000
H	-2.7206920000	1.1617110000	0.6307960000
C	-1.9557110000	-0.8538010000	1.1791190000
H	-1.9583870000	-0.8222780000	2.2573190000
C	2.3522320000	0.2284770000	-0.3456870000
H	2.6985680000	1.1928720000	-0.6757400000

C	1.9604040000	-0.8444430000	-1.1794270000
H	1.9544500000	-0.8340180000	-2.2580670000
C	1.5284590000	-1.8983930000	-0.3585650000
H	1.1448100000	-2.8475900000	-0.6970410000
C	1.6401990000	-1.4811760000	0.9885370000
H	1.3753320000	-2.0632620000	1.8570300000
C	2.1685930000	-0.1705040000	0.9932590000
H	2.3805240000	0.4278670000	1.8626590000
H	-2.3725960000	0.3530530000	-1.8897650000
H	0.0617090000	1.5110850000	-2.4709100000
H	-0.0854720000	1.5102140000	2.4709790000

2. -588.862468297

Zr	0.0000250000	-0.0294560000	0.0007900000
C	0.0085160000	1.6531050000	-1.4801070000
C	0.0023460000	2.7791530000	-0.7422030000
H	0.0063690000	3.7630610000	-1.2123380000
C	-0.0049960000	2.7798970000	0.7408710000
H	-0.0099480000	3.7643070000	1.2099570000
C	-0.0101210000	1.6546450000	1.4800420000
C	1.6295710000	-1.9290840000	-0.4372140000
H	1.2345660000	-2.8524390000	-0.8315890000
C	1.7511730000	-1.5962000000	0.9338210000
H	1.4747990000	-2.2254140000	1.7658000000
C	2.3192130000	-0.3054390000	1.0184560000
H	2.5328500000	0.2376240000	1.9241890000
C	2.5255720000	0.1660280000	-0.2939960000
H	2.9025120000	1.1385600000	-0.5659940000
C	2.1073280000	-0.8409630000	-1.1930020000
H	2.1264140000	-0.7721740000	-2.2694670000
C	-2.1071200000	-0.8440080000	1.1924620000
C	-1.6280430000	-1.9309200000	0.4357260000
C	-1.7492800000	-1.5966730000	-0.9349900000
H	-1.2318900000	-2.8541100000	0.8293060000
C	-2.3184020000	-0.3063430000	-1.0185400000
H	-1.4718890000	-2.2247390000	-1.7674960000
C	-2.5258010000	0.1635860000	0.2943190000
H	-2.5318080000	0.2375830000	-1.9237830000
H	-2.1269800000	-0.7764570000	2.2689820000
H	-2.9040210000	1.1353600000	0.5671740000
H	0.0188160000	1.7616910000	-2.5619670000
H	-0.0205370000	1.7646760000	2.5617540000

3. -631.869584213

Nb	0.0142280000	-0.1326400000	-0.0049500000
C	-2.1713560000	0.5197550000	-0.0008720000
C	-1.1977360000	-2.0331160000	-0.0041460000

C	-2.5266710000	-1.8741380000	-0.0123210000
C	-3.0464160000	-0.4918270000	-0.0173110000
H	-4.1228590000	-0.3258840000	-0.0309890000
H	-2.5595620000	1.5349660000	-0.0026890000
H	-0.8136670000	-3.0529400000	-0.0027440000
H	-3.2358610000	-2.7010030000	-0.0177750000
C	-0.2313730000	1.4181140000	1.3759610000
C	-0.2122480000	1.4492840000	-1.3590210000
C	2.1287130000	-0.2332380000	1.1557680000
C	2.3028020000	0.6026160000	0.0188850000
C	2.1460000000	-0.2055830000	-1.1400640000
C	1.9038120000	-1.5329640000	-0.7128760000
H	2.5446910000	1.6527120000	0.0335580000
H	2.2436800000	0.1230390000	-2.1616890000
O	-0.3711780000	2.3048850000	-2.0889040000
O	-0.4010520000	2.2585880000	2.1212840000
C	1.8935160000	-1.5500210000	0.6931790000
H	1.7057770000	-2.3761810000	-1.3555870000
H	2.2113450000	0.0708310000	2.1862650000
H	1.6866930000	-2.4083870000	1.3124820000

4. -1518.88175258

V	0.0864760000	-0.1095660000	-0.0031000000
C	-2.0856900000	0.3932620000	-0.0011530000
C	-0.9281710000	-1.9891890000	-0.0039570000
C	-2.2635450000	-1.9885020000	-0.0135340000
C	-2.8985920000	-0.6631530000	-0.0190200000
H	-3.9818030000	-0.5602390000	-0.0322030000
H	-2.5114120000	1.3934310000	-0.0016560000
H	-0.4204960000	-2.9531580000	-0.0010540000
H	-2.8768930000	-2.8874460000	-0.0190730000
C	-0.3535140000	1.2761130000	1.3406430000
C	-0.3393680000	1.3073510000	-1.3227160000
C	2.0842110000	-0.0927000000	1.1473920000
C	2.2063640000	0.7404960000	0.0058050000
C	2.0878920000	-0.0814610000	-1.1444570000
C	1.8872610000	-1.4053560000	-0.7100690000
H	2.3813050000	1.8039590000	0.0115110000
H	2.1474820000	0.2482570000	-2.1688480000
O	-0.6119370000	2.1028070000	-2.0814080000
O	-0.6341220000	2.0556530000	2.1132740000
C	1.8853830000	-1.4121880000	0.6996560000
H	1.7060880000	-2.2574250000	-1.3448290000
H	2.1395340000	0.2270540000	2.1751740000
H	1.7023300000	-2.2701450000	1.3258090000

