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Supporting Information for:

Beryllium Chemistry the Safe Way: A Theoretical Evaluation of Low Oxidation State Beryllium Compounds

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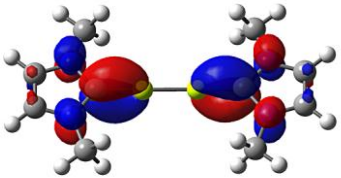
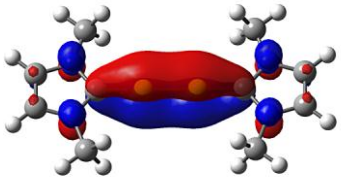
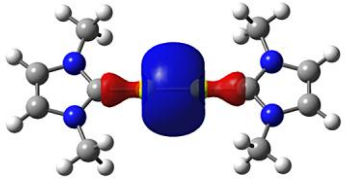
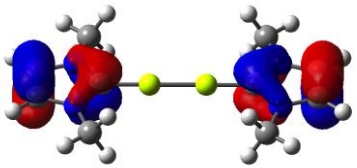
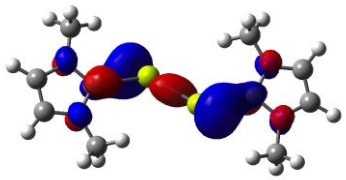
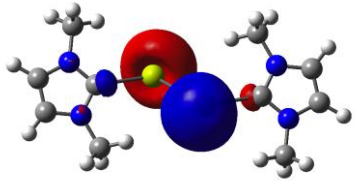
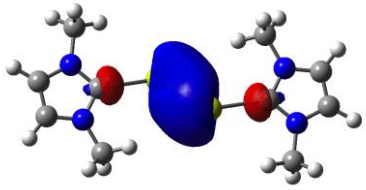
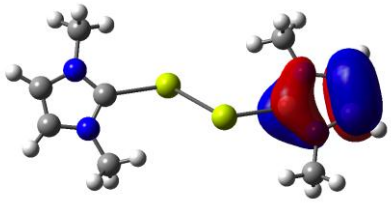
(i) L = NHC^{Me}

	LUMO	**HOMO**	**HOMO-1**	**HOMO-2**
Be				
Mg				

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(ii) L = NHC^{Ph}

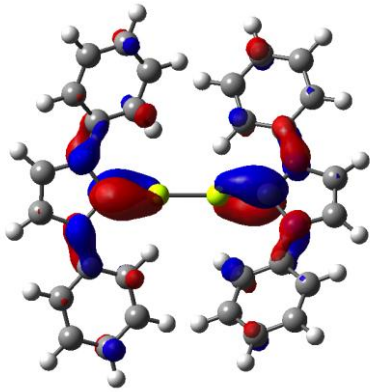
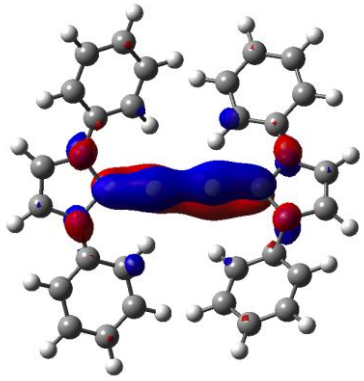
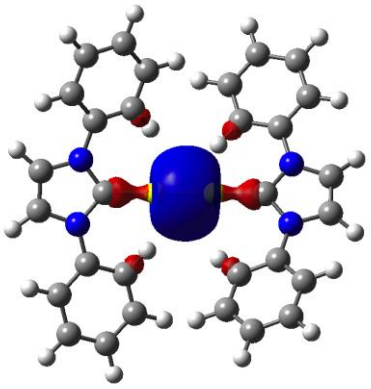
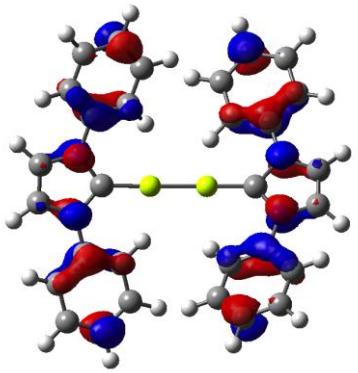
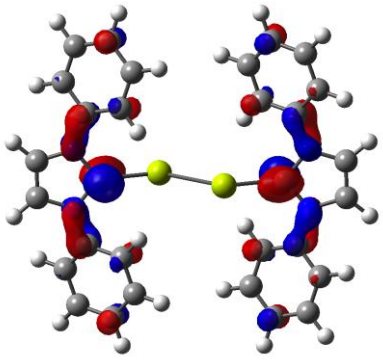
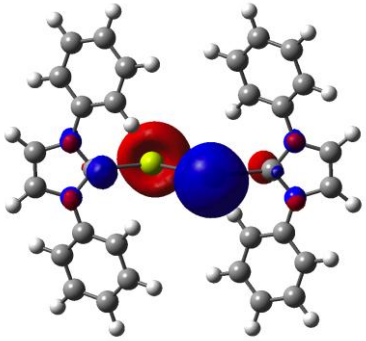
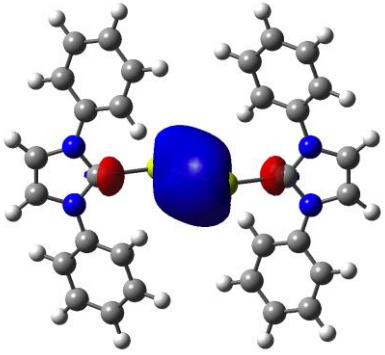
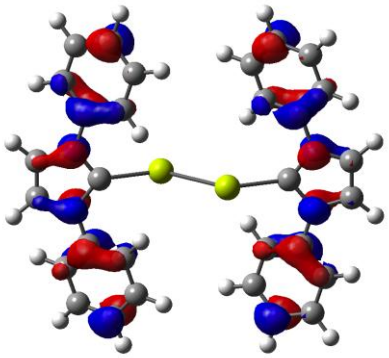
E	LUMO	HOMO	HOMO-1	HOMO-2
Be				
Mg				

Table S2. B3LYP/def2-TZVPP frontier molecular orbitals for L_2-EE-L_2 (**3E^{R}**, E = Be, Mg; L = NHC^{R}; R = Me, Ph).

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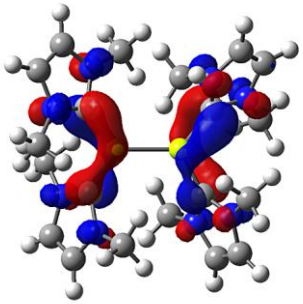
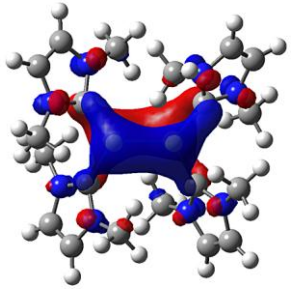
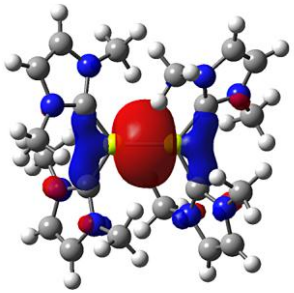
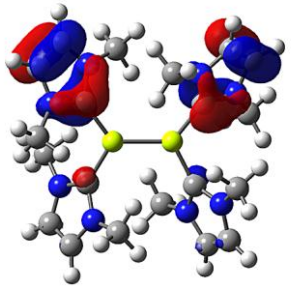
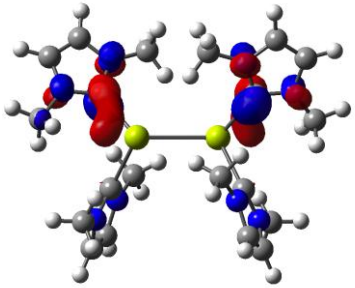
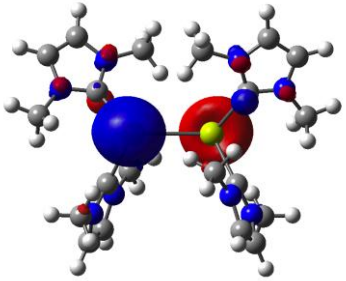
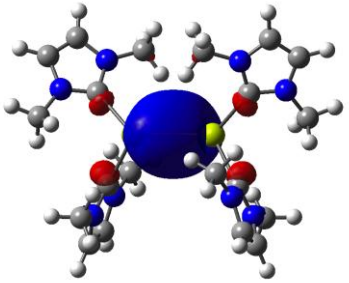
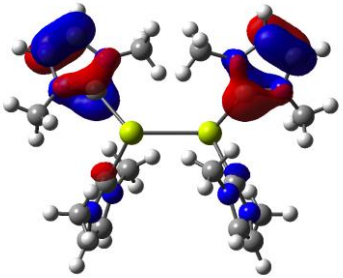
(i) L = NHC^{Me}

	LUMO	HOMO	HOMO-1	HOMO-2
Be				
Mg				

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(ii) L = NHC^{Ph}

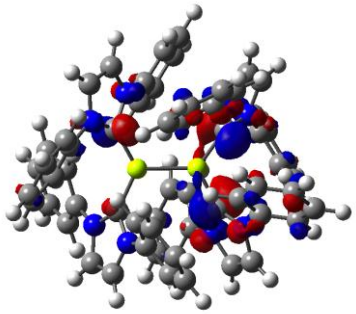
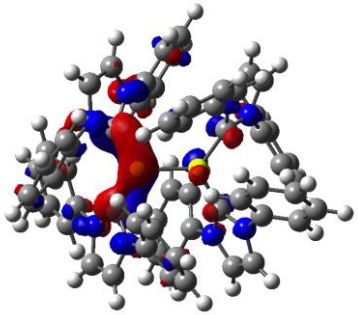
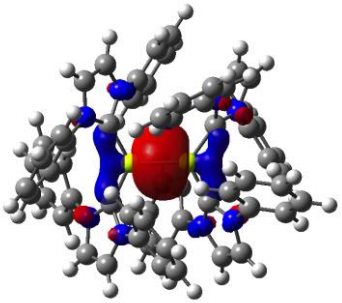
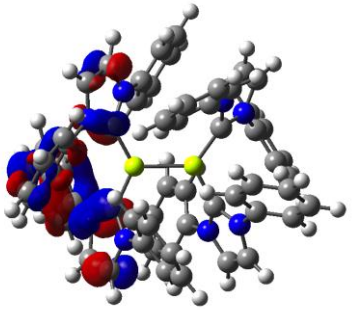
	LUMO	HOMO	HOMO-1	HOMO-2
Be				

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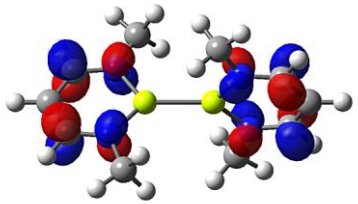
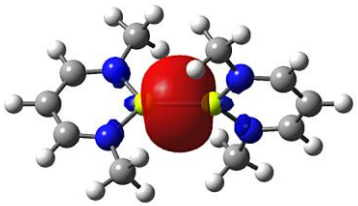
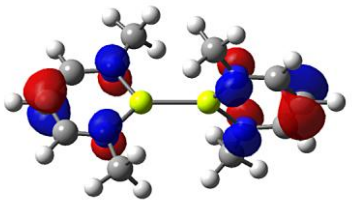
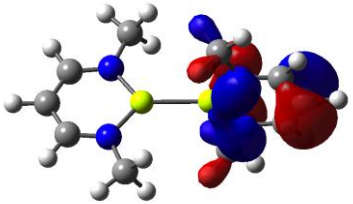
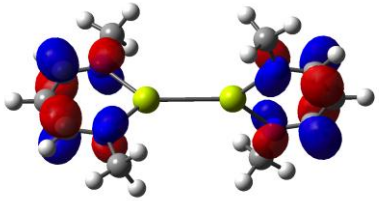
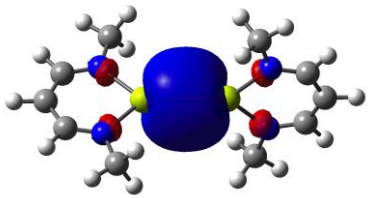
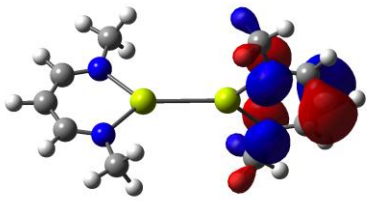
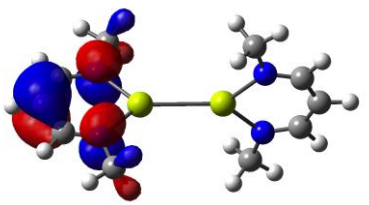
Table S3. B3LYP/def2-TZVPP frontier molecular orbitals for L-EE-L (**1E^{R}**, E = Be, Mg; L = Nac^{R}; R = Me, Ph)

