

Supporting Information for:

**Chemical Bonding in Transition Metal Complexes with Beryllium
Ligands $[(\text{PMe}_3)_2\text{M}-\text{BeCl}_2]$, $[(\text{PMe}_3)_2\text{M}-\text{BeClMe}]$ and $[(\text{PMe}_3)_2\text{M}-\text{BeMe}_2]$ (M = Ni, Pd, Pt)**

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Table S1: Optimized coordinates and energies (kcal/mol) of **1M-3M** at BP86/TZ2P. Nimg is the number of imaginary frequencies

1Ni (C_{2v})

Nimg = 0

E = -3356.15

P	0.000000	-2.154599	-0.768539
P	0.000000	2.154599	-0.768539
C	0.000000	-2.825029	-2.501036
H	0.000000	-3.924944	-2.485067
H	-0.891693	-2.473982	-3.037161
H	0.891693	-2.473982	-3.037161
C	-1.440703	-3.043075	-0.033031
H	-1.329200	-4.129928	-0.156206
H	-1.522737	-2.792492	1.032378
H	-2.362379	-2.709405	-0.527845
C	1.440703	-3.043075	-0.033031
H	1.329200	-4.129928	-0.156206
H	2.362379	-2.709405	-0.527845
H	1.522737	-2.792492	1.032378
C	0.000000	2.825029	-2.501036
H	-0.891693	2.473982	-3.037161
H	0.000000	3.924944	-2.485067
H	0.891693	2.473982	-3.037161
C	-1.440703	3.043075	-0.033031
H	-1.522737	2.792492	1.032378
H	-1.329200	4.129928	-0.156206
H	-2.362379	2.709405	-0.527845
C	1.440703	3.043075	-0.033031
H	2.362379	2.709405	-0.527845
H	1.329200	4.129928	-0.156206
H	1.522737	2.792492	1.032378
Ni	0.000000	0.000000	-0.701026
Be	0.000000	0.000000	1.392960
Cl	1.720705	0.000000	2.189498
Cl	-1.720705	0.000000	2.189498

1Pd (C_{2v})

Nimg = 0

E = -3336.84

P	0.000000	2.314074	-0.684591
P	0.000000	-2.314074	-0.684591
C	0.000000	3.019675	-2.397845
H	0.000000	4.119134	-2.366459
H	0.890829	2.674841	-2.939329
H	-0.890829	2.674841	-2.939329
C	1.438123	3.179545	0.077458
H	1.331886	4.270121	-0.015432
H	1.514870	2.900683	1.136613
H	2.360991	2.855908	-0.421786

C	-1.438123	3.179545	0.077458
H	-1.331886	4.270121	-0.015432
H	-2.360991	2.855908	-0.421786
H	-1.514870	2.900683	1.136613
C	0.000000	-3.019675	-2.397845
H	0.890829	-2.674841	-2.939329
H	0.000000	-4.119134	-2.366459
H	-0.890829	-2.674841	-2.939329
C	1.438123	-3.179545	0.077458
H	1.514870	-2.900683	1.136613
H	1.331886	-4.270121	-0.015432
H	2.360991	-2.855908	-0.421786
C	-1.438123	-3.179545	0.077458
H	-2.360991	-2.855908	-0.421786
H	-1.331886	-4.270121	-0.015432
H	-1.514870	-2.900683	1.136613
Pd	0.000000	0.000000	-0.650253
Be	0.000000	0.000000	1.544254
Cl	-1.711766	0.000000	2.359037
Cl	1.711766	0.000000	2.359037

1Pt(C_{2v})

Nimg = 0

E = -3397.49

P	0.000000	-2.290178	-0.577526
P	0.000000	2.290178	-0.577526
C	0.000000	-2.975178	-2.293960
H	0.000000	-4.074644	-2.268478
H	-0.891690	-2.626256	-2.831498
H	0.891690	-2.626256	-2.831498
C	-1.441461	-3.137634	0.189730
H	-1.338621	-4.228963	0.104435
H	-1.514704	-2.849369	1.246909
H	-2.362340	-2.812518	-0.312135
C	1.441461	-3.137634	0.189730
H	1.338621	-4.228963	0.104435
H	2.362340	-2.812518	-0.312135
H	1.514704	-2.849369	1.246909
C	0.000000	2.975178	-2.293960
H	-0.891690	2.626256	-2.831498
H	0.000000	4.074644	-2.268478
H	0.891690	2.626256	-2.831498
C	-1.441461	3.137634	0.189730
H	-1.514704	2.849369	1.246909
H	-1.338621	4.228963	0.104435
H	-2.362340	2.812518	-0.312135
C	1.441461	3.137634	0.189730
H	2.362340	2.812518	-0.312135
H	1.338621	4.228963	0.104435

H	1.514704	2.849369	1.246909
Pt	0.000000	0.000000	-0.505536
Be	0.000000	0.000000	1.691502
Cl	1.708337	0.000000	2.528532
Cl	-1.708337	0.000000	2.528532

2Ni (C_s)