5. -2072.07615297

Fe	0.0752840000	-0.1742700000	-0.0006360000
C	-1.2672670000	0.4495700000	-1.2228920000
C	-1.2675800000	0.4468500000	1.2229940000
C	-2.4267360000	0.8916140000	0.7238340000
C	-2.4265540000	0.8932460000	-0.7230540000
H	-3.2694650000	1.2109500000	-1.3277280000
H	-1.0283590000	0.4000170000	-2.2817990000
H	-1.0293140000	0.3941660000	2.2818930000
H	-3.2698880000	1.2077480000	1.3289970000
C	2.2816870000	-0.3489420000	-0.0004620000
C	1.8644490000	0.3694180000	-1.1418160000
C	1.1768180000	1.5296590000	-0.7094990000
H	1.9821510000	0.0545060000	-2.1664700000
C	1.1765540000	1.5279220000	0.7127770000
C	1.8640750000	0.3666150000	1.1424840000
H	1.9812770000	0.0490760000	2.1663830000
H	2.7632300000	-1.3129300000	-0.0015510000
H	0.7343200000	2.2821690000	-1.3392630000
H	0.7337930000	2.2788730000	1.3442140000
Cl	-0.4357540000	-2.2817220000	-0.0008440000

6. -903.295121832

Ru	-0.0268230000	0.1474270000	0.0004670000
C	1.2890080000	-0.5936590000	1.2218140000
C	1.2899420000	-0.5903250000	-1.2220310000
C	2.4454540000	-1.0984810000	-0.7089290000
C	2.4449190000	-1.1003140000	0.7080270000
H	1.0692300000	-0.6279430000	2.2866560000
H	3.2593020000	-1.4789360000	1.3153480000
H	1.0707720000	-0.6218340000	-2.2870910000
H	3.2601390000	-1.4758320000	-1.3166130000
Cl	0.7129010000	2.3280860000	0.0008830000
C	-2.3503880000	0.2235740000	0.6986340000
C	-1.6345480000	-0.9286990000	1.1401870000
C	-1.2417580000	-1.6795610000	-0.0018170000
H	-1.4624280000	-1.2118450000	2.1661300000
C	-1.6337560000	-0.9261150000	-1.1423470000
C	-2.3499190000	0.2251410000	-0.6985320000
H	-2.7464190000	1.0015090000	-1.3335200000
H	-2.7475820000	0.9983720000	1.3350830000
H	-0.7347740000	-2.6301410000	-0.0027540000
H	-1.4610760000	-1.2069430000	-2.1688310000

7. -1650.54743988

Fe	-0.1046680000	-0.0000110000	-0.1526380000
C	-1.5878370000	-1.3282000000	-0.0077180000
C	-1.5878150000	1.3282480000	-0.0076110000

C	-2.7901180000	0.7438770000	-0.0397620000
C	-2.7901400000	-0.7438140000	-0.0397150000
H	-3.7352750000	-1.2863260000	-0.0482640000
H	-1.5276050000	-2.4171520000	0.0013460000
H	-1.5275300000	2.4171950000	0.0011830000
H	-3.7352490000	1.2864010000	-0.0485810000
H	1.0974020000	1.2339620000	2.2065980000
C	1.3512750000	0.6981600000	1.3041370000
C	1.3514790000	-0.6998950000	1.3031760000
H	1.0977120000	-1.2369900000	2.2049030000
C	1.5933640000	-1.4070650000	0.1095490000
H	1.5324400000	-2.4852510000	0.0998980000
C	1.7851780000	-0.7056130000	-1.0780730000
H	1.8828360000	-1.2403620000	-2.0119360000
C	1.7851530000	0.7073090000	-1.0770910000
H	1.8827850000	1.2433790000	-2.0101970000
C	1.5931080000	1.4070310000	0.1114830000
H	1.5319650000	2.4852190000	0.1033860000

8. -481.724694879

Ru	-0.2040850000	0.0002910000	0.0009950000
C	-1.5916720000	-1.2041870000	0.0005520000
C	-1.5922560000	1.2048390000	0.0003010000
C	-2.9774570000	0.6691520000	-0.0006310000
C	-2.9771750000	-0.6691410000	0.0001800000
H	-3.8656260000	-1.2905490000	0.0001400000
H	-1.5023490000	-2.2970880000	-0.0015150000
H	-1.5034990000	2.2977500000	0.0007380000
H	-3.8662260000	1.2901070000	-0.0015550000
H	1.8495990000	2.1533220000	1.2351600000
C	1.8192420000	1.2182700000	0.6931270000
C	1.6874590000	-0.0008320000	1.4028220000
H	1.6685270000	-0.0012640000	2.4822180000
C	1.8171190000	-1.2196320000	0.6921570000
H	1.8456990000	-2.1551460000	1.2334960000
C	1.8151450000	-1.2191890000	-0.6953550000
H	1.8421000000	-2.1543010000	-1.2374600000
C	1.6831180000	0.0001670000	-1.4046410000
H	1.6610360000	0.0006090000	-2.4839780000
C	1.8172260000	1.2188010000	-0.6943790000
H	1.8459680000	2.1542510000	-1.2358090000

9. -2349.26160760

Ni	-0.0967800000	0.0000610000	-0.0011950000
C	1.3662350000	1.3252950000	-0.0001700000
C	1.3636040000	-1.3286470000	-0.0009420000
C	2.5643820000	-0.7400900000	0.0006570000

C	2.5658240000	0.7342760000	0.0012940000
H	3.5070570000	1.2822180000	0.0027460000
H	1.3356550000	2.4175210000	0.0006200000
H	1.3305350000	-2.4207930000	-0.0016180000
H	3.5045750000	-1.2898150000	0.0013410000
P	-1.4530320000	1.8629740000	0.0002790000
H	-2.8561110000	1.9981610000	0.0000790000
H	-1.1797270000	2.7426440000	-1.0570450000
P	-1.4584120000	-1.8595760000	0.0006390000
H	-1.1887270000	-2.7413930000	-1.0557610000
H	-2.8619010000	-1.9897730000	0.0008910000
H	-1.1809280000	2.7387990000	1.0610720000
H	-1.1891990000	-2.7352440000	1.0623330000