(i) L = Nac^{Me}

	LUMO	HOMO	HOMO-1	HOMO-2
Be				
Mg				

(ii) L = Nac^{Ph}

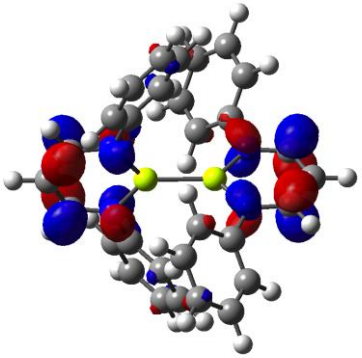
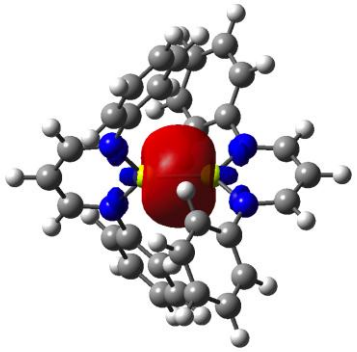
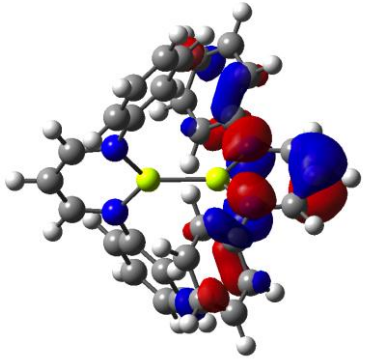
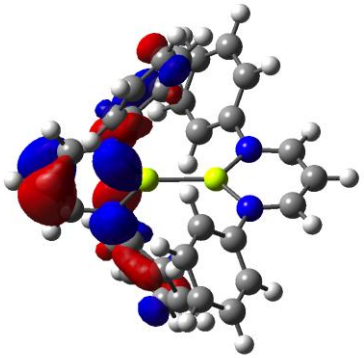
	LUMO	HOMO	HOMO-1	HOMO-2
Be				

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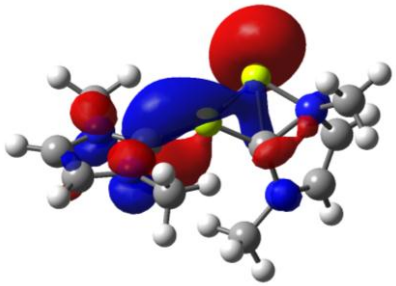
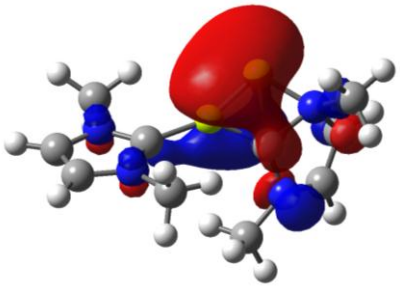
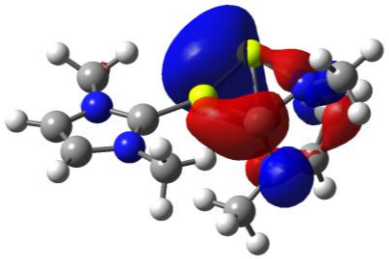
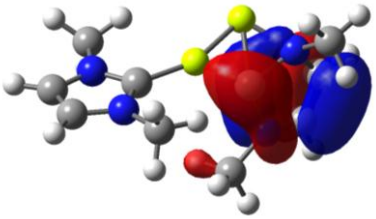
Table S4. B3LYP/def2-TZVPP frontier molecular orbitals for *bridged* L-EE-L (**2Be^{R}(B)**; L = NHC^{R}; R = Me, Ph)

(i) L = NHC^{Me}

	LUMO	**HOMO**	**HOMO-1**	**HOMO-2**
Be				

(ii) L = NHC^{Ph}

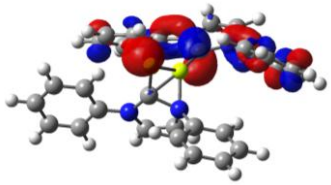
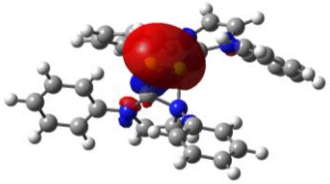
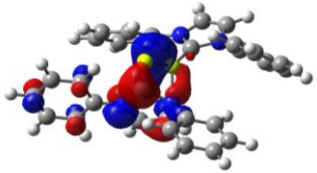
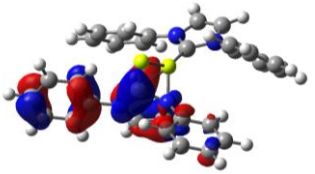
	LUMO	**HOMO**	**HOMO-1**	**HOMO-2**
Be				

Table S5. B3LYP/def2-TZVPP frontier molecular orbitals for *bridged* L_2-EE-L_2 (**3Be^{R}(B)**; L = NHC^{R}; R = Me, Ph)

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(i) L = NHC^{Me}

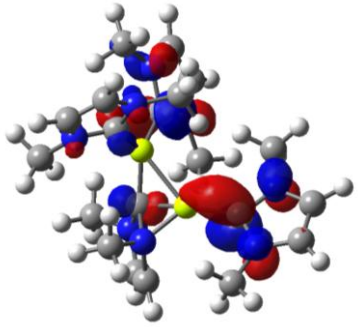
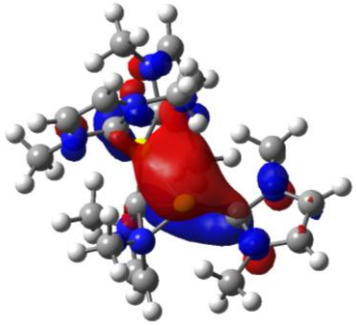
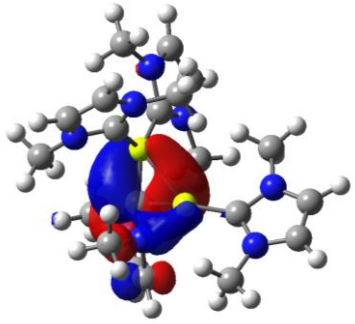
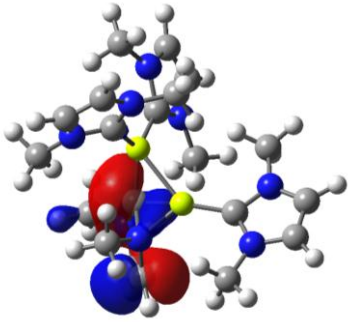
	LUMO	HOMO	HOMO-1	HOMO-2
Be				

Table S6. B3LYP/def2-TZVPP frontier molecular orbitals for E-L_3 (**4Be^{R}**; L = NHC^{R}; R = Me, Ph)

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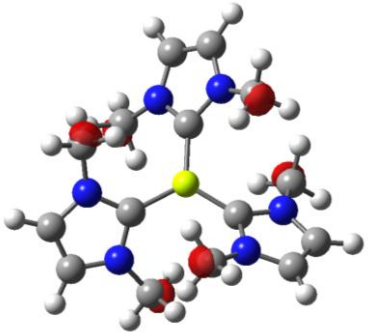
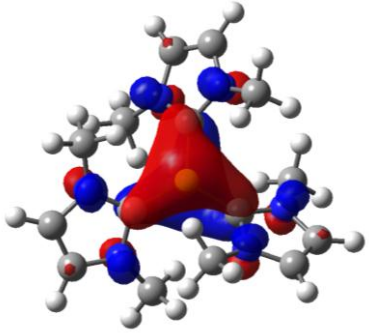
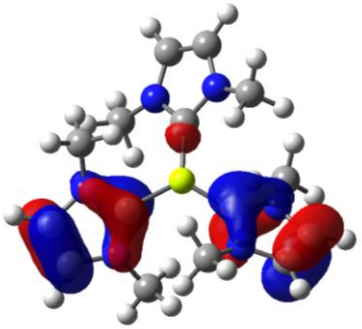
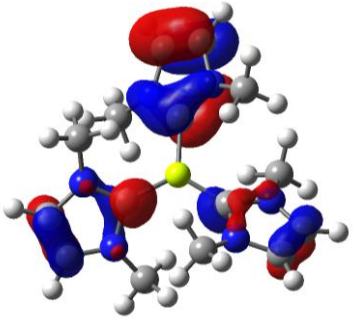
(i) L = NHC^{Me}

	LUMO	HOMO	HOMO-1	HOMO-2
Be				

(ii) L = NHC^{Ph}

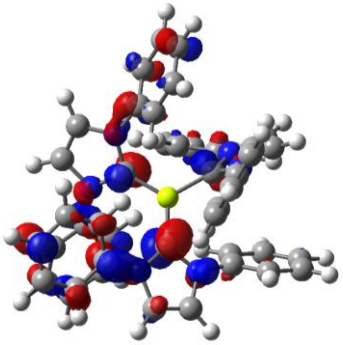
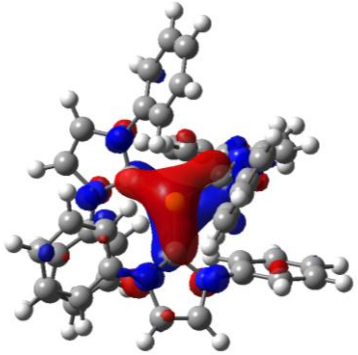
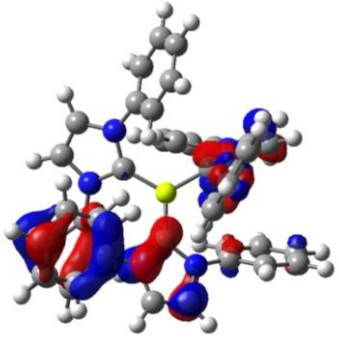
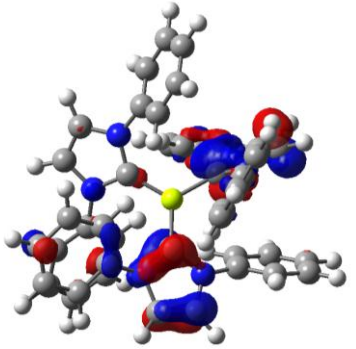
	LUMO	HOMO	HOMO-1	HOMO-2
Be				

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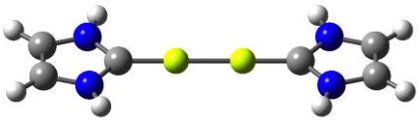
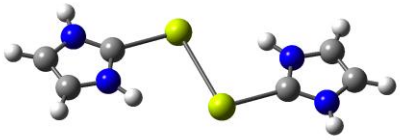
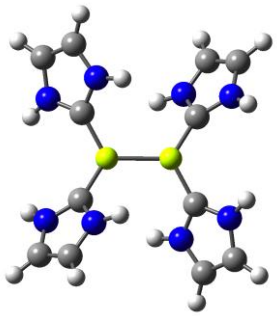
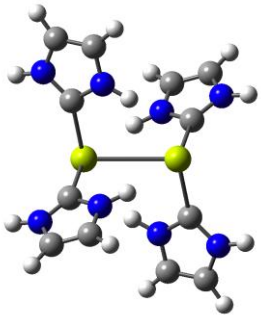
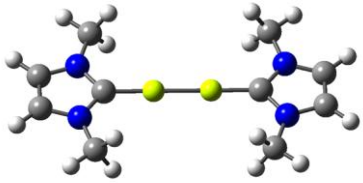
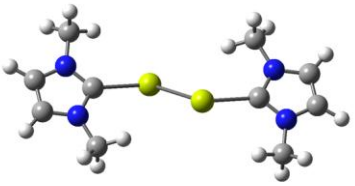
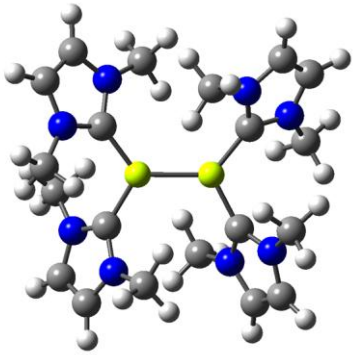
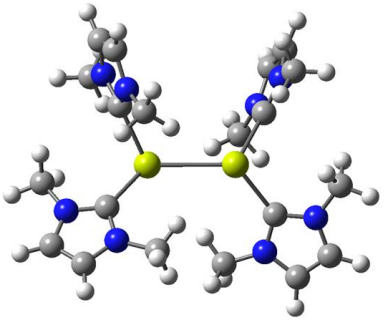
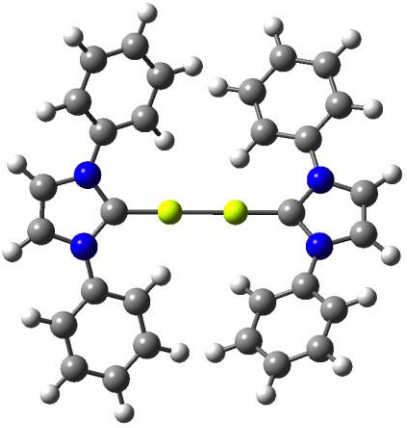
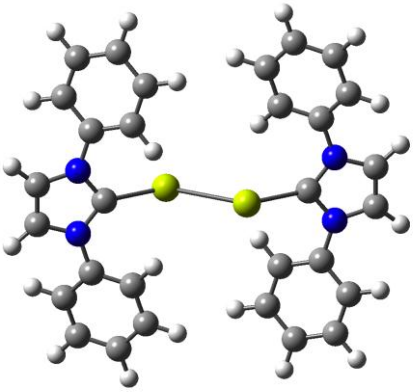
Table S7. B3LYP/def2-TZVPP optimised geometries of L-EE-L compounds **1E^{R}**, **2E^{R}**, **3E^{R}** (E = Be, Mg; L = NHC^{R}, Nac^{R}; R = H, Me, Ph).