Nimg = 0

E = -3720.73

P	0.627053	-0.022031	-2.146686
P	0.627053	-0.022031	2.146686
C	2.298997	-0.500857	-2.801194
H	2.297473	-0.501090	-3.901367
H	3.057080	0.207817	-2.442113
H	2.562472	-1.504520	-2.441881
C	0.329420	1.560282	-3.056443
H	0.445937	1.413634	-4.140050
H	-0.684145	1.921528	-2.840293
H	1.043093	2.320346	-2.712093
C	-0.464812	-1.198560	-3.060307
H	-0.290085	-1.127910	-4.143684
H	-0.259765	-2.222014	-2.719937
H	-1.515579	-0.976715	-2.833667
C	2.298997	-0.500857	2.801194
H	3.057080	0.207817	2.442113
H	2.297473	-0.501090	3.901367
H	2.562472	-1.504520	2.441881
C	0.329420	1.560282	3.056443
H	-0.684145	1.921528	2.840293
H	0.445937	1.413634	4.140050
H	1.043093	2.320346	2.712093
C	-0.464812	-1.198560	3.060307
H	-0.259765	-2.222014	2.719937
H	-0.290085	-1.127910	4.143684
H	-1.515579	-0.976715	2.833667
Ni	0.520062	0.007868	0.000000
Be	-1.527917	0.553380	0.000000
Cl	-2.637666	-0.995767	0.000000
C	-1.860392	2.250984	0.000000
H	-0.990883	2.924191	0.000000
H	-2.474987	2.514393	-0.878845
H	-2.474987	2.514393	0.878845

2Pd (C_s)

Nimg = 1(i74.3cm⁻¹)

E = -3700.85

P	0.566678	-0.046929	-2.309079
P	0.566678	-0.046929	2.309079
C	2.213729	-0.557691	-2.988952
H	2.195732	-0.566147	-4.088989

H	2.989015	0.140306	-2.646255
H	2.467077	-1.562204	-2.625062
C	0.277628	1.530155	-3.226314
H	0.399196	1.380811	-4.309146
H	-0.737527	1.892546	-3.019311
H	0.989013	2.291252	-2.879691
C	-0.564802	-1.207404	-3.189469
H	-0.419373	-1.144176	-4.277843
H	-0.367245	-2.232975	-2.850981
H	-1.605943	-0.967822	-2.936682
C	2.213729	-0.557691	2.988952
H	2.989015	0.140306	2.646255
H	2.195732	-0.566147	4.088989
H	2.467077	-1.562204	2.625062
C	0.277628	1.530155	3.226314
H	-0.737527	1.892546	3.019311
H	0.399196	1.380811	4.309146
H	0.989013	2.291252	2.879691
C	-0.564802	-1.207404	3.189469
H	-0.367245	-2.232975	2.850981
H	-0.419373	-1.144176	4.277843
H	-1.605943	-0.967822	2.936682
Pd	0.477795	0.000203	0.000000
Be	-1.677250	0.621226	0.000000
Cl	-2.819213	-0.905630	0.000000
C	-1.989929	2.323033	0.000000
H	-3.077176	2.511117	0.000000
H	-1.574315	2.845788	0.876498
H	-1.574315	2.845788	-0.876498

2Pt(C_s)

Nimg = 1(i72.5 cm⁻¹)

E = -3761.02

P	0.593803000	-0.065074000	-2.281023000
P	0.593803000	-0.065074000	2.281023000
C	2.253842000	-0.569840000	-2.919977000
H	2.253267000	-0.595326000	-4.019591000
H	3.015299000	0.141845000	-2.574242000
H	2.507725000	-1.566332000	-2.534853000
C	0.291566000	1.504117000	-3.198911000
H	0.419758000	1.351672000	-4.280275000
H	-0.729015000	1.853688000	-2.995864000
H	0.993099000	2.273219000	-2.849917000
C	-0.530100000	-1.249753000	-3.130797000
H	-0.392116000	-1.201775000	-4.220617000
H	-0.318676000	-2.266782000	-2.775347000
H	-1.571118000	-1.014527000	-2.872045000
C	2.253842000	-0.569840000	2.919977000
H	3.015299000	0.141845000	2.574242000
H	2.253267000	-0.595326000	4.019591000

H	2.507725000	-1.566332000	2.534853000
C	0.291566000	1.504117000	3.198911000
H	-0.729015000	1.853688000	2.995864000
H	0.419758000	1.351672000	4.280275000
H	0.993099000	2.273219000	2.849917000
C	-0.530100000	-1.249753000	3.130797000
H	-0.318676000	-2.266782000	2.775347000
H	-0.392116000	-1.201775000	4.220617000
H	-1.571118000	-1.014527000	2.872045000
Pt	0.482751000	0.001317000	0.000000000
Be	-1.671907000	0.622197000	0.000000000
Cl	-2.853253000	-0.887641000	0.000000000
C	-2.013350000	2.323920000	0.000000000
H	-3.103699000	2.492870000	0.000000000
H	-1.606284000	2.854617000	0.876278000
H	-1.606284000	2.854617000	-0.876278000

3Ni (C_{2v})