10. -968.836783688

Pd	-0.0891410000	-0.0000040000	-0.0000040000
C	1.4844110000	1.3112190000	0.0000050000
C	1.4845360000	-1.3111270000	-0.0000130000
C	2.6893810000	-0.7327400000	0.0000020000
C	2.6893150000	0.7329540000	0.0000100000
H	3.6178310000	1.3001790000	0.0000110000
H	1.3984830000	2.3976980000	-0.0000030000
H	1.3987260000	-2.3976150000	-0.0000210000
H	3.6179560000	-1.2998710000	0.0000110000
P	-1.5040070000	1.9270200000	0.0000000000
H	-2.9092490000	2.0161390000	0.0000000000
H	-1.2707420000	2.8256740000	-1.0536110000
P	-1.5038310000	-1.9271290000	0.0000030000
H	-1.2706510000	-2.8257240000	-1.0536760000
H	-2.9090660000	-2.0163520000	0.0001920000
H	-1.2707410000	2.8256540000	1.0536270000
H	-1.2703520000	-2.8257850000	1.0535640000

11. -1586.15815206

Cr	0.1604160000	0.0438820000	-0.0003560000
C	-1.4132840000	-0.3370280000	1.2847280000
C	-1.4133260000	-0.3381480000	-1.2847770000
C	-2.5827950000	-0.6753010000	-0.7284180000
C	-2.5826260000	-0.6750510000	0.7285910000
H	-3.4732060000	-0.9220640000	1.2998720000
H	-1.2956550000	-0.2756310000	2.3657370000
H	-1.2953410000	-0.2787650000	-2.3658740000
H	-3.4734800000	-0.9226380000	-1.2993840000
C	-0.6722020000	1.9928580000	0.7103920000
C	-0.6699950000	1.9933110000	-0.7132160000
C	0.6706430000	1.8918660000	-1.1471250000
H	-1.5354580000	2.1117300000	-1.3389510000

C	1.4876050000	1.8295960000	0.0018910000
C	0.6672980000	1.8915170000	1.1482890000
H	0.9948470000	1.8338080000	2.1732930000
H	-1.5393650000	2.1121390000	1.3335840000
H	1.0013630000	1.8347540000	-2.1711460000
H	2.5590830000	1.7132240000	0.0035600000
C	2.0552040000	-1.0211370000	-0.7072160000
C	2.0486520000	-1.0248980000	0.7180630000
C	0.9319560000	-1.7457560000	1.1472350000
H	2.7616970000	-0.5244710000	1.3533600000
C	0.2153720000	-2.1610220000	-0.0063060000
C	0.9425030000	-1.7392060000	-1.1509790000
H	0.6487190000	-1.8979950000	-2.1745120000
H	2.7740630000	-0.5171240000	-1.3330630000
H	0.6289240000	-1.9111010000	2.1669960000
H	-0.7162100000	-2.6986490000	-0.0118350000

12. -609.942886556

Mo	-0.0002870000	0.1917700000	-0.0000720000
C	0.0020150000	-1.5340950000	1.3153460000
C	0.0018380000	-1.5342030000	-1.3153210000
C	0.0035720000	-2.7395810000	-0.7296550000
C	0.0036920000	-2.7395170000	0.7297660000
H	0.0051600000	-3.6733700000	1.2871860000
H	0.0019190000	-1.4480800000	2.4011590000
H	0.0016450000	-1.4482570000	-2.4011390000
H	0.0049580000	-3.6734860000	-1.2869880000
C	-2.2259650000	-0.1524710000	0.7072980000
C	-2.2261090000	-0.1525330000	-0.7069700000
C	-1.7707080000	1.1104070000	-1.1594830000
H	-2.5182900000	-0.9795780000	-1.3293700000
C	-1.4933580000	1.8914830000	0.0000240000
C	-1.7704620000	1.1104850000	1.1596120000
H	-1.6873820000	1.4257230000	2.1858450000
H	-2.5180290000	-0.9794710000	1.3298110000
H	-1.6878210000	1.4255700000	-2.1857540000
H	-1.1646670000	2.9166190000	-0.0000300000
C	1.4886670000	1.8952460000	-0.0009830000
C	1.7676380000	1.1157770000	1.1592130000
C	2.2261790000	-0.1463850000	0.7078540000
H	1.6835880000	1.4315040000	2.1852170000
C	2.2263590000	-0.1474790000	-0.7064270000
C	1.7680010000	1.1140510000	-1.1598660000
H	1.6844530000	1.4282480000	-2.1863790000
H	1.1571900000	2.9194950000	-0.0018260000
H	2.5204040000	-0.9721340000	1.3310070000
H	2.5207780000	-0.9742060000	-1.3281840000

13. -2117.60542740

Cr	-0.1372550000	-0.0473280000	-0.0000530000
C	1.3279370000	0.8074560000	1.3122650000
C	1.3280870000	0.8081790000	-1.3117130000
C	2.3575540000	1.4467800000	-0.7255530000
C	2.3574600000	1.4463940000	0.7265640000
H	3.1208320000	1.9890740000	1.2823150000
H	1.2623370000	0.8827680000	2.4031620000
H	1.2626180000	0.8839680000	-2.4025820000
H	3.1210200000	1.9897300000	-1.2809130000
H	-2.7161120000	-1.1669340000	-1.2363570000
C	-2.2950250000	-0.3292730000	-0.6969810000
C	-2.2950280000	-0.3291740000	0.6971840000
H	-2.7160840000	-1.1667840000	1.2366690000
C	-1.6820320000	0.7242520000	1.3994520000
H	-1.6274270000	0.6999520000	2.4783660000
C	-1.1566480000	1.8320010000	0.6976800000
H	-0.7061030000	2.6498780000	1.2384310000
C	-1.1568430000	1.8320060000	-0.6977610000
H	-0.7064480000	2.6499010000	-1.2386150000
C	-1.6822130000	0.7241960000	-1.3994040000
H	-1.6277790000	0.6998610000	-2.4783250000
P	0.5670530000	-1.6667420000	-1.5418260000
H	0.0535200000	-2.9852590000	-1.7006090000
H	1.9169530000	-2.0473360000	-1.4710690000
P	0.5665670000	-1.6674900000	1.5412170000
H	0.5312830000	-1.3367990000	2.9073620000
H	1.9164960000	-2.0480130000	1.4706820000
H	0.5321920000	-1.3354620000	-2.9078240000
H	0.0530200000	-2.9860870000	1.6993130000