Ligand	Be	Mg
NHC^{H}		
NHC^{H}		
NHC^{Me}		
NHC^{Me}		
NHC^{Ph}		

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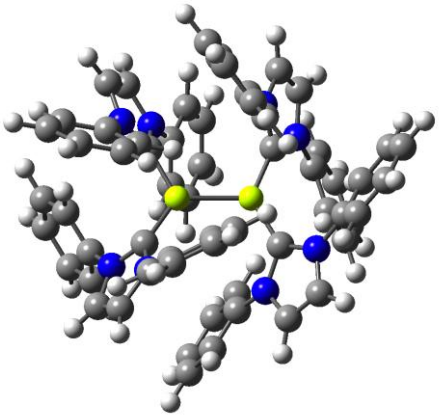
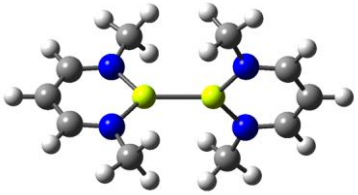
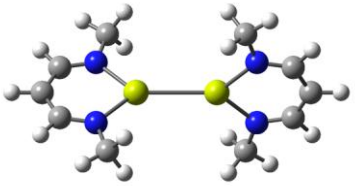
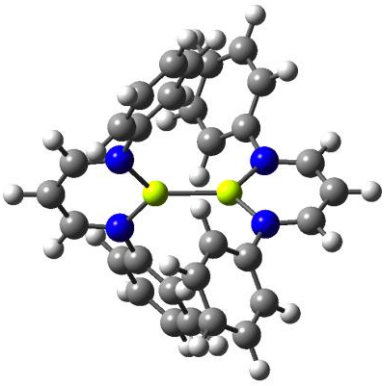
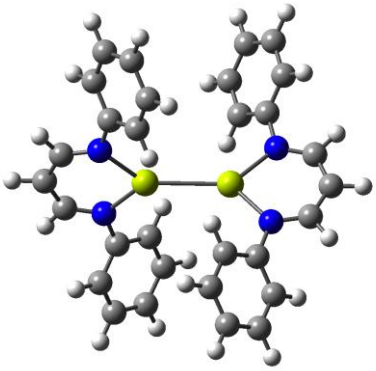
NHC^{Ph}		No Stable Minimum
NAC^{Me}		
NAC^{Ph}		

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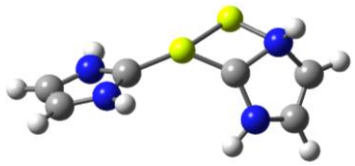
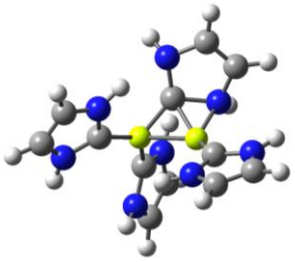
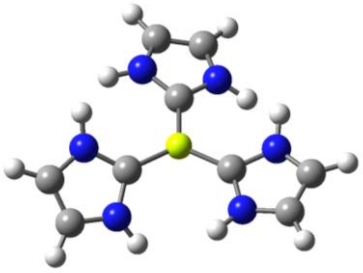
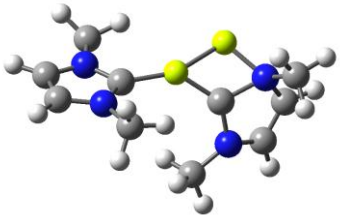
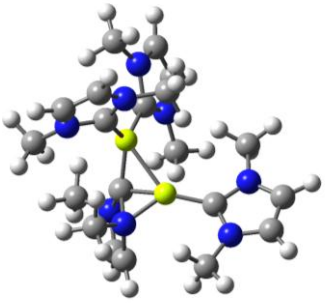
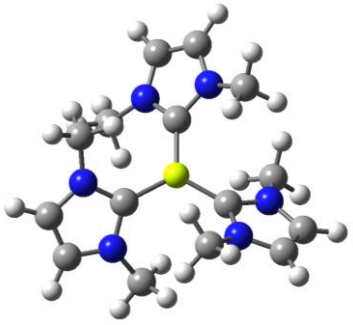
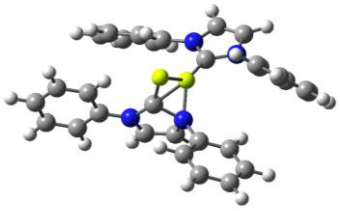
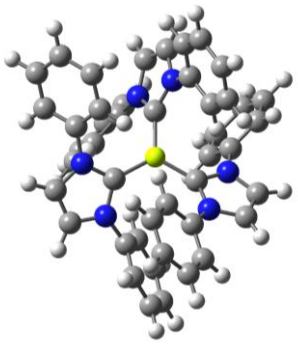
Table S8. B3LYP/def2-TZVPP optimised geometries of **2Be^{R}(B)** (L-Be$_2$-L), **3Be^{R}(B)** (L$_2$-Be$_2$-L$_2$) and **4Be^{R}** (BeL$_3$) compounds (L = NHC^{R}; R = H, Ph).

L	2Be^{R}(B)	3Be^{R}(B)	4Be^{R}
NHC^{H}			
NHC^{Me}			
NHC^{Ph}		No stable minimum	

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Cartesian Coordinates of Optimized geometries

$2E^R$

NHC^R–EE–NHC^R

BERYLLIUM

$2Be^R$

NHC^R–BeBe–NHC^R

$2Be^H$ (NHC^H-BeBe-NHC^H)

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	0.972669	0.000187	0.000007
4	-0.972674	-0.000276	-0.000032
6	-2.655682	-0.000104	-0.000046
7	-3.528288	1.072986	0.000442
7	-3.528480	-1.073032	-0.000388
1	-3.218647	2.026383	0.000966
6	-4.853432	0.674705	0.000280
1	-3.219008	-2.026484	-0.000832
6	-4.853550	-0.674507	-0.000299
6	2.655677	0.000070	0.000015
7	3.528321	-1.072986	0.000425
7	3.528447	1.073021	-0.000445
1	3.218711	-2.026393	0.000914
6	4.853456	-0.674660	0.000260
1	3.218942	2.026461	-0.000966
6	4.853534	0.674551	-0.000245
1	5.671049	-1.371265	0.000526
1	5.671204	1.371065	-0.000501
1	-5.671001	1.371338	0.000561
1	-5.671243	-1.370993	-0.000592

$2Be^{Me}$ (NHC^{Me}-BeBe-NHC^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	0.974389	0.000000	-0.000112
4	-0.974389	0.000000	-0.000110
6	2.661263	0.000000	-0.000087
7	3.512914	1.083934	0.000190
7	3.512914	-1.083934	-0.000208
6	4.832612	0.676293	0.000046
6	4.832612	-0.676293	-0.000036
6	-2.661263	0.000000	-0.000083
7	-3.512914	-1.083934	0.000190
7	-3.512914	1.083934	-0.000207
6	-4.832612	-0.676293	0.000048
6	-4.832612	0.676293	-0.000031
6	-3.039744	2.446576	-0.000329
1	-2.428270	2.635815	0.886295
1	-2.427608	2.635363	-0.886592
1	-3.887356	3.127997	-0.000822
6	-3.039744	-2.446576	0.000410
1	-2.428323	-2.635890	-0.886235
1	-2.427555	-2.635287	0.886653
1	-3.887356	-3.127997	0.001014
6	3.039744	-2.446576	-0.000324
1	2.428271	-2.635811	0.886302
1	2.427607	-2.635366	-0.886585
1	3.887356	-3.127997	-0.000816
6	3.039744	2.446576	0.000415
1	2.428323	2.635893	-0.886229
1	2.427556	2.635285	0.886658
1	3.887356	3.127997	0.001020
1	5.650969	1.372847	0.000160
1	5.650969	-1.372847	-0.000012
1	-5.650969	1.372847	-0.000009
1	-5.650969	-1.372847	0.000159

2Be^{Ph} (NHC^{Ph}-BeBe-NHC^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1			
4	-0.004318	0.988959	-0.084386
4	0.004318	-0.988959	-0.084386
6	-0.001060	2.674735	-0.038667
7	-1.032627	3.566641	-0.325678
7	1.054354	3.495684	0.347692
6	-0.602598	4.871569	-0.126627
6	0.675252	4.827314	0.285195
6	0.001060	-2.674735	-0.038667
7	1.032627	-3.566641	-0.325678
7	-1.054354	-3.495684	0.347692
6	0.602598	-4.871569	-0.126627
6	-0.675252	-4.827314	0.285195
1	-1.216401	5.725934	-0.331479
1	1.350990	5.633419	0.494452
1	-1.350990	-5.633419	0.494452
1	1.216401	-5.725934	-0.331479
6	2.317792	3.049643	0.772653
6	3.125772	3.865316	1.575858
6	2.769716	1.772549	0.427159
6	4.361616	3.413636	2.007243
1	2.778301	4.838342	1.891507
6	4.008933	1.328168	0.873857
1	2.183057	1.141595	-0.230102
6	4.813185	2.141220	1.659895
1	4.969251	4.054006	2.632839
1	4.341752	0.337306	0.596510
1	5.775437	1.789153	2.005383
6	2.317792	-3.218641	-0.782218
6	2.581519	-1.924894	-1.242757
6	3.358174	-4.157715	-0.773677
6	3.849315	-1.590076	-1.699651
1	1.788118	-1.186881	-1.304245
6	4.621014	-3.807842	-1.223936
1	3.197656	-5.156655	-0.396928
6	4.879571	-2.521399	-1.691356
1	4.024404	-0.588658	-2.071009
1	5.410965	-4.546901	-1.202203
1	5.867377	-2.252175	-2.039115
6	-2.317792	-3.049643	0.772653
6	-3.125772	-3.865316	1.575858
6	-2.769716	-1.772549	0.427159
6	-4.361616	-3.413636	2.007243
1	-2.778301	-4.838342	1.891507
6	-4.008933	-1.328168	0.873857
1	-2.183057	-1.141595	-0.230102
6	-4.813185	-2.141220	1.659895
1	-4.969251	-4.054006	2.632839
1	-4.341752	-0.337306	0.596510
1	-5.775437	-1.789153	2.005383
6	-2.317792	3.218641	-0.782218
6	-2.581519	1.924894	-1.242757
6	-3.358174	4.157715	-0.773677
6	-3.849315	1.590076	-1.699651
1	-1.788118	1.186881	-1.304245
6	-4.621014	3.807842	-1.223936
1	-3.197656	5.156655	-0.396928
6	-4.879571	2.521399	-1.691356
1	-4.024404	0.588658	-2.071009
1	-5.410965	4.546901	-1.202203
1	-5.867377	2.252175	-2.039115

MAGNESIUM

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$2Mg^{R}$ (NHC^{R}–MgMg–NHC^{R})

$2Mg^{H}$ (NHC^{H}-MgMg-NHC^{H})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	-0.701329	1.518489	-0.001132
12	0.701293	-1.518008	-0.000726
6	2.881879	-0.564245	-0.002481
7	3.031065	0.777652	-0.001040
7	4.163564	-1.004429	-0.000438
1	2.214320	1.393222	-0.001708
6	4.353909	1.170005	0.001836
1	4.400961	-1.980952	-0.001132
6	5.083997	0.029411	0.002204
6	-2.881491	0.563480	0.000138
7	-4.162930	1.004399	-0.000034
7	-3.031426	-0.778311	0.000813
1	-4.399775	1.981059	-0.000599
6	-5.083952	-0.028936	0.000519
1	-2.215001	-1.394264	0.001180
6	-4.354501	-1.169936	0.001117
1	6.147084	-0.127607	0.004176
1	4.660997	2.199495	0.003324
1	-4.662157	-2.199257	0.001552
1	-6.146952	0.128682	0.000393

$2Mg^{Me}$ (NHC^{Me}-MgMg-NHC^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	1.036636	-0.739339	0.859077
12	-1.034805	0.735262	-0.859139
6	-3.203694	0.096207	-0.103372
7	-3.726196	-1.158435	-0.058940
7	-4.292955	0.896603	0.053555
6	-5.096202	-1.138906	0.118751
6	-5.455866	0.162887	0.195358
6	3.203623	-0.096373	0.103018
7	3.725233	1.158819	0.063260
7	4.293350	-0.895378	-0.057933
6	5.095108	1.140969	-0.115530
6	5.455621	-0.160267	-0.197672
6	4.229456	-2.344667	-0.132987
1	5.085523	-2.779699	0.381358
1	3.315269	-2.680659	0.354431
1	4.224299	-2.682225	-1.169641
6	2.933528	2.370393	0.210088
1	1.928821	2.187349	-0.172604
1	2.872988	2.670778	1.256598
1	3.389852	3.172714	-0.366906
6	-4.228356	2.346186	0.122503
1	-4.228512	2.688281	1.157679
1	-3.311304	2.679240	-0.361478
1	-5.081266	2.779674	-0.398383
6	-2.935499	-2.371379	-0.200011
1	-3.388903	-3.168942	0.385856
1	-2.880374	-2.680260	-1.244343
1	-1.928917	-2.185477	0.176232
1	-6.419623	0.617432	0.338438
1	-5.689217	-2.033796	0.175555
1	5.687470	2.036486	-0.169123
1	6.419579	-0.613535	-0.343400