Nimg = 0

E = -4082.97

P	0.000000	2.137279	-0.436663
P	0.000000	-2.137279	-0.436663
C	0.000000	2.787322	-2.177754
H	0.000000	3.887725	-2.181501
H	0.890725	2.424790	-2.707898
H	-0.890725	2.424790	-2.707898
C	1.431641	3.067408	0.278551
H	1.315845	4.149135	0.116634
H	1.501663	2.860239	1.354159
H	2.361874	2.725209	-0.193847
C	-1.431641	3.067408	0.278551
H	-1.315845	4.149135	0.116634
H	-2.361874	2.725209	-0.193847
H	-1.501663	2.860239	1.354159
C	0.000000	-2.787322	-2.177754
H	0.890725	-2.424790	-2.707898
H	0.000000	-3.887725	-2.181501
H	-0.890725	-2.424790	-2.707898
C	1.431641	-3.067408	0.278551
H	1.501663	-2.860239	1.354159
H	1.315845	-4.149135	0.116634
H	2.361874	-2.725209	-0.193847
C	-1.431641	-3.067408	0.278551
H	-2.361874	-2.725209	-0.193847
H	-1.315845	-4.149135	0.116634
H	-1.501663	-2.860239	1.354159
Ni	0.000000	0.000000	-0.279782
Be	0.000000	0.000000	1.868557
C	1.626389	0.000000	2.473568
H	2.448061	0.000000	1.742278
H	1.780291	0.879090	3.126439

H	1.780291	-0.879090	3.126439
C	-1.626389	0.000000	2.473568
H	-1.780291	0.879090	3.126439
H	-2.448061	0.000000	1.742278
H	-1.780291	-0.879090	3.126439

3Pd(C_{2v})

Nimg = 2 (i94.4, i86.9 cm⁻¹)

E = -4062.34

P	0.000000	-2.299689	-0.413825
P	0.000000	2.299689	-0.413825
C	0.000000	-2.944895	-2.152296
H	0.000000	-4.045310	-2.162282
H	-0.889920	-2.578779	-2.681110
H	0.889920	-2.578779	-2.681110
C	-1.426691	-3.233175	0.300718
H	-1.319402	-4.312897	0.119378
H	-1.481167	-3.047424	1.381276
H	-2.361202	-2.877460	-0.152809
C	1.426691	-3.233175	0.300718
H	1.319402	-4.312897	0.119378
H	2.361202	-2.877460	-0.152809
H	1.481167	-3.047424	1.381276
C	0.000000	2.944895	-2.152296
H	-0.889920	2.578779	-2.681110
H	0.000000	4.045310	-2.162282
H	0.889920	2.578779	-2.681110
C	-1.426691	3.233175	0.300718
H	-1.481167	3.047424	1.381276
H	-1.319402	4.312897	0.119378
H	-2.361202	2.877460	-0.152809
C	1.426691	3.233175	0.300718
H	2.361202	2.877460	-0.152809
H	1.319402	4.312897	0.119378
H	1.481167	3.047424	1.381276
Pd	0.000000	0.000000	-0.248731
Be	0.000000	0.000000	2.054366
C	-1.633074	0.000000	2.644531
H	-1.636221	0.000000	3.750157
H	-2.223196	0.876021	2.328919
H	-2.223196	-0.876021	2.328919
C	1.633074	0.000000	2.644531
H	2.223196	-0.876021	2.328919
H	2.223196	0.876021	2.328919
H	1.636221	0.000000	3.750157

3Pt(C_{2v})

Nimg = 2 (i99.0, i89.1 cm⁻¹)

E = -4121.64

P	0.000000	-2.273894	-0.432657
P	0.000000	2.273894	-0.432657
C	0.000000	-2.908415	-2.169998

H	0.000000	-4.008501	-2.179853
H	-0.890898	-2.540606	-2.696077
H	0.890898	-2.540606	-2.696077
C	-1.432194	-3.179021	0.295370
H	-1.333496	-4.261606	0.128867
H	-1.481816	-2.974855	1.372881
H	-2.362703	-2.819390	-0.163158
C	1.432194	-3.179021	0.295370
H	1.333496	-4.261606	0.128867
H	2.362703	-2.819390	-0.163158
H	1.481816	-2.974855	1.372881
C	0.000000	2.908415	-2.169998
H	-0.890898	2.540606	-2.696077
H	0.000000	4.008501	-2.179853
H	0.890898	2.540606	-2.696077
C	-1.432194	3.179021	0.295370
H	-1.481816	2.974855	1.372881
H	-1.333496	4.261606	0.128867
H	-2.362703	2.819390	-0.163158
C	1.432194	3.179021	0.295370
H	2.362703	2.819390	-0.163158
H	1.333496	4.261606	0.128867
H	1.481816	2.974855	1.372881
Pt	0.000000	0.000000	-0.280889
Be	0.000000	0.000000	2.008504
C	-1.620830	0.000000	2.652964
H	-1.586217	0.000000	3.758128
H	-2.223126	0.875178	2.357283
H	-2.223126	-0.875178	2.357283
C	1.620830	0.000000	2.652964
H	2.223126	-0.875178	2.357283
H	2.223126	0.875178	2.357283
H	1.586217	0.000000	3.758128