14. -1141.36970977

Mo	0.1163890000	0.0196540000	0.0340510000
C	-1.3410680000	-1.5217170000	0.5676720000
C	-1.2963070000	-0.0469730000	-1.5990430000
C	-2.2789230000	-0.9799240000	-1.5371910000
C	-2.2945030000	-1.7939460000	-0.3495540000
H	-3.0257240000	-2.5886460000	-0.2179440000
H	-1.3068870000	-2.1201080000	1.4787060000
H	-1.2516050000	0.5293520000	-2.5271320000
H	-2.9969760000	-1.1408220000	-2.3375210000
H	2.5773880000	1.5352400000	1.0493980000
C	2.2398450000	0.6178190000	0.5900040000
C	2.0353160000	-0.5467200000	1.3835930000
H	2.1673740000	-0.5042820000	2.4558980000
C	1.5809640000	-1.7052520000	0.7822420000
H	1.3177920000	-2.5604910000	1.3885550000

C	1.3580290000	-1.7590630000	-0.6345550000
H	0.9516040000	-2.6498860000	-1.0877490000
C	1.8456280000	-0.7014830000	-1.4396120000
H	1.8024130000	-0.7780150000	-2.5168120000
C	2.2661390000	0.4778830000	-0.8373700000
H	2.5698760000	1.3128300000	-1.4559910000
P	-0.3266450000	2.3048260000	-0.6440400000
H	0.5426630000	3.3736930000	-0.3127480000
H	-1.5129610000	2.9300880000	-0.2148330000
P	-1.3695560000	0.6572450000	1.7498680000
H	-1.5481550000	-0.1639700000	2.8756060000
H	-2.7229660000	0.8363810000	1.3946850000
H	-0.4519040000	2.6046260000	-2.0122040000
H	-1.2479720000	1.8837290000	2.4654060000

15. -1993.71135616

Fe	0.0880180000	-0.0682220000	-0.0001820000
C	-1.2842290000	0.5869550000	1.3088330000
C	-1.2846870000	0.5866120000	-1.3091780000
C	-2.3431190000	1.1863080000	-0.7316490000
C	-2.3428260000	1.1865920000	0.7315580000
H	-3.1697960000	1.6287430000	1.2849660000
H	-1.2509050000	0.5402930000	2.4003550000
H	-1.2522770000	0.5389390000	-2.4006720000
H	-3.1705330000	1.6279040000	-1.2848490000
H	2.1963950000	-1.8518840000	-1.2468550000
C	2.0414640000	-0.9272750000	-0.7089290000
C	1.7904110000	0.2471710000	-1.4017150000
H	1.7311480000	0.2395040000	-2.4803720000
C	1.5265570000	1.4468360000	-0.6939700000
H	1.2584960000	2.3413810000	-1.2357470000
C	1.5261460000	1.4469780000	0.6937670000
H	1.2575540000	2.3416150000	1.2351360000
C	1.7892430000	0.2474570000	1.4020210000
H	1.7285940000	0.2400280000	2.4805990000
C	2.0408080000	-0.9271750000	0.7096980000
H	2.1951520000	-1.8517070000	1.2479150000
P	-1.2907690000	-1.8280360000	0.0000710000
H	-2.6512390000	-1.5220720000	-0.0000440000
H	-1.2790750000	-2.7803360000	1.0445650000
H	-1.2790420000	-2.7808550000	-1.0439530000

16. -824.945894379

Ru	0.0603690000	-0.0508630000	-0.0141410000
C	-1.4315470000	0.4528320000	1.2873230000
C	-1.3594650000	0.7286990000	-1.2445690000
C	-2.4760240000	1.2185950000	-0.6735340000

C	-2.5176610000	1.0584840000	0.7704620000
H	-3.3604150000	1.3927880000	1.3685290000
H	-1.3685650000	0.2582180000	2.3576120000
H	-1.2338640000	0.7740330000	-2.3261500000
H	-3.2863990000	1.6790680000	-1.2306520000
H	2.1409870000	-0.7688100000	-2.2263500000
C	2.0278340000	-0.3188290000	-1.2516350000
C	2.1022740000	-1.1052480000	-0.0824310000
H	2.2714260000	-2.1702500000	-0.1706240000
C	2.0050410000	-0.5251200000	1.2008550000
H	2.0976930000	-1.1342470000	2.0875010000
C	1.7019290000	0.8428770000	1.3026400000
H	1.5459040000	1.2867150000	2.2760030000
C	1.5851080000	1.6461520000	0.1473900000
H	1.3301870000	2.6913310000	0.2330650000
C	1.7248100000	1.0474110000	-1.1238350000
H	1.5821270000	1.6488950000	-2.0108000000
P	-1.2948700000	-1.7816420000	-0.0925440000
H	-2.6523710000	-1.5417740000	-0.3302780000
H	-1.3946710000	-2.6255570000	1.0304630000
H	-1.0790290000	-2.8029000000	-1.0439620000

17. -1895.21145582

Ni	0.2510120000	0.0005580000	0.0007040000
C	1.6709510000	-1.2989790000	0.0000510000
C	1.6715350000	1.2995970000	0.0001120000
C	2.8841960000	0.7376930000	-0.0004060000
C	2.8838550000	-0.7376380000	-0.0004290000
H	3.8159870000	-1.2999450000	-0.0009060000
H	1.5612080000	-2.3840210000	0.0001280000
H	1.5623210000	2.3846760000	0.0002300000
H	3.8165720000	1.2995960000	-0.0006440000
H	-1.7417690000	-0.5134780000	-2.4306450000
C	-1.7522050000	-0.2878390000	-1.3738630000
C	-1.7085460000	-1.3201230000	-0.4348800000
H	-1.6512720000	-2.3474800000	-0.7665190000
C	-1.7261270000	-1.0355970000	0.9350450000
H	-1.6870410000	-1.8442030000	1.6513110000
C	-1.7533800000	0.2869010000	1.3731480000
H	-1.7438810000	0.5124550000	2.4299570000
C	-1.7113900000	1.3191940000	0.4342630000
H	-1.6567340000	2.3467280000	0.7657990000
C	-1.7278110000	1.0345770000	-0.9357850000
H	-1.6901880000	1.8433370000	-1.6519570000