$2Mg^{Ph}$ (NHC^{Ph}-MgMg-NHC^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	1.209779	0.000021	0.853723
12	-1.209776	0.000025	-0.853725
6	-3.306928	0.000005	0.069605
7	-4.159418	-1.077677	0.114149
7	-4.159453	1.077662	0.114117
6	-5.487472	-0.673065	0.169815
6	-5.487493	0.673010	0.169810
6	3.306928	0.000001	-0.069613
7	4.159454	1.077657	-0.114123
7	4.159417	-1.077682	-0.114158
6	5.487494	0.673002	-0.169812
6	5.487470	-0.673072	-0.169843
1	-6.306368	1.361726	0.253878
1	-6.306326	-1.361805	0.253892
1	6.306371	1.361717	-0.253874
1	6.306322	-1.361814	-0.253934
6	3.727748	2.425983	-0.114959
6	4.555065	3.433577	0.385016
6	2.455286	2.746302	-0.590595
6	4.119680	4.750599	0.385820
1	5.525398	3.190439	0.794414
6	2.029623	4.069571	-0.580117
1	1.825451	1.976686	-1.017853
6	2.855389	5.076641	-0.098410
1	4.768117	5.523321	0.776747
1	1.047454	4.306426	-0.966933
1	2.519692	6.104745	-0.095462
6	3.727665	-2.425995	-0.115033
6	4.554945	-3.433631	0.384918
6	2.455194	-2.746255	-0.590684
6	4.119515	-4.750638	0.385680
1	5.525283	-3.190537	0.794329
6	2.029486	-4.069509	-0.580249
1	1.825386	-1.976601	-1.017914
6	2.855216	-5.076622	-0.098569
1	4.767923	-5.523395	0.776588
1	1.047310	-4.306320	-0.967076
1	2.519484	-6.104715	-0.095654
6	-3.727669	-2.425990	0.115031
6	-4.554951	-3.433627	-0.384916
6	-2.455198	-2.746254	0.590684
6	-4.119523	-4.750635	-0.385676
1	-5.525288	-3.190533	-0.794328
6	-2.029493	-4.069509	0.580252
1	-1.825390	-1.976603	1.017920
6	-2.855225	-5.076621	0.098573
1	-4.767934	-5.523391	-0.776582
1	-1.047319	-4.306321	0.967082
1	-2.519495	-6.104714	0.095660
6	-3.727745	2.425988	0.114959
6	-4.555058	3.433586	-0.385015
6	-2.455284	2.746302	0.590600
6	-4.119671	4.750607	-0.385811
1	-5.525389	3.190450	-0.794419
6	-2.029618	4.069571	0.580130
1	-1.825450	1.976681	1.017851
6	-2.855381	5.076645	0.098426
1	-4.768105	5.523332	-0.776737
1	-1.047450	4.306422	0.966951
1	-2.519683	6.104748	0.095485

3E^{R}
(NHC^{R})$_2$–EE–(NHC^{R})$_2$

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$3Be^{H}$ $(NHC^{H})_2$-BeBe-$(NHC^{H})_2$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-0.000039	1.050825	0.137282
4	-0.000005	-1.050828	-0.137280
6	1.496677	-1.907757	-0.005427
7	2.082601	-2.992736	-0.618939
7	2.478885	-1.518949	0.868169
1	1.643960	-3.488390	-1.371224
6	3.376921	-3.221509	-0.174641
1	2.327195	-0.705199	1.446852
6	3.623396	-2.283685	0.767477
6	1.496624	1.907789	0.005427
7	2.082532	2.992772	0.618946
7	2.478833	1.519008	-0.868180
1	1.643888	3.488408	1.371241
6	3.376846	3.221572	0.174643
1	2.327155	0.705258	-1.446866
6	3.623332	2.283762	-0.767485
6	-1.496697	1.907772	0.005283
7	-2.082675	2.992743	0.618759
7	-2.478816	1.518998	-0.868429
1	-1.644110	3.488370	1.371107
6	-3.376945	3.221540	0.174329
1	-2.327074	0.705263	-1.447119
6	-3.623329	2.283743	-0.767839
6	-1.496646	-1.907807	-0.005281
7	-2.478765	-1.519058	0.868441
7	-2.082610	-2.992780	-0.618766
1	-2.327033	-0.705322	1.447134
6	-3.623269	-2.283817	0.767846
1	-1.644043	-3.488390	-1.371124
6	-3.376876	-3.221600	-0.174334
1	4.497299	-2.115900	1.369516
1	3.994573	-4.017936	-0.547774
1	3.994486	4.018005	0.547782
1	4.497234	2.115998	-1.369531
1	-3.994628	4.017964	0.547417
1	-4.497170	2.115983	-1.369976
1	-3.994549	-4.018028	-0.547429
1	-4.497109	-2.116076	1.369989

$3Be^{Me}$ $(NHC^{Me})_2$-BeBe-$(NHC^{Me})_2$

B3LYP/def2-TZVPP optimized geometry (Å).

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0 1

4	-1.047373	0.112083	0.061725
4	1.047388	0.111997	-0.061630
6	2.098061	1.511632	-0.088330
7	3.251278	1.690477	-0.832790
7	1.958670	2.732403	0.545670
6	3.776822	2.956864	-0.668044
6	2.967846	3.607568	0.196612
6	-2.097910	1.511820	0.088359
7	-3.251129	1.690802	0.832783
7	-1.958365	2.732566	-0.545653
6	-3.776541	2.957238	0.667988
6	-2.967467	3.607841	-0.196654
6	-1.882859	-1.432199	-0.025381
7	-1.675032	-2.589371	0.693717
7	-2.785766	-1.832509	-0.988710
6	-2.398900	-3.647637	0.181617
6	-3.095002	-3.174401	-0.876314
6	1.882725	-1.432366	0.025399
7	2.785662	-1.832779	0.988656
7	1.674691	-2.589520	-0.693668
6	3.094749	-3.174702	0.876225
6	2.398500	-3.647862	-0.181643
6	-3.264481	-0.966999	-2.045219
1	-2.430411	-0.358623	-2.404761
1	-3.659769	-1.576507	-2.857436
1	-4.048034	-0.296014	-1.691528
6	-0.863432	-2.673288	1.891737
1	-1.490196	-2.867388	2.766710
1	-0.123973	-3.469584	1.797373
1	-0.354553	-1.715840	2.007529
6	0.862946	-2.673349	-1.891597
1	1.489596	-2.867461	-2.766649
1	0.123451	-3.469603	-1.797170
1	0.354112	-1.715867	-2.007303
6	3.264551	-0.967324	2.045132
1	3.659886	-1.576877	2.857292
1	4.048112	-0.296387	1.691368
1	2.430565	-0.358894	2.404777
6	3.778333	0.706854	-1.751644
1	4.290488	-0.101781	-1.229058
1	2.953669	0.274006	-2.322717
1	4.481190	1.190922	-2.429168
6	0.942617	3.038069	1.531215
1	0.260528	3.808179	1.167886
1	0.375502	2.123653	1.718420
1	1.409549	3.387533	2.455512
6	-0.942248	3.038103	-1.531173
1	-0.260132	3.808199	-1.167865
1	-0.375180	2.123639	-1.718288
1	-1.409114	3.387528	-2.455519
6	-3.778314	0.707255	1.751644
1	-4.290542	-0.101336	1.229061
1	-2.953712	0.274331	2.322748
1	-4.481138	1.191412	2.429139
1	4.663694	3.287252	-1.177916
1	3.027437	4.606988	0.587956
1	-3.026940	4.607259	-0.588019
1	-4.663394	3.287728	1.177824
1	-3.767730	-3.673467	-1.550178
1	-2.362366	-4.634229	0.606951
1	2.361818	-4.634451	-0.606972
1	3.767481	-3.673842	1.550030

3Be^{Ph} (NHC^{Ph})$_2$-BeBe-(NHC^{Ph})$_2$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	0.749058	0.928372	0.219256
4	-0.597719	-0.818187	-0.076854
6	-0.651938	-1.468740	-1.693758
7	-1.782125	-1.633852	-2.510738
7	0.396891	-1.841840	-2.546791
6	-1.430867	-2.067584	-3.795940
6	-0.084536	-2.198776	-3.820153
6	1.517991	1.521914	-1.223260
7	2.891968	1.606284	-1.598710
7	0.860124	1.782716	-2.449086
6	3.018898	1.867343	-2.977123
6	1.778424	1.968328	-3.496924
6	0.803535	1.636510	1.797852
7	0.716549	0.938351	3.040885
7	0.503405	2.984836	2.204031
6	0.294790	1.794379	4.078273
6	0.168005	3.035714	3.567760
6	-1.557406	-1.617766	1.179913
7	-1.365148	-2.945936	1.600946
7	-2.480318	-1.139314	2.131460
6	-2.067567	-3.228871	2.778691
6	-2.762450	-2.117675	3.104306
1	-2.164105	-2.210571	-4.569756
1	0.566408	-2.544354	-4.601873
1	1.460339	2.233235	-4.489497
1	3.973918	2.016864	-3.446288
1	-0.063286	3.962920	4.061561
1	0.210547	1.460147	5.096151
1	-3.398429	-1.915473	3.946606
1	-2.008372	-4.190853	3.256328

6	-3.143754	-1.410330	-2.137877
6	-3.514776	-0.254635	-1.441278
6	-4.119513	-2.344651	-2.527911
6	-4.860208	-0.035569	-1.133479
1	-2.762173	0.475943	-1.171963
6	-5.464244	-2.114309	-2.219094
1	-3.824657	-3.247256	-3.053182
6	-5.838722	-0.962674	-1.518614
1	-5.139127	0.863435	-0.595982
1	-6.213754	-2.840016	-2.519039
1	-6.881754	-0.787106	-1.275747
6	-0.636337	-3.975815	0.918707
6	-1.028172	-4.379718	-0.365695
6	0.417722	-4.623906	1.576597
6	-0.345311	-5.423442	-0.998328
1	-1.866271	-3.889889	-0.844284
6	1.086193	-5.675543	0.940568
1	0.723981	-4.283001	2.559191
6	0.709525	-6.074885	-0.347735
1	-0.644738	-5.732832	-1.994348
1	1.907064	-6.172722	1.447110
1	1.235081	-6.885899	-0.841310
6	1.774079	-2.013758	-2.205629
6	2.157159	-2.455229	-0.930439
6	2.750881	-1.838904	-3.202908
6	3.500043	-2.737672	-0.668206
1	1.412788	-2.605446	-0.162483
6	4.091104	-2.128383	-2.929949
1	2.471083	-1.447692	-4.174226
6	4.473919	-2.581599	-1.663594
1	3.778916	-3.094638	0.316733
1	4.834712	-1.991457	-3.709261
1	5.514433	-2.802684	-1.451241
6	-0.522258	2.069418	-2.648058
6	-1.229586	2.902381	-1.762037
6	-1.147535	1.637369	-3.834717
6	-2.534324	3.294109	-2.063326
6	-1.147535	1.637369	-3.834717
6	-2.534324	3.294109	-2.063326
1	-0.739932	3.260951	-0.867554
6	-2.455944	2.037793	-4.126788
1	-0.616358	0.974864	-4.509316
6	-3.159050	2.865967	-3.247007
1	-3.059481	3.952101	-1.378451
1	-2.926639	1.692031	-5.042339
1	-4.174633	3.172843	-3.474221
6	4.031885	1.397798	-0.780653
6	5.237200	0.943584	-1.359435
6	4.000005	1.654758	0.604579
6	6.382371	0.787323	-0.580392
1	5.269116	0.675043	-2.407885
6	5.152189	1.474804	1.377845
1	3.078542	1.970503	1.073488
6	6.353037	1.056535	0.796746
1	7.298734	0.439165	-1.047839
1	5.104181	1.675012	2.443990
1	7.246834	0.937292	1.400303
6	0.459888	4.144375	1.396607
6	-0.547330	5.111381	1.617294
6	1.406776	4.367191	0.375518
6	-0.597270	6.271097	0.843784
1	-1.296505	4.940234	2.383046
6	1.337384	5.529229	-0.399918
1	2.206419	3.661298	0.220103
6	0.344558	6.488644	-0.174870
1	-1.377722	7.002926	1.029537
1	2.078400	5.687286	-1.177431
1	0.302118	7.389212	-0.778339
6	1.195073	-0.363669	3.335310
6	0.620134	-1.082684	4.408451
6	2.326414	-0.902956	2.687130
6	1.180410	-2.289133	4.835113
1	-0.275296	-0.706560	4.889980
6	2.883923	-2.100047	3.133104
1	2.775642	-0.363739	1.865189
6	2.321810	-2.807380	4.211278
1	0.722720	-2.821991	5.663968
1	3.782151	-2.472854	2.650163
1	2.770293	-3.732958	4.558477
6	-3.222656	0.086589	2.111916
6	-2.643391	1.293174	1.698428
6	-4.564952	0.066673	2.536529
6	-3.406203	2.465378	1.711618
1	-1.612658	1.299461	1.357251
6	-5.309820	1.247477	2.567850
1	-5.035823	-0.871578	2.807601
6	-4.734670	2.456408	2.154034
1	-2.947906	3.393130	1.384668
1	-6.343583	1.217612	2.898096
1	-5.313197	3.374551	2.176510

MAGNESIUM

3Mg^{R}

$(NHC^{R})_2$–EE–$(NHC^{R})_2$

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$3Mg^{H}$ $(NHC^{H})_2$-MgMg-$(NHC^{H})_2$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	1.020447	-0.000129	1.208000
12	-1.020440	-0.000129	-1.208003
6	2.410937	-1.667511	0.427410
7	3.297326	-2.573653	0.916701
7	2.232055	-2.095077	-0.844557
1	3.625952	-2.548678	1.865150
6	3.654307	-3.534397	-0.016576
1	1.566591	-1.616097	-1.458470
6	2.967585	-3.224807	-1.141110
6	-2.410937	-1.667505	-0.427417
7	-3.297300	-2.573670	-0.916713
7	-2.232090	-2.095036	0.844566
1	-3.625893	-2.548727	-1.865174
6	-3.654306	-3.534389	0.016581
1	-1.566652	-1.616032	1.458488
6	-2.967625	-3.224760	1.141129
6	-2.410766	1.667467	-0.427582
7	-3.296971	2.573736	-0.916975
7	-2.231948	2.095024	0.844396
1	-3.625496	2.548806	-1.865459
6	-3.653940	3.534518	0.016267
1	-1.566620	1.615948	1.458384
6	-2.967348	3.224861	1.140863
6	2.410776	1.667463	0.427575
7	2.231943	2.095035	-0.844396
7	3.296992	2.573721	0.916966
1	1.566601	1.615973	-1.458379
6	2.967344	3.224873	-1.140858
1	3.625531	2.548777	1.865446
6	3.653955	3.534511	-0.016270
1	2.943931	-3.704992	-2.101948
1	4.342891	-4.332608	0.192774
1	-4.342877	-4.332612	-0.192769
1	-2.944002	-3.704916	2.101983
1	-4.342406	4.332812	-0.193153
1	-2.943720	3.705055	2.101697
1	4.342430	4.332798	0.193151
1	2.943705	3.705078	-2.101687

$3Mg^{Me}$ $(NHC^{Me})_2$-MgMg-$(NHC^{Me})_2$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	-1.344264	0.189250	0.602679
12	1.344257	0.189215	-0.602668

6	2.554344	-1.673299	0.112228
7	2.738901	-2.064606	1.403082
7	2.912751	-2.777613	-0.601875
6	3.191186	-3.366173	1.487905
6	3.303038	-3.820007	0.218358
6	-2.554372	-1.673248	-0.112219
7	-2.738902	-2.064573	-1.403072
7	-2.912842	-2.777536	0.601892
6	-3.191236	-3.366123	-1.487885
6	-3.303144	-3.819930	-0.218333
6	-2.927331	1.734228	0.032312
7	-2.793240	2.918913	-0.642373
7	-4.164658	1.852609	0.611149
6	-3.893529	3.737115	-0.472775
6	-4.759719	3.064539	0.318344
6	2.927367	1.734171	-0.032332
7	4.164649	1.852573	-0.611260
7	2.793339	2.918818	0.642429
6	4.759748	3.064478	-0.318425
6	3.893626	3.737017	0.472798
6	-4.733442	0.840173	1.473706
1	-4.004003	0.570545	2.244933
1	-5.631033	1.231654	1.948796
1	-4.987175	-0.055668	0.907472
6	-1.624351	3.291602	-1.416221
1	-1.925644	3.668913	-2.394814
1	-1.050318	4.062929	-0.900457
1	-0.988886	2.414913	-1.550335
6	1.624528	3.291462	1.416420
1	1.925907	3.668534	2.395079
1	1.050549	4.062958	0.900850
1	0.988986	2.414807	1.550383
6	4.733362	0.840174	-1.473907
1	5.630852	1.231713	-1.949140
1	4.987242	-0.055654	-0.907718
1	4.003817	0.570509	-2.245019
6	2.489954	-1.205635	2.552861
1	3.261574	-0.439277	2.629067
1	1.516757	-0.721919	2.441469
1	2.490587	-1.813720	3.456007
6	2.888233	-2.854088	-2.051633
1	2.417030	-3.785026	-2.368147
1	2.307601	-2.011557	-2.430790
1	3.898185	-2.809327	-2.462065
6	-2.888366	-2.853988	2.051653
1	-2.417164	-3.784916	2.368197
1	-2.307753	-2.011445	2.430813
1	-3.898331	-2.809229	2.462053
6	-2.489890	-1.205632	-2.552859
1	-3.261492	-0.439262	-2.629118
1	-1.516689	-0.721933	-2.441434
1	-2.490491	-1.813738	-3.455992
1	3.386591	-3.854471	2.425388
1	3.613482	-4.776615	-0.161274
1	-3.613635	-4.776520	0.161307
1	-3.386630	-3.854432	-2.425365
1	-5.730369	3.341360	0.688762
1	-3.968961	4.710997	-0.921833
1	3.969101	4.710874	0.921905
1	5.730371	3.341311	-0.688905

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$1E^{R}$
$(Nac^{R}–EE–Nac^{R})$

BERYLLIUM

$1Be^{Me}$ $(Nac^{Me})–BeBe–(Nac^{Me})$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

7	0.000000	1.327902	2.093939
7	0.000000	-1.327902	2.093939
6	0.000000	1.213947	3.407827
6	0.000000	-1.213947	3.407827
6	0.000000	0.000000	4.088922
1	0.000000	2.129406	3.998940
1	0.000000	-2.129406	3.998940
1	0.000000	0.000000	5.167354
4	0.000000	0.000000	1.080941
7	1.327902	0.000000	-2.093939
7	-1.327902	0.000000	-2.093939
6	1.213947	0.000000	-3.407827
6	-1.213947	0.000000	-3.407827
6	0.000000	0.000000	-4.088922
1	2.129406	0.000000	-3.998940
1	-2.129406	0.000000	-3.998940
1	0.000000	0.000000	-5.167354
4	0.000000	0.000000	-1.080941
6	2.675278	0.000000	-1.535682
1	2.824916	0.877152	-0.904861
1	2.824916	-0.877152	-0.904861
1	3.434784	0.000000	-2.321770
6	-2.675278	0.000000	-1.535682
1	-2.824916	-0.877152	-0.904861
1	-2.824916	0.877152	-0.904861
1	-3.434784	0.000000	-2.321770
6	0.000000	2.675278	1.535682
1	0.877152	2.824916	0.904861
1	-0.877152	2.824916	0.904861
1	0.000000	3.434784	2.321770
6	0.000000	-2.675278	1.535682
1	-0.877152	-2.824916	0.904861
1	0.877152	-2.824916	0.904861
1	0.000000	-3.434784	2.321770

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1Be^{Ph} (Nac^{Ph})–BeBe–(Nac^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-0.000395	-0.000161	-1.066756
4	0.000431	-0.000010	1.066771
7	-0.906725	0.987710	-2.093246
7	0.905154	-0.988373	-2.093621
6	-0.825205	0.893667	-3.413533
6	0.822370	-0.894998	-3.413875
6	-0.001760	-0.000853	-4.085131
1	-1.431963	1.572741	-4.007428
1	1.428607	-1.574330	-4.008006
1	-0.002283	-0.001127	-5.163716
7	-0.987504	-0.905681	2.093801
7	0.989210	0.905507	2.093092
6	-0.893063	-0.823818	3.414038
6	0.896184	0.823126	3.413398
6	0.001950	-0.000508	4.085145
1	-1.572195	-1.430150	4.008300
1	1.575894	1.429300	4.007161
1	0.002534	-0.000723	5.163730
6	-1.849794	1.918651	-1.573769
6	-1.464279	2.815503	-0.575024
6	-3.168905	1.943728	-2.033954
6	-2.378319	3.725749	-0.061481
1	-0.444096	2.799214	-0.220630
6	-4.080457	2.856053	-1.513996
1	-3.486349	1.229562	-2.782424
6	-3.689809	3.751377	-0.526097
1	-2.061341	4.422648	0.703366
1	-5.100396	2.856503	-1.875951
1	-4.399566	4.459258	-0.119441
6	1.848842	-1.918932	-1.574583
6	1.464375	-2.815402	-0.575092
6	3.167541	-1.944000	-2.035947
6	2.379026	-3.725262	-0.061956
1	0.444502	-2.799130	-0.219810
6	4.079711	-2.855942	-1.516395
1	3.484194	-1.230125	-2.785030
6	3.690103	-3.750881	-0.527739
1	2.062855	-4.421866	0.703494
1	5.099323	-2.856391	-1.879271
1	4.400346	-4.458456	-0.121399
6	1.919936	1.848735	1.573518
6	2.815974	1.463695	0.573860
6	1.945590	3.167549	2.034521
6	3.725998	2.377899	0.060215
1	2.799239	0.443736	0.218843
6	2.857692	4.079268	1.514462
1	1.232040	3.484644	2.783727
6	3.752208	3.689089	0.525646
1	4.422262	2.061287	-0.705362
1	2.858598	5.098976	1.877067
1	4.459909	4.398979	0.118909
6	-1.918971	-1.848519	1.574850
6	-2.815936	-1.462907	0.576246
6	-1.944459	-3.167497	2.035394
6	-3.726687	-2.376714	0.063183
1	-2.799328	-0.442823	0.221585
6	-2.857292	-4.078817	1.515917
1	-1.230224	-3.485033	2.783760
6	-3.752720	-3.688070	0.528152
1	-4.423663	-2.059657	-0.701562
1	-2.858059	-5.098660	1.878143
1	-4.460994	-4.397650	0.121872

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MAGNESIUM

$1Mg^{Me}$ (Nac^{Me})–MgMg–(Nac^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	1.437450	-0.000012	0.000059
12	-1.437450	0.000066	0.000093
7	-2.857378	1.066038	-1.065717
7	-2.857434	-1.065952	1.065777
6	-4.147656	0.884997	-0.884890
6	-4.147703	-0.885041	0.884754
6	-4.770997	-0.000059	-0.000122
1	-4.824324	1.492331	-1.492167
1	-4.824403	-1.492425	1.491944
1	-5.850863	-0.000112	-0.000204
7	2.857469	1.065844	1.065856
7	2.857343	-1.065912	-1.065872
6	4.147732	0.884890	0.884833
6	4.147627	-0.884966	-0.884993
6	4.770997	-0.000038	-0.000117
1	4.824452	1.492187	1.492089
1	4.824275	-1.492274	-1.492316
1	5.850863	-0.000043	-0.000176
6	2.458819	2.057126	2.057204
1	1.850799	2.841731	1.599195
1	1.851210	1.598973	2.842047
1	3.323471	2.531343	2.531102
6	2.458575	-2.057201	-2.057165
1	1.850553	-2.841766	-1.599090
1	1.850929	-1.599043	-2.841976
1	3.323171	-2.531471	-2.531114
6	-2.458642	2.057516	-2.056834
1	-1.851117	2.842328	-1.598517
1	-1.850511	1.599619	-2.841419
1	-3.323254	2.531439	-2.531102
6	-2.458751	-2.057352	2.056993
1	-1.851086	-2.842126	1.598798
1	-1.850777	-1.599366	2.841648
1	-3.323388	-2.531335	2.531155