18. -514.782422399

Pd	0.7664610000	-0.0269270000	0.0091420000
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C	2.2737020000	-1.2831800000	-0.2667920000
C	3.5337580000	0.6500440000	0.1132240000
H	4.4080600000	-1.3776830000	-0.3137970000
H	2.0625630000	-2.3295660000	-0.4791770000
H	-1.5732590000	-2.4595990000	0.2638000000
C	-1.5823820000	-1.3821440000	0.1682630000
C	-1.5823750000	-0.5829420000	1.3112530000
H	-1.5710900000	-1.0385480000	2.2918030000
C	2.3165660000	1.1857660000	0.2383540000
C	3.5089300000	-0.7821440000	-0.1798640000
H	4.4532710000	1.2196290000	0.2180370000
H	2.1417950000	2.2377000000	0.4560470000
H	-1.5293580000	2.4659300000	-0.1799300000
C	-1.5577510000	1.3888030000	-0.0839850000
C	-1.6058620000	0.5902710000	-1.2261470000
H	-1.6130920000	1.0458180000	-2.2067660000
H	-1.5262670000	1.4276050000	2.0665120000
C	-1.5558170000	0.8034050000	1.1837470000
H	-1.6102340000	-1.4207800000	-1.9822720000
C	-1.6038900000	-0.7964880000	-1.0991210000

Table S2. CSD search of metallacyclopentadienes.

Number of structures 287

Nfrag	Refcode	TOR M1-C2-C3-C4
1	ADEXIQ	-.682
2	AGAHUL	7.438
3	AJEBAU	2.561
4	AJOGIP	-2.954
5	AJOGOV	1.593
6	AKIMIR	-1.859
7	AKIMOX	1.213
8	ASASIX	8.903
9	ASODAN	16.388
10	ATANIT	-.556
11	BACQAZ	2.018
12	BAVDUY	-4.527
13	BEKVUK	.725
14	BEQLEQ	-7.512
15	BIXTOS	-.382
16	BODQUG	-1.896
17	BULPED	-.996
18	CATLIV	-3.354
19	CBFBNB10	.000
20	CEQFEJ	-2.664
21	CEXKUN	.727
22	CIFMUC	2.800
23	COJS AV	3.729
24	COJSEZ	5.303
25	CPFPCO	-3.977

26	CPFPRH	-4.573
27	CPPHZR	-8.055
28	CPTPHF	-4.667
29	CPTPTI	-4.834
30	CSMRHC10	-3.446
31	CUPFEY	10.930
32	DAMBIE	1.042
33	DAMBOK	3.596
34	DANDAA	-2.340
35	DAVZIJ	-7.392
36	DOZQEO	-4.656
37	DUGHAQ	-7.008
38	DUGHEU	-4.449
39	EBAWUA	-1.684
40	EFIPUE	10.828
41	EFIPUE	7.359
42	EKAFUR	6.962
43	FEHFII	9.948
44	FEZDUJ	.632
45	FEZDUJ	1.110
46	FEZFAR	-19.011
47	FOPDOF	-6.474
48	FOSPOU	.406
49	FOZNOX	1.934
50	FUDGUH	-2.245
51	FUDHAO	13.143
52	FUDHIW	-4.575
53	FUDNEX	7.794
54	GABJIC	-8.619
55	GABJIC	.273
56	GECWUG	2.812
57	GIBWIY	3.690
58	GIJRAV	-3.169
59	GIMVON	-6.061
60	GINJUI	-4.729
61	GINJUI10	-4.729
62	GIZGAZ	7.688
63	GIZGON	2.509
64	HABMOP	-5.520
65	HEHDIH	-2.427
66	HEJQOE	29.751
67	HIJFUD	-4.084
68	HIJFUD	-4.371
69	HOCTAV	9.014
70	HOCTEZ	-6.321
71	HONHEA	2.399
72	HONHEA	5.835
73	HOSGAY	-.507
74	HOSGAY	.242

75	HOYPOB	-8.578
76	HUJCUK	-5.124
77	HULSOW	-4.601
78	HULSOW	4.634
79	HXPAUP	-5.166
80	HXPAUP	10.918
81	ICUKAS	-3.658
82	IDATAJ	4.023
83	IDUYEN	1.750
84	IFAVUG	-3.355
85	IFAVUG	4.246
86	IFIZAA	-1.312
87	IHUTUA	1.442
88	IRASEA	-8.420
89	IRAYIJ	3.169
90	IRAYIJ	4.856
91	JAJDUT	.217
92	JASCOY01	-5.819
93	JAYLEA	-3.209
94	JAYLIE	-6.285
95	JAYLOK	-7.061
96	JITZIV	.495
97	JOCSAV	2.057
98	JOFWUY	.877
99	JOFXAF	1.145
100	JOFXEJ	.755
101	JOFXIN	.741
102	JOFXOT	.623
103	JOFXUZ	.591
104	JOFYAG	3.879
105	JOFYAG	8.253
106	JOFYEK	2.464
107	JOGKEX	-1.307
108	JOGKIB	1.101
109	JOGKOH	-2.122
110	JOGKUN	1.723
111	JOGLAU	-2.551
112	JOGLAU	.221
113	JOGLEY	-.595
114	JOGLOI	-1.275
115	JOMREL	2.723
116	JOMRIP	7.915
117	JOMRIP	8.617
118	JOMVAL	-1.423
119	KAHDIF10	-3.060
120	KASWUW	-.348
121	KAXHUM	3.811
122	KAYHOI	-.770
123	KEHLIS	2.809