1Mg^{Ph} (Nac^{Ph})–MgMg–(Nac^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1			
20	0.000000	0.000000	-1.899105
20	0.000000	0.000000	1.899602
7	0.274902	1.542257	-3.689755
7	-0.274902	-1.542257	-3.689755
6	0.261304	1.236628	-4.974776
6	-0.261304	-1.236628	-4.974776
6	0.000000	0.000000	-5.570042
1	0.453672	2.048812	-5.677748
1	-0.453672	-2.048812	-5.677748
1	0.000000	0.000000	-6.650722
7	0.536880	1.468651	3.693878
7	-0.536880	-1.468651	3.693878
6	0.391543	1.201092	4.979160
6	-0.391543	-1.201092	4.979160
6	0.000000	0.000000	5.575672
1	0.627480	2.003328	5.680439
1	-0.627480	-2.003328	5.680439
1	0.000000	0.000000	6.656327
6	0.672649	2.844697	-3.323201
6	0.000000	3.496547	-2.280829
6	1.760072	3.498640	-3.921488
6	0.387050	4.763995	-1.865468
1	-0.849326	3.016047	-1.810344
6	2.136913	4.768833	-3.507682
1	2.324731	2.995186	-4.694772
6	1.453344	5.410610	-2.479695
1	-0.151111	5.246813	-1.060662
1	2.979618	5.254331	-3.983053
1	1.752693	6.398803	-2.157641
6	0.848832	2.793480	3.324551
6	1.776609	3.014759	2.298017
6	0.221141	3.906088	3.903721
6	2.081592	4.303296	1.879476
1	2.284975	2.170684	1.848197
6	0.535818	5.192094	3.486432
1	-0.532431	3.754763	4.665016
6	1.467591	5.399621	2.473990
1	2.805053	4.448125	1.088257
1	0.039285	6.036882	3.946404
1	1.706952	6.403153	2.149143
6	-0.848832	-2.793480	3.324551
6	-1.776609	-3.014759	2.298017
6	-0.221141	-3.906088	3.903721
6	-2.081592	-4.303296	1.879476
1	-2.284975	-2.170684	1.848197
6	-0.535818	-5.192094	3.486432
1	0.532431	-3.754763	4.665016
6	-1.467591	-5.399621	2.473990
1	-2.805053	-4.448125	1.088257
1	-0.039285	-6.036882	3.946404
1	-1.706952	-6.403153	2.149143
6	-0.672649	-2.844697	-3.323201
6	0.000000	-3.496547	-2.280829
6	-1.760072	-3.498640	-3.921488
6	-0.387050	-4.763995	-1.865468
1	0.849326	-3.016047	-1.810344
6	-2.136913	-4.768833	-3.507682
1	-2.324731	-2.995186	-4.694772
6	-1.453344	-5.410610	-2.479695
1	0.151111	-5.246813	-1.060662
1	-2.979618	-5.254331	-3.983053
1	-1.752693	-6.398803	-2.157641

2E^{R}(B) (*bridged structure*)

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(NHC^{R}–EE–NHC^{R})

BERYLLIUM

2Be^{H}(B) (NHC^{H})–BeBe–(NHC^{H})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-1.539781	1.821215	-0.135006
4	0.017229	0.755857	-0.484438
6	1.632154	0.259459	-0.187144
7	2.483367	0.825436	0.706007
7	2.404194	-0.691236	-0.777059
6	3.739306	0.253751	0.674492
6	3.691743	-0.711924	-0.271802
1	4.545809	0.575286	1.306669
1	4.448095	-1.389639	-0.621366
6	-1.447570	0.014705	-0.406394
7	-1.960792	-1.217135	0.136699
7	-2.748009	0.813294	-0.613303
6	-3.198780	-0.984447	0.703524
6	-3.699120	0.194250	0.308778
1	-3.654833	-1.706084	1.363171
1	-4.661594	0.634802	0.494968
1	2.197106	1.603457	1.276850
1	2.053155	-1.293041	-1.501053
1	-3.087714	0.796648	-1.571169
1	-1.307529	-1.796998	0.634574

2Be^{Me}(B) (NHC^{Me})–BeBe–(NHC^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-1.483496	1.354653	-1.308805
4	0.038549	0.329869	-0.707668
6	1.685709	0.092303	-0.273911
7	2.615003	1.063428	-0.054660
7	2.397072	-1.069468	-0.220694
6	3.870066	0.519673	0.120379
6	3.735320	-0.822480	0.010917
1	4.740308	1.122403	0.305341
1	4.466764	-1.607180	0.075360
6	-1.466283	-0.063717	-0.145913
7	-2.003769	-0.377802	1.141028
7	-2.718634	0.346581	-0.933089
6	-3.223461	0.231973	1.285517
6	-3.665556	0.721480	0.113246
1	-3.707186	0.283489	2.248547
1	-4.609159	1.173352	-0.134067
6	-1.115648	-0.611692	2.246689
1	-0.450668	0.247686	2.419721
1	-1.692369	-0.802477	3.150972
1	-0.490681	-1.482869	2.048047
6	-3.274101	-0.669591	-1.855156
1	-4.148194	-0.253029	-2.359170
1	-2.513428	-0.916070	-2.591707
1	-3.565706	-1.564029	-1.299408
6	1.825371	-2.386621	-0.440141
1	2.019734	-3.032030	0.416383
1	0.751861	-2.274435	-0.571053
1	2.249937	-2.841223	-1.335874
6	2.302871	2.482377	-0.023244
1	1.416038	2.647248	-0.638162
1	2.095173	2.812507	0.994696
1	3.143924	3.047161	-0.422131

2Be^{Ph}(B) (NHC^{Ph})–BeBe–(NHC^{Ph})

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B3LYP/def2-TZVPP optimized geometry (Å).

0 1

6	-0.751052	-1.258480	0.496508
7	-1.852866	-1.386057	-0.422476
7	0.478722	-1.220021	-0.388299
6	-1.402464	-1.102295	-1.696690
6	-0.072596	-0.959605	-1.718292
1	-2.076933	-0.979418	-2.526251
1	0.577925	-0.766163	-2.551253
4	0.401248	0.179147	0.636655
4	-0.362194	-1.002069	2.065106
6	0.847613	1.819717	0.235709
7	2.113116	2.335193	0.188024
7	0.043401	2.907284	0.031194
6	2.090445	3.701664	-0.038320
6	0.795370	4.060107	-0.134463
1	2.987637	4.290429	-0.070267
1	0.341938	5.023869	-0.268148
6	-1.384569	2.901179	-0.043700
6	-2.132472	2.219713	0.908709
6	-2.011681	3.600215	-1.072173
6	-3.518840	2.232569	0.820670
1	-1.629147	1.683021	1.701737
6	-3.398537	3.617484	-1.142694
1	-1.420417	4.106977	-1.822774
6	-4.154777	2.931378	-0.198824
1	-4.100966	1.688935	1.551855
1	-3.885435	4.155746	-1.944789
1	-5.234417	2.934401	-0.262149
6	3.329492	1.601702	0.371445
6	4.361645	1.763498	-0.548456
6	3.484097	0.773066	1.477123
6	5.562421	1.089616	-0.356129
1	4.222892	2.401412	-1.411073
6	4.684445	0.096829	1.652703
1	2.665100	0.643675	2.173226
6	5.724580	0.254181	0.742677
1	6.364838	1.212916	-1.070995
1	4.802825	-0.554400	2.507965
1	6.656676	-0.275237	0.887584
6	1.433972	-2.324165	-0.395251
6	1.096091	-3.572517	0.109786
6	2.693376	-2.113036	-0.947032
6	2.020724	-4.608437	0.062418
1	0.120904	-3.712774	0.553657
6	3.614585	-3.152708	-0.991534
1	2.957562	-1.134275	-1.325431
6	3.282352	-4.404837	-0.487071
1	1.752267	-5.579512	0.457895
1	4.596293	-2.978647	-1.412437
1	4.001208	-5.212843	-0.516984
6	-3.157707	-1.629696	-0.040172
6	-3.493295	-1.699120	1.323468
6	-4.188650	-1.809458	-0.981603
6	-4.801477	-1.938242	1.721214
1	-2.723898	-1.579056	2.075003
6	-5.490651	-2.036060	-0.568036
1	-3.971071	-1.791034	-2.039697
6	-5.815471	-2.102573	0.785385
1	-5.025578	-1.992427	2.779000
1	-6.261195	-2.173919	-1.316051
1	-6.833666	-2.284899	1.099976

$3E^{R}(B)$ (*bridged structure*)
$(NHC^{R})_2$–EE–$(NHC^{R})_2$

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BERYLLIUM

$3Be^{H}(B)\ (NHC^{H})_2–BeBe–(NHC^{H})_2$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-0.587140	-0.928651	-0.126610
4	1.144257	0.301168	0.295588
6	0.123671	-0.553534	1.380041
7	-0.584932	-0.178102	2.609077
7	-0.218037	-2.036433	1.155384
6	-1.421477	-1.262207	2.941163
6	-1.239867	-2.306693	2.128825
1	-2.123444	-1.195903	3.760093
1	-1.750691	-3.257040	2.149133
1	0.019743	0.066566	3.393348
1	0.535034	-2.727215	1.180103
6	0.684674	1.973478	0.256063
7	1.127838	3.135974	-0.323493
7	-0.391540	2.407692	0.985287
6	0.341588	4.229230	0.011532
1	1.930010	3.170959	-0.923609
6	-0.617885	3.760151	0.841732
1	-0.891775	1.756647	1.581781
1	0.530798	5.221940	-0.352744
1	-1.419109	4.276535	1.337841
6	2.561135	-0.401289	-0.386810
7	3.208344	-0.246044	-1.594698
7	3.277509	-1.431028	0.179096
6	4.204253	-1.190428	-1.789436
1	2.816461	0.316690	-2.325698
6	4.253596	-1.935236	-0.664812
1	3.093073	-1.736578	1.116643
1	4.789086	-1.247515	-2.688987
1	4.895338	-2.755081	-0.399318
6	-2.064485	-0.817915	-0.947872
7	-3.094452	-1.714951	-1.112259
7	-2.504150	0.253279	-1.687453
6	-4.112014	-1.216692	-1.910381
1	-3.108291	-2.606154	-0.653221
6	-3.735024	0.028728	-2.272810
1	-1.936688	1.075224	-1.799146
1	-4.993377	-1.779692	-2.156527
1	-4.227686	0.752275	-2.895585

$3Be^{Me}(B)\ (NHC^{Me})_2–BeBe–(NHC^{Me})_2$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1			
4	-1.297189	-0.278527	0.163975
4	0.946789	-0.079471	0.247965
6	-0.178592	-0.548209	1.470571
7	-0.343743	-0.211177	2.876017
7	-1.246010	-1.637920	1.204412
6	-1.516928	-0.794544	3.321081
6	-2.081038	-1.562756	2.377921
1	-1.896799	-0.596123	4.313155
1	-3.000217	-2.123195	2.433990
6	1.631418	1.555317	0.283914
7	2.818520	1.994929	-0.277099
7	1.167171	2.688944	0.922623
6	3.054880	3.328811	0.004344
6	2.024985	3.756692	0.762450
1	3.923092	3.849265	-0.356612
1	1.827546	4.721705	1.192990
6	1.700095	-1.250646	-0.856873
7	1.739376	-1.238298	-2.237188
7	2.268878	-2.468736	-0.545108
6	2.268115	-2.413697	-2.738036
6	2.602672	-3.182376	-1.678865
1	2.353218	-2.603729	-3.792437
1	3.046275	-4.160919	-1.639435
6	-2.621776	0.414761	-0.657507
7	-3.832860	-0.181491	-0.973270
7	-2.690155	1.620084	-1.337299
6	-4.571474	0.600405	-1.839499
6	-3.859517	1.725685	-2.064357
1	-5.533747	0.298447	-2.211234
1	-4.086991	2.585470	-2.667813
6	-4.224381	-1.490851	-0.516926
1	-3.467925	-2.229460	-0.795311
1	-4.337347	-1.505824	0.567988
1	-5.172668	-1.762460	-0.976263
6	-1.624618	2.589326	-1.355216
1	-1.680921	3.269505	-0.504392
1	-0.669159	2.055033	-1.308006
1	-1.676544	3.173348	-2.274173
6	-0.001447	2.751743	1.782418
1	-0.659072	1.920344	1.551099
1	0.289591	2.678450	2.831783
1	-0.518265	3.698126	1.624558
6	3.777205	1.164509	-0.971911
1	3.888316	0.217981	-0.445115
1	3.470095	0.947177	-1.995503
1	4.735417	1.681094	-0.998169
6	1.049758	-0.258396	-3.048201
1	1.593068	0.683929	-3.107343
1	0.920187	-0.654102	-4.055408
1	0.075490	-0.065009	-2.578727
6	2.611107	-2.889808	0.796891
1	2.159440	-2.189266	1.493872
1	2.223868	-3.889683	0.995960
1	3.695894	-2.895841	0.933911
6	-0.875023	-3.026801	0.874315
1	-0.275991	-3.029781	-0.030911
1	-0.325983	-3.499716	1.696158
1	-1.785587	-3.603802	0.687886
6	0.801636	-0.256495	3.771250
1	0.517060	0.125555	4.754758
1	1.200548	-1.274624	3.898205
1	1.599012	0.369741	3.374567

3Be^{Ph}(B) (NHC^{Ph})$_2$–BeBe–(NHC^{Ph})$_2$

B3LYP/def2-TZVP optimized geometry (Å).