124	KEHLOY	.365
125	KEYVOZ	28.022
126	KEYVOZ	9.925
127	KEYVOZ10	28.022
128	KEYVOZ10	9.925
129	KOBIW	1.156
130	KOCRIF	2.896
131	KOCRUR	.000
132	KOXVOI	-4.074
133	KUJHIH	1.528
134	KUJHON	8.573
135	KUJHUT	9.118
136	KULJOS	4.925
137	KUPVAT	-3.029
138	KUPVEX	4.382
139	KUPVIB	-3.592
140	KUPVOH	.465
141	LAHQER	-.402
142	LAHQER	.181
143	LAXVEO	-.643
144	LEXGUR	-2.837
145	LEXGUR	-8.349
146	MAFCPR10	-2.883
147	MAQPUQ	-1.984
148	MAQQAX	3.597
149	MAQQEB	-1.566
150	MAQQIF	7.276
151	MAQQOL	-4.751
152	MAWREI	4.163
153	MAWRIM	2.870
154	MESJAV	2.914
155	MOJHOI	9.856
156	MOJHUO	1.847
157	MOKLED	1.438
158	MOPFUS	-6.390
159	MUCWIS	8.472
160	MXCPDL	3.883
161	MXCPDL	7.475
162	MXCPDN	-3.503
163	NACTOB	-2.921
164	NACTUH	4.886
165	NACVAP	-1.875
166	NACVAP	6.402
167	NACVAP	-2.946
168	NACVAP	-3.528
169	NAVBIY	-.608
170	NICTID	-3.388
171	NICTID	7.379
172	NIGCOV	8.182

173	NITMAF	-2.258
174	NOGGUN	-.770
175	NOLHOO	-8.142
176	NULKIQ	7.792
177	OBIGIR	-2.269
178	OBIGIR01	-6.735
179	OBOLIB	-.372
180	ODUKON	-5.978
181	OHIWAD	-.858
182	OYISEW	.241
183	PETBIZ	2.795
184	POSCEI	.508
185	POTNEU	3.261
186	POTNIY	-2.647
187	POTNOE	-3.273
188	POTNUK	5.263
189	POTNUK	-8.712
190	POTPAS	-13.430
191	POTVAY	-26.184
192	POTVAY	21.354
193	POTVAY	21.987
194	POTVAY	22.867
195	POVLOC	-11.930
196	POVLOC	-14.824
197	PUKRIW	1.005
198	PUNJIR	-5.390
199	PUNJOX	4.580
200	QOCHAT	4.792
201	QOCHEX	.223
202	QOCJEY	4.274
203	QOCJEY01	-4.024
204	QOCJEY02	3.423
205	QOCJID	-3.134
206	QOCJID	1.657
207	QOCKEB	.289
208	QOCKIF	-1.221
209	RABYAX	4.475
210	RABYEB	.146
211	RAVCOJ	-22.521
212	RAXDEB	-4.920
213	RAXDIF	-4.177
214	RAXDOL	5.833
215	REPMEF	9.087
216	REPMIJ	7.370
217	RIFKIA	-1.557
218	RIZWAA	-49.284
219	ROPGUY	2.649
220	RUKZAY	2.614
221	RUQREA	.321

222	RUQRIE	1.294
223	SEQVAL	4.503
224	SIDDAM	-16.329
225	SIYKES	-5.983
226	SIYKIW	-5.762
227	SOQCAC	-3.611
228	SOQCAC	-3.264
229	TEGXIN	-8.549
230	TEGXIN	-9.662
231	TEJXAK	5.107
232	TEXPIW	8.212
233	TICFIX	-.247
234	TICFUJ	-3.868
235	TIPJIN	1.760
236	TUWRAG	-.376
237	UDITAD	14.550
238	UDITIL	12.562
239	UDITOR	11.169
240	UJACEO	7.042
241	UJACOY	-6.050
242	UMUZOT	-1.578
243	URAJOO	-.666
244	URAJUU	-.472
245	URAKIJ	-.621
246	URAKOP	.437
247	URALIK	-.442
248	UVODUG	-3.307
249	UVODUG	-3.773
250	UZOFOG	-1.767
251	VAHHER	.337
252	VAHNOH	-4.126
253	VARPOT	4.195
254	VASSOX	-.406
255	VATTUF	.756
256	VIJFUP	5.313
257	VIQHEI	4.268
258	VIQHEI	4.463
259	VIQHEI	.880
260	VIQHIM	-3.335
261	VIQHIM	-5.857
262	VIQHIM	-3.285
263	VIQHIM	-5.615
264	VIRCEH	-4.194
265	VIRCEH	5.652
266	VIRCIL	6.060
267	VIRCIL	7.999
268	VIRCOR	8.771
269	VOCQUC	-.596
270	VOKWEX	-10.200

271	VOZXEP	10.236
272	VUWXUI	-11.026
273	WAWROB	11.882
274	WELQUB	-1.213
275	WELQUB	-1.266
276	WEQDED	13.418
277	WEQDIH	5.911
278	WIWKIW	-.400
279	WIWKIW	6.467
280	WOFXAR	4.822
281	WOFXEV	4.916
282	WOFXIZ	-4.136
283	WOFZAT	-.025
284	XALXEQ	.293
285	XALXIU	.595
286	XALXOA	-1.408
287	XAMJIE	-1.783
288	XAYGEM	-7.986
289	XEXHIS	-6.519
290	XICMOL	-5.110
291	XICMOL	-8.867
292	XICNAY	-2.287
293	XICNAY	-2.831
294	XICNAY	-3.147
295	XIGHUQ	-.942
296	XIMMAJ	-2.779
297	XIPQAR	3.664
298	XIWHER	-4.784
299	XOFXIZ	-13.521
300	XOPYEH	-3.564
301	XOSNEY	4.386
302	YABWAB	-3.857
303	YAWQOC	-4.756
304	YAWQUI	8.567
305	YEJWIU	-2.231
306	YIQWOK	.715
307	YOWYOZ	-.258
308	YUBKUD	-.311
309	YUBLAK	.150
310	YUBLEO	.563
311	YUSXOZ	3.751
312	YUSXOZ	-1.217
313	YUVGEB	-1.822
314	YUVGEB	.758
315	YUVGEB	-1.239
316	YUVGEB01	-1.822
317	YUVGEB01	.758
318	YUVGEB01	-1.239
319	YUWPAH	-2.619

320	YUWPAH	-10.051
321	ZAJROR	-.154
322	ZAJROR	-1.655
323	ZAJRUX	-2.634
324	ZAZXIH	-.690
325	ZEDWUC	6.496
326	ZEDXAJ	-6.087
327	ZEXFUD	-1.597
328	ZEXGAK	-1.800
329	ZOCBAU	1.222
330	ZOLDIN	.024
331	ZOMVEF	-6.676
332	ZUXSEQ	4.300
333	GUDDIV	-11.026
334	GUDDIV	-7.888
335	GUFROC	12.601
336	GUFROC	7.462
337	UHARUT	-3.473
338	PUTTOQ	-5.155
339	PUTTOQ	-9.387
340	YUHXOR	-.715
	Nobs	340
	Mean	.125
	SDSample	7.149
	SDMean	.388
	Minimum	-49.284
	Maximum	29.751

Table S3. CSD search of metallabenzenes.