0 1			
4	-1.172076	0.067312	0.191357
4	1.101689	0.081733	0.118811
6	1.784619	0.373613	-1.511195
7	2.583180	-0.491079	-2.261366
7	1.547321	1.421123	-2.395982
6	2.777469	0.002248	-3.541054
6	2.146077	1.175955	-3.624512
6	-1.800184	-0.016897	-1.467004
7	-2.601344	0.903384	-2.179402
7	-1.367246	-0.892382	-2.477069
6	-2.592843	0.603627	-3.537698
6	-1.840965	-0.483427	-3.719885
6	-2.228354	-0.049014	1.623886
7	-2.023864	0.445209	2.937561
7	-3.261156	-1.018066	1.820187
6	-2.820593	-0.234170	3.848766
6	-3.567575	-1.111655	3.174419
6	2.304652	-0.245462	1.394786
7	2.245737	-1.380011	2.209349
7	3.575825	0.273361	1.652649
6	3.444520	-1.554053	2.882896
6	4.251538	-0.539746	2.554262
1	3.330044	-0.531532	-4.285915
1	2.103607	1.870152	-4.437298
1	-1.668895	-1.046017	-4.613787
1	-3.168214	1.152832	-4.253823
1	-4.335647	-1.757916	3.543614
1	-2.856845	0.019475	4.886803
1	5.261240	-0.349522	2.851699
1	3.616230	-2.385180	3.535374

6	3.177873	-1.736814	-1.880298
6	3.914195	-2.474649	-2.811488
6	3.090784	-2.196588	-0.570583
6	4.542606	-3.652226	-2.432843
1	4.016546	-2.123081	-3.824946
6	3.723034	-3.376778	-0.199503
1	2.533136	-1.621186	0.164555
6	4.447785	-4.113240	-1.126692
1	5.111015	-4.207540	-3.166461
1	3.644310	-3.720845	0.822605
1	4.939593	-5.031599	-0.834489
6	1.148815	-2.274871	2.470260
6	1.368110	-3.405853	3.270208
6	-0.118683	-2.084538	1.907231
6	0.337603	-4.305251	3.504687
1	2.342510	-3.590343	3.694158
6	-1.157856	-2.961342	2.196001
1	-0.366368	-1.173710	1.308144
6	-0.929406	-4.085124	2.977843
1	0.522106	-5.170966	4.127166
1	-2.168291	-2.671394	1.856952
1	-1.740001	-4.763280	3.209823
6	0.948389	2.692749	-2.150011
6	0.803308	3.614223	-3.193699
6	0.439658	3.019418	-0.891076
6	0.149054	4.817862	-2.982652
1	1.178674	3.389093	-4.177699
6	-0.211082	4.231359	-0.690593
1	0.580115	2.345903	-0.060657
6	-0.364314	5.135171	-1.730181
1	0.039146	5.508742	-3.807655
1	-0.591456	4.468105	0.291722
1	-0.869723	6.076836	-1.567532
6	-0.775548	-2.172714	-2.343223
6	-0.389531	-2.916509	-3.469294
6	-0.450498	-2.666885	-1.077781
6	0.308484	-4.102779	-3.321383
1	-0.608330	-2.551777	-4.459052
6	0.245568	-3.861406	-0.940147
1	-0.763594	-2.130672	-0.201387
6	0.632810	-4.587462	-2.055126
1	0.612349	-4.647992	-4.205435
1	0.475257	-4.225183	0.051536
1	1.173666	-5.516992	-1.944733
6	-3.309730	2.030781	-1.693968
6	-3.354233	2.326753	-0.325546
6	-3.986582	2.886878	-2.575751
6	-4.012754	3.455147	0.135549
1	-2.903633	1.656422	0.389531
6	-4.655816	4.004734	-2.100195
1	-4.007027	2.677163	-3.632348
6	-4.665129	4.311638	-0.745834
1	-4.027094	3.656664	1.198993
1	-5.168942	4.645614	-2.805651
1	-5.174642	5.194059	-0.383316
6	-3.939352	-1.853759	0.903722
6	-3.628492	-1.835298	-0.461918
6	-4.946155	-2.740384	1.334103
6	-4.279375	-2.674911	-1.354465
1	-2.866141	-1.143542	-0.825279
6	-5.596582	-3.566066	0.429966
1	-5.201563	-2.814083	2.376277
6	-5.271084	-3.548533	-0.921263
1	-4.013506	-2.637334	-2.402973
1	-6.360464	-4.240841	0.794397
1	-5.778859	-4.199535	-1.620063
6	-1.408750	1.657233	3.311727
6	-0.815974	2.476274	2.335410
6	-1.270599	2.038504	4.661891
6	-0.095690	3.609219	2.698111
1	-0.948124	2.235543	1.294695
6	-0.532430	3.155153	5.007878
1	-1.717499	1.444512	5.440891
6	0.064607	3.956975	4.031471
1	0.344011	4.223278	1.922902
1	-0.411375	3.397929	6.055921
1	0.641696	4.828157	4.309789
6	4.157857	1.518548	1.255660
6	5.475229	1.837128	1.604562
6	3.413970	2.453386	0.533787
6	6.022505	3.056518	1.229454
1	6.079482	1.126292	2.145026
6	3.961834	3.678497	0.183294
1	2.415839	2.214292	0.225722
6	5.272953	3.989881	0.526708
1	7.045412	3.278691	1.503572
1	3.362304	4.384960	-0.375158
1	5.701819	4.943984	0.251574

$4E^R$
$E–(NHC^R)_3$

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4Be^{H} Be–(NHC^{H})$_3$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-0.030920	-0.000091	-0.000321
6	-1.729138	-0.000975	-0.000139
7	-2.611733	0.909739	0.571977
7	-2.610919	-0.912584	-0.572063
6	-3.942017	0.560747	0.369199
1	-2.310900	1.544879	1.286068
6	-3.941513	-0.565023	-0.368932
1	-2.309570	-1.547584	-1.286059
1	-4.762245	1.135513	0.758701
1	-4.761227	-1.140625	-0.758281
6	0.840768	1.455241	0.031465
7	0.414811	2.770121	0.177257
7	2.205543	1.635854	-0.205375
6	1.424136	3.688226	-0.074286
1	-0.559863	3.008168	0.209222
6	2.543639	2.981907	-0.318803
1	2.746265	0.907419	-0.636933
1	1.271315	4.750730	-0.019380
1	3.545489	3.315543	-0.519061
6	0.842460	-1.454432	-0.031770
7	2.207416	-1.633328	0.205256
7	0.418121	-2.769855	-0.177216
6	2.547167	-2.978925	0.319000
1	2.747268	-0.904083	0.636535
6	1.428548	-3.686675	0.074556
1	-0.556243	-3.009108	-0.209466
1	3.549406	-3.311280	0.519438
1	1.277022	-4.749377	0.019902

4Be^{Me} Be–(NHC^{Me})$_3$

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	0.000573	-0.001981	-0.001026
6	1.442211	-0.955375	0.001123
7	1.667853	-2.187070	0.606062
7	2.665325	-0.679994	-0.601780
6	2.959745	-2.633378	0.376153
6	3.579040	-1.697640	-0.375827
1	3.326402	-3.566182	0.767648
1	4.580784	-1.671774	-0.767663
6	-1.546641	-0.769921	0.002040
7	-2.725164	-0.354135	0.612861
7	-1.925866	-1.959171	-0.611761
6	-3.759414	-1.246200	0.377832
6	-3.261974	-2.245343	-0.382764
1	-4.750487	-1.098948	0.769874
1	-3.742684	-3.120820	-0.783039
6	0.106723	1.722193	0.000076
7	1.059651	2.534961	0.604161
7	-0.739846	2.644369	-0.606733
6	0.802140	3.876937	0.372489
6	-0.318545	3.945077	-0.378027
1	1.427716	4.661010	0.761743
1	-0.840524	4.799529	-0.771699
6	2.043525	2.053473	1.548677
1	1.615863	1.189915	2.068338
1	2.968219	1.733956	1.063779
1	2.277181	2.844003	2.263944
6	0.758576	-2.794825	1.551959
1	0.219796	-1.991983	2.065325
1	0.021706	-3.438787	1.067727
1	1.326056	-3.386980	2.272030
6	2.867971	0.392465	-1.551988
1	1.921895	0.557617	-2.079116
1	3.152371	1.331795	-1.072556
1	3.648143	0.108113	-2.260460
6	-1.779752	2.287072	-1.546314
1	-1.461120	1.381161	-2.071358
1	-2.732523	2.073287	-1.056185
1	-1.925999	3.103003	-2.257197
6	-1.096781	-2.671446	-1.559078
1	-0.485545	-1.936938	-2.094161
1	-0.420546	-3.379477	-1.074876
1	-1.732951	-3.215206	-2.259941
6	-2.796220	0.736236	1.562172
1	-1.844954	0.784132	2.103044
1	-2.953423	1.702068	1.077176
1	-3.614946	0.556755	2.260929

4Be^{Ph} Be–(NHC^{Ph})$_3$

B3LYP/def2-TZVP optimized geometry (Å).

0 1

4	0.041558	-0.010114	0.016640
6	1.004315	-0.194981	-1.411173
7	2.313346	0.184676	-1.776099

7	0.528422	-0.792462	-2.584644
6	2.578768	-0.184029	-3.098289
6	1.477923	-0.763025	-3.594126
1	3.507626	0.040385	-3.583406
1	1.291382	-1.189485	-4.561991
6	0.810781	0.112667	1.573151
7	0.394767	0.816256	2.696650
7	2.011009	-0.443353	1.990350
6	1.293369	0.666978	3.749189
6	2.301698	-0.100830	3.303047
1	1.147153	1.152248	4.695548
1	3.187044	-0.450740	3.799930
6	-1.727823	0.064253	-0.112291
7	-2.512451	0.969029	-0.837685
7	-2.687480	-0.786908	0.449164
6	-3.860658	0.654173	-0.730322
6	-3.967741	-0.416884	0.065611
1	-4.622000	1.210336	-1.241417
1	-4.840889	-0.939904	0.404280
6	-2.123170	2.188338	-1.451650
6	-2.966733	3.302200	-1.338457
6	-0.925166	2.317874	-2.158765
6	-2.627691	4.509344	-1.926752
1	-3.873009	3.233141	-0.754093
6	-0.583957	3.544108	-2.728890
1	-0.279842	1.469481	-2.278440
6	-1.426420	4.638851	-2.628075
1	-3.292022	5.356969	-1.820889
1	0.348775	3.626048	-3.271468
1	-1.159091	5.581761	-3.085820
6	-2.488408	-1.974281	1.195980
6	-1.503083	-2.065831	2.181236
6	-3.307909	-3.082672	0.950264
6	-1.337564	-3.254688	2.891706
1	-0.906206	-1.206918	2.418012
6	-3.146202	-4.254129	1.672240
1	-4.049418	-3.038301	0.165804
6	-2.151547	-4.349137	2.648401
1	-0.572490	-3.308023	3.655429
1	-3.785605	-5.101164	1.461394
1	-2.023045	-5.264080	3.210929
6	-0.721730	1.695452	2.810857
6	-0.899259	2.748536	1.915505
6	-1.582567	1.561558	3.901585
6	-1.929527	3.654841	2.110054
1	-0.230888	2.852859	1.074431
6	-2.615736	2.474503	4.088310
1	-1.452112	0.737206	4.589451
6	-2.796561	3.520892	3.194786
1	-2.052171	4.471967	1.412452
1	-3.282145	2.357710	4.932810
1	-3.601773	4.228637	3.339555
6	2.769905	-1.446424	1.313545
6	2.161225	-2.628571	0.897596
6	4.141826	-1.275909	1.163088
6	2.929885	-3.632596	0.325641
1	1.098593	-2.754251	1.040555
6	4.907346	-2.289784	0.591553
1	4.603483	-0.349342	1.474043
6	4.304852	-3.464610	0.165884
1	2.456955	-4.555426	0.016589
1	5.973786	-2.150361	0.474453
1	4.899436	-4.250339	-0.281092
6	3.198685	1.065583	-1.109827
6	4.572756	1.008808	-1.393811
6	2.742431	2.049433	-0.228685
6	5.453471	1.899858	-0.800646
1	4.960572	0.243549	-2.050204
6	3.630735	2.940502	0.353741
1	1.686476	2.111189	-0.020878
6	4.994965	2.872150	0.083858
1	6.509641	1.825577	-1.026151
1	3.248420	3.702314	1.021396
1	5.685031	3.561909	0.550300
6	-0.670460	-1.538889	-2.765773
6	-1.523858	-1.203302	-3.818703
6	-0.924912	-2.681634	-2.007530
6	-2.621195	-2.008805	-4.109653
1	-1.329835	-0.310803	-4.397712
6	-2.018132	-3.478914	-2.304865
1	-0.252860	-2.937810	-1.201968
6	-2.875809	-3.145331	-3.355938
1	-3.278801	-1.738209	-4.925533
1	-2.197981	-4.370782	-1.719772
1	-3.728439	-3.771438	-3.582902

L-E-L

(NHC^R)–E–(NHC^R)

BERYLLIUM

(NHC^H)–Be–(NHC^H)

B3LYP/def2-TZVPP optimized geometry (Å).