Number of structures		123
Nfrag	Refcode	TOR M-C2-C3-C4
1	FOXTEU	1.037
2	NOWREZ	21.543
3	NOWRID	1.165
4	NOWROJ	1.637
5	NOWRUP	23.581
6	NOWSEA	1.137
7	NOWSOK	.067
8	NOWSUQ	.305
9	AKULAU	8.700
10	AYAMOE	.452
11	AYANAR	10.976
12	BEKVUK	178.703
13	BIXHIB	5.503
14	BIXHOH	17.767
15	BIXHUN	13.181
16	BIXJAV	9.147
17	BIXJEZ	9.898

18	BIXJOJ	6.962
19	BIXTUY	12.503
20	BIXVAG	2.154
21	COQNIH	1.213
22	COQNIH	4.765
23	ETASUO	1.706
24	ETATAV	3.836
25	ETATEZ	23.539
26	EVICAN	3.431
27	EVICAN	4.938
28	FEYVUC	.013
29	FIJPAR	9.369
30	FILVOM	1.410
31	FILWAZ	3.008
32	FILWED	1.204
33	GIFWEY	7.283
34	GIFWIC	6.893
35	GIFWOI	24.780
36	GIFWOI	23.759
37	GIXQIO	5.941
38	GIXQIO01	5.941
39	IHIXED	.033
40	IHIXIH	1.930
41	IHIXON	.147
42	IHIXUT	3.201
43	ILEZEE	19.953
44	ILEZII	30.040
45	ILEZII	30.522
46	IZOKOX	9.704
47	IZOKUD	1.789
48	JAMWID	8.270
49	JAMWID10	8.270
50	JEGGEI	6.867
51	JEGGIM	6.731
52	JEGGUY	5.571
53	JELSOJ	17.594
54	JOJTAF	18.299
55	JOJTEJ	16.841
56	JOJTIN	.247
57	JOQWOD	15.727
58	JUQMUD	2.191
59	KEHNUH	3.605
60	KEHPAP	20.642
61	KISHEA	1.557
62	KULJIM	.706
63	LIMKAT	3.966
64	LIMMID	5.613
65	MUXSEE	17.881
66	MUXSEE	20.992

67	MUXSII	.684
68	NIPZIV	4.396
69	NIPZOB	1.572
70	ODEFAG	3.655
71	ODEFEK	2.992
72	ODEFIO	5.533
73	OGOJAV	1.571
74	ONEPED	2.145
75	OYIZON	7.777
76	POMQAK	.818
77	PUXVEL	16.981
78	PUXVIP	11.031
79	QIHBUH	4.221
80	QIHCAO	8.858
81	QOYKAR	6.807
82	QOYKOF	4.923
83	QOYKUL	18.353
84	QOYLAS	7.212
85	QUGHUW	4.886
86	QUGJAE	1.771
87	QUGJAE	3.724
88	RESYOE	34.053
89	RESYUK	32.154
90	RIFCEO	1.942
91	RIFCEO	10.083
92	RUDVUI	10.741
93	RUHSET	5.204
94	SILTIS	2.176
95	TAFHOA	.177
96	TAFHUG	3.478
97	TAFJAO	1.649
98	TAFJES	2.642
99	TAFJIW	2.144
100	TAFJOC	.337
101	TECHIU	18.748
102	TECHOA	13.176
103	TECJAO	6.484
104	TECJIW	14.003
105	TIPJAF	5.678
106	TIPJEJ	6.748
107	TUXROU	13.940
108	TUXRUA	13.125
109	UDIPEE	4.385
110	UDIPII	10.555
111	UDIRAC	4.273
112	UDIRAC	5.143
113	UGIBOC	29.440
114	UGIBOC	29.476
115	UGIBOC	28.135

116	UGIBOC	29.290
117	UKIHAX	1.239
118	VOZXIT	31.383
119	VOZYEQ	34.244
120	VOZYIU	23.867
121	VOZYIU	27.380
122	VOZYIU	29.392
123	VOZYOA	39.251
124	VUGJUE	6.600
125	WEXTAW	3.843
126	WEXTEA	3.118
127	WOFZUN	7.593
128	WUSNAB	7.394
129	WUSNEF	4.468
130	YOTKOJ	.091
131	YOTLAW	8.895
132	ZIHTUH	5.450
133	ZIHVAP	28.112
134	ZIHVET	1.741
135	ZOWMUV	8.239
136	WUCYEB	21.304

Nobs	136
Mean	10.965
SDSample	17.370
SDMean	1.489
Minimum	.013
Maximum	178.703

Table S4. CSD search of bended metallacyclopentadienes M-C2-C3-C4 > 20°.

Number of structures 6		
Nfrag	Refcode	TOR1
2	HEJQOE	29.751
3	HXPAUP	23.748
4	KEYVOZ10	28.022
5	POTVAY	21.354
6	POTVAY	21.987
7	POTVAY	22.867
8	RAVCOJ	22.521
9	RIZWAA	49.284

Nobs	9
Mean	26.505
SDSample	9.162
SDMean	3.054
Minimum	19.011
Maximum	49.284

Table S5. CSD search of bended metallabenzenes M-C2-C3-C4 > 20°.

Number of structures 18

Nfrag	Refcode	TOR1
1	NOWREZ	21.543
2	NOWRUP	23.581
3	ETATEZ	23.539
4	GIFWOI	24.780
5	GIFWOI	23.759
6	ILEZEE	25.585
7	ILEZII	30.040
8	ILEZII	30.522
9	KEHPAP	20.642
10	MUXSEE	20.992
11	QOYKUL	25.853
12	RESYOE	34.053
13	RESYUK	32.154
14	UGIBOC	29.440
15	UGIBOC	29.476
16	UGIBOC	28.135
17	UGIBOC	29.290
18	VOZXIT	31.383
19	VOZYEQ	34.244
20	VOZYIU	23.867
21	VOZYIU	27.380
22	VOZYIU	29.392
23	VOZYOA	39.251
24	ZIHVAP	28.112
25	WUCYEB	21.304

Nobs	25
Mean	27.533
SDSample	4.696
SDMean	.939
Minimum	20.642
Maximum	39.251

Table S6. CSD search of 16e d⁸ metallacyclopentadienes.

Number of structures 30

Nfrag	Refcode	DIST M-C2
1	DUGHAQ	2.071
2	DUGHEU	2.039
3	GIBWIY	2.060
4	IDATAJ	2.053
5	IFAVUG	2.024
6	IFAVUG	2.029
7	IHUTUA	2.041
8	KASWUW	2.020
9	LAXVEO	2.007
10	MAQPUQ	1.986

11	MAQQAX	2.002
12	MAQQEB	2.019
13	MAQQIF	2.047
14	MAQQOL	2.037
15	MAWREI	2.040
16	MAWRIM	2.013
17	MOPFUS	2.000
18	MXCPDL	1.985
19	MXCPDL	1.981
20	NACTOB	2.009
21	NACTUH	2.066
22	NACVAP	1.977
23	NACVAP	2.004
24	NACVAP	1.991
25	NACVAP	2.004
26	NOLHOO	2.079
27	NULKIQ	2.030
28	PUNJIR	2.008
29	PUNJOX	2.024
30	SIDDAM	1.977
31	UZOFOG	2.020
32	WIWKIW	2.000
33	WIWKIW	2.041
34	XIGHUQ	2.078
35	YABWAB	2.073
36	ZOMVEF	2.065

Nobs	36
Mean	2.025
SDSample	.030
SDMean	.005
Minimum	1.977
Maximum	2.079

Table S7. CSD search of 16e d⁰ metallacyclopentadienes.

Number of structures		94
Nfrag	Refcode	DIST1
1	AJEBAU	2.280
2	AJOGIP	2.241
3	AJOGOV	2.278
4	ASASIX	2.271
5	BODQUG	2.162
6	CEQFEJ	2.245
7	CPPHZR	2.249
8	CPTPHF	2.190
9	CPTPTI	2.141
10	DAVZIJ	2.282
11	EFIPUE	2.192
12	EFIPUE	2.207

13	FEZDUJ	2.204
14	FEZDUJ	2.211
15	FEZFAR	2.217
16	FOPDOF	2.139
17	FUDGUH	2.270
18	FUDHAO	2.253
19	FUDHIW	2.231
20	GABJIC	2.250
21	GABJIC	2.260
22	GECWUG	2.215
23	GIJRAV	2.288
24	HEJQOE	2.242
25	HIJFUD	2.248
26	HIJFUD	2.252
27	HOCTAV	2.267
28	HOCTEZ	2.221
29	HOYPOB	2.327
30	ICUKAS	2.270
31	IDUYEN	2.264
32	IFIZAA	2.250
33	JAYLEA	2.310
34	JAYLIE	2.324
35	JAYLOK	2.290
36	KAYHOI	2.157
37	KEHLIS	2.264
38	KEHLOY	2.245
39	KOBIW	2.250
40	KOCRIF	2.259
41	KOCRUR	2.255
42	KUJHIH	2.241
43	KUJHON	2.257
44	KUJHUT	2.222
45	MOKLED	2.259
46	NIGCOV	2.159
47	OBIGIR	2.279
48	OBIGIR01	2.271
49	OBOLIB	2.240
50	ODUKON	2.236
51	POSCEI	2.146
52	POTNEU	2.253
53	POTNIY	2.270
54	POTNOE	2.268
55	POTNUK	2.247
56	POTNUK	2.245
57	POTPAS	2.268
58	POTVAY	2.249
59	POTVAY	2.255
60	POTVAY	2.265
61	POTVAY	2.266

62	POVLOC	2.264
63	POVLOC	2.277
64	PUKRIW	2.254
65	QOCHAT	2.234
66	QOCHEX	2.225
67	QOCJID	2.242
68	QOCJID	2.247
69	RAVCOJ	2.235
70	RIZWAA	2.134
71	SOQCAC	2.264
72	SOQCAC	2.251
73	TEXPIW	2.244
74	UJACEO	2.269
75	UJACOY	2.301
76	UVODUG	2.258
77	UVODUG	2.267
78	VAHNOH	2.160
79	VARPOT	2.271
80	VASSOX	2.240
81	VIQHEI	2.265
82	VIQHEI	2.255
83	VIQHEI	2.269
84	VIQHIM	2.221
85	VIQHIM	2.264
86	VIQHIM	2.228
87	VIQHIM	2.261
88	VOCQUC	2.263
89	WAWROB	2.171
90	WOFXAR	2.249
91	WOFXEV	2.271
92	WOFXIZ	2.239
93	WOFZAT	2.235
94	XICMOL	2.263
95	XICMOL	2.254
96	XICNAY	2.271
97	XICNAY	2.249
98	XICNAY	2.250
99	XIPQAR	2.145
100	XIWHER	2.275
101	XOSNEY	2.279
102	YAWQOC	2.245
103	YAWQUI	2.251
104	YIQWOK	2.241
105	YOWYOZ	2.257
106	YUVGEB	2.248
107	YUVGEB	2.238
108	YUVGEB	2.245
109	YUVGEB01	2.248
110	YUVGEB01	2.238

111	YUVGEB01	2.245
112	YUWPAH	2.241
113	YUWPAH	2.247
114	ZAJROR	2.257
115	ZAJROR	2.228
116	ZAJRUX	2.197
117	ZOCBAU	2.148
118	ZOLDIN	2.157
119	GUFLOC	2.238
120	GUFLOC	2.242
121	PUTTOQ	2.280
122	PUTTOQ	2.288

Nobs	122
Mean	2.243
SDSample	.038
SDMean	.003
Minimum	2.134
Maximum	2.327