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0 1

4	0.000000	-0.000181	0.917244
6	-1.556006	-0.000125	0.334404
7	-2.389196	-1.075871	0.051447
7	-2.388962	1.075818	0.051430
1	-2.126263	-2.027449	0.219365
6	-3.662480	-0.673113	-0.323695
1	-2.126030	2.027282	0.219992
6	-3.662360	0.673321	-0.323620
6	1.556006	-0.000123	0.334405
7	2.389198	-1.075870	0.051454
7	2.388959	1.075820	0.051420
1	2.126262	-2.027448	0.219367
6	3.662492	-0.673111	-0.323655
1	2.126029	2.027284	0.219983
6	3.662349	0.673324	-0.323658
1	-4.445851	-1.369606	-0.558302
1	-4.445593	1.369976	-0.558206
1	4.445871	-1.369604	-0.558233
1	4.445573	1.369978	-0.558273
6	-3.802464	-0.674803	-0.132863
6	1.631461	0.000042	0.077056
7	2.486188	-1.088806	-0.017105
7	2.486448	1.088703	-0.016730
6	3.802368	-0.675067	-0.133025
6	3.802529	0.674695	-0.132859
6	2.018980	2.442412	0.054963
1	1.364942	2.675351	-0.793166
1	1.446401	2.594535	0.979389
1	2.862944	3.128627	0.045197
6	2.018443	-2.442418	0.054535
1	1.446797	-2.594869	0.979485
1	1.363440	-2.674753	-0.793017
1	2.862211	-3.128852	0.043501
6	-2.018805	-2.442369	0.055142
1	-1.364106	-2.675214	-0.792500
1	-1.446918	-2.594489	0.979997
1	-2.862692	-3.128672	0.044666
6	-2.018640	2.442458	0.054649
1	-1.446915	2.594762	0.979567
1	-1.363766	2.675030	-0.792934
1	-2.862469	3.128827	0.043854
1	-4.618396	1.370142	-0.210126
1	-4.618484	-1.369945	-0.209818
1	4.618588	1.369795	-0.209770
1	4.618270	-1.370331	-0.210135

(NHC^{Me})–Be–(NHC^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-0.000004	0.000095	0.335600
6	-1.631445	0.000034	0.076940
7	-2.486272	1.088811	-0.017201
7	-2.486343	-1.088708	-0.016940
6	-3.802424	0.674963	-0.132997

(NHC^{Ph})–Be–(NHC^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	0.004938	0.087564	-0.003803
6	0.007014	-1.590901	-0.002210
7	-0.963996	-2.455672	-0.493946
7	0.980793	-2.452296	0.489859
6	-0.594153	-3.779403	-0.295266

6	0.615555	-3.777316	0.291244
6	-0.005591	1.720691	-0.000382
7	-0.998305	2.592201	0.495618
7	0.981252	2.599202	-0.495649
6	-0.613924	3.912289	0.299076
6	0.587662	3.916579	-0.300031
1	-1.210866	-4.596211	-0.619643
1	1.235035	-4.591971	0.615768
1	-1.233390	4.742541	0.578077
1	1.201169	4.751063	-0.579653
6	2.133781	-2.085927	1.239025
6	3.368409	-2.644771	0.912413
6	2.022649	-1.227594	2.332578
6	4.490088	-2.338669	1.677400
1	3.450471	-3.303084	0.058031
6	3.147045	-0.925710	3.085605
1	1.059726	-0.803888	2.579370
6	4.386011	-1.474947	2.758679
1	5.447116	-2.770468	1.416375
1	3.053888	-0.264785	3.936983
1	5.260690	-1.231719	3.346538
6	-2.119143	-2.093403	-1.241798
6	-3.350990	-2.658140	-0.914768
6	-2.012897	-1.232968	-2.334162
6	-4.474752	-2.355901	-1.678185
1	-3.429345	-3.317948	-0.061195
6	-3.139369	-0.934973	-3.085624
1	-1.052136	-0.804507	-2.581179
6	-4.375574	-1.490157	-2.758318
1	-5.429611	-2.792259	-1.416798
1	-3.049980	-0.272366	-3.936100
1	-5.251906	-1.249896	-3.344932
6	-2.146152	2.178354	1.157097
6	-2.849726	3.039427	2.016079
6	-2.595515	0.856596	1.014076
6	-3.961535	2.588082	2.703310
1	-2.506488	4.051940	2.172502
6	-3.713871	0.416183	1.715357
1	-2.150875	0.207600	0.273285
6	-4.403366	1.269416	2.562901
1	-4.482256	3.265756	3.367321
1	-4.052440	-0.601937	1.576430
1	-5.272786	0.922379	3.104136
6	2.132011	2.191055	-1.154826
6	2.831832	3.053670	-2.015222
6	2.587047	0.871385	-1.008766
6	3.945227	2.605592	-2.701882
1	2.484300	4.064525	-2.173087
6	3.707346	0.434362	-1.709420
1	2.149165	0.224135	-0.261978
6	4.392464	1.288790	-2.559098
1	4.463129	3.284081	-3.367252
1	4.050856	-0.581757	-1.568122
1	5.263052	0.944340	-3.100112

L-E-L

(NHC^{R})–E–(NHC^{R})

MAGNESIUM

(NHC^{H})–Mg–(NHC^{H})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	-1.014596	2.719178	-0.000044
6	1.631110	-0.551940	-0.000027
7	2.721458	-1.361994	-0.000005
7	2.199745	0.676538	0.000002
6	3.921615	-0.666425	0.000046
6	3.582167	0.642008	0.000036
6	-2.069386	0.500187	-0.000026
7	-1.379170	-0.659625	-0.000021
7	-3.361727	0.084585	-0.000047
6	-2.207454	-1.762886	0.000042
6	-3.478342	-1.294092	0.000071
1	4.883266	-1.145838	0.000070
1	4.191028	1.527298	0.000065
1	-4.422366	-1.807773	0.000125
1	-1.837877	-2.772275	0.000063
1	2.649234	-2.363292	-0.000018
1	1.645714	1.530126	-0.000003
1	-4.138026	0.723177	-0.000099
1	-0.336225	-0.699204	-0.000036

(NHC^{Me})–Mg–(NHC^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	-0.000001	-0.000014	1.735934
6	1.731564	-0.000030	0.145810
7	2.526679	-1.069324	-0.164102
7	2.527099	1.069039	-0.163798
6	3.770685	-0.676531	-0.632438
6	3.770938	0.675891	-0.632279
6	-1.731560	0.000034	0.145803
7	-2.526692	1.069326	-0.164072
7	-2.527084	-1.069034	-0.163833
6	-3.770673	0.676532	-0.632473
6	-3.770912	-0.675888	-0.632347
6	-2.099017	-2.443554	0.006140
1	-1.434078	-2.751657	-0.802960
1	-1.570217	-2.536762	0.960253
1	-2.968902	-3.099100	0.020550
6	-2.098118	2.443724	0.005604
1	-1.569406	2.536979	0.959762
1	-1.432956	2.751360	-0.803490
1	-2.967754	3.099605	0.019732
6	2.099033	2.443560	0.006178
1	1.434120	2.751678	-0.802937
1	1.570207	2.536759	0.960277
1	2.968922	3.099100	0.020621
6	2.098071	-2.443723	0.005490
1	1.569376	-2.537028	0.959653
1	1.432884	-2.751287	-0.803610
1	2.967691	-3.099627	0.019554
1	4.535588	-1.378393	-0.915353
1	4.536104	1.377533	-0.915025
1	-4.536062	-1.377533	-0.915133
1	-4.535575	1.378394	-0.915391

(NHC^{Ph})–Mg–(NHC^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	0.180925	0.075311	1.275482
6	0.903767	-1.599154	-0.202904
7	2.091292	-2.251121	0.005935
7	0.202144	-2.495605	-0.968606
6	2.114889	-3.500995	-0.591520
6	0.922753	-3.661076	-1.198616
6	-0.958108	1.628682	0.194983

7	-0.480429	2.839729	-0.300769
7	-2.263989	1.937281	0.562620
6	-1.453576	3.830169	-0.217317
6	-2.553112	3.273680	0.317028
1	2.968617	-4.150057	-0.528332
1	0.536554	-4.470574	-1.789268
1	-1.308687	4.832934	-0.568075
1	-3.516594	3.709095	0.500343
6	-1.085953	-2.272395	-1.545255
6	-2.083263	-3.229284	-1.381270
6	-1.320197	-1.131233	-2.305519
6	-3.322809	-3.040951	-1.983146
1	-1.893786	-4.105642	-0.776206
6	-2.562413	-0.949991	-2.899720
1	-0.536254	-0.397981	-2.421608
6	-3.564768	-1.901771	-2.740279
1	-4.100072	-3.781139	-1.849526
1	-2.744179	-0.063212	-3.491567
1	-4.531123	-1.754083	-3.203157
6	3.203184	-1.739940	0.756081
6	3.151675	-1.728255	2.146372
6	4.337582	-1.306563	0.082503
6	4.255887	-1.280794	2.864163
1	2.261902	-2.073332	2.652450
6	5.436081	-0.852985	0.807866
1	4.355985	-1.323496	-0.998958
6	5.393046	-0.839175	2.196847
1	4.221211	-1.272321	3.944990
1	6.320311	-0.512360	0.286472
1	6.246811	-0.486434	2.759978
6	0.829698	3.042307	-0.761246
6	1.313710	4.331085	-1.024453
6	1.696621	1.950802	-0.915879
6	2.618696	4.520016	-1.447668
1	0.682496	5.195706	-0.884602
6	3.004002	2.158109	-1.344665
1	1.331701	0.942333	-0.785716
6	3.477502	3.433365	-1.612479
1	2.969653	5.524869	-1.642666
1	3.655243	1.302855	-1.466080
1	4.497646	3.585051	-1.937749
6	-3.124068	1.034257	1.199958
6	-4.196670	1.485653	1.979984
6	-2.858448	-0.341372	1.137145
6	-5.005809	0.582113	2.646316
1	-4.383227	2.544057	2.090997
6	-3.685401	-1.238967	1.811108
1	-2.105857	-0.705978	0.455405
6	-4.758267	-0.791026	2.562342
1	-5.827426	0.949703	3.246793
1	-3.479617	-2.298356	1.735964
1	-5.392915	-1.493239	3.085511

E-L

E–(NHC^{R})

BERYLLIUM

Be–(NHC^{H})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-2.793886	-0.000732	0.001099
6	-0.921379	-0.002342	-0.000715

7	-0.091745	-1.057636	-0.000365
7	-0.095938	1.056165	-0.000292
6	1.234777	-0.675714	0.000273
6	1.232090	0.679554	0.000351
1	2.048855	-1.377551	0.000645
1	2.043314	1.384671	0.000770
1	-0.442054	2.005664	-0.000211
1	-0.433714	-2.008545	-0.000459

Be–(NHC^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	-0.000004	2.525414	-0.440626
6	0.000000	0.747635	0.146223
7	1.072939	-0.081570	0.049928
7	-1.072938	-0.081571	0.049927
6	0.677913	-1.390858	-0.118813
6	-0.677912	-1.390859	-0.118806
6	-2.449854	0.383422	0.112434
1	-2.811562	0.393129	1.139729
1	-2.492778	1.396548	-0.291652
1	-3.081671	-0.268594	-0.487458
6	2.449855	0.383424	0.112436
1	2.492780	1.396545	-0.291664
1	2.811558	0.393145	1.139731
1	3.081674	-0.268600	-0.487445
1	-1.377922	-2.199212	-0.229277
1	1.377924	-2.199210	-0.229288

Be–(NHC^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	0.000170	-1.636667	1.133055
6	-0.000002	-0.224165	-0.012707
7	-1.085667	0.609042	-0.159613
7	1.085662	0.609058	-0.159619
6	-0.674867	1.918496	-0.348477
6	0.674841	1.918511	-0.348431
1	-1.360147	2.728219	-0.511396
1	1.360110	2.728246	-0.511339
6	2.416241	0.149016	-0.086993
6	3.454462	1.014227	0.264448
6	2.682398	-1.205750	-0.307122
6	4.749355	0.531688	0.366037
1	3.250843	2.052179	0.486443
6	3.985579	-1.678281	-0.188070
1	1.889020	-1.867011	-0.624255
6	5.021778	-0.816640	0.139444
1	5.547759	1.208208	0.639715
1	4.183956	-2.727099	-0.361553
1	6.033637	-1.188398	0.224325
6	-2.416250	0.148999	-0.086966
6	-3.454473	1.014221	0.264436
6	-2.682406	-1.205769	-0.307068
6	-4.749371	0.531685	0.366010
1	-3.250861	2.052177	0.486412
6	-3.985585	-1.678295	-0.188034
1	-1.889004	-1.867047	-0.624104
6	-5.021794	-0.816643	0.139439
1	-5.547777	1.208213	0.639662
1	-4.183960	-2.727117	-0.361495
1	-6.033655	-1.188396	0.224310

E-L

E–(NHC^{R})

MAGNESIUM

Mg–(NHC^{H})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	2.940347	-0.004755	-0.003799
6	0.274142	-0.076862	0.008957
7	-0.642941	-1.072895	0.003319

7	-0.511396	1.025090	0.004136
1	-0.379574	-2.043406	0.005309
6	-1.951082	-0.614556	-0.004648
1	-0.125929	1.954892	0.005738
6	-1.866093	0.734424	-0.004113
1	-2.806809	-1.264699	-0.010089
1	-2.633300	1.486866	-0.008733

Mg–(NHC^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	2.900215	-0.000179	-0.226555
6	0.269927	-0.000023	0.296939
7	-0.547769	1.064322	0.077288
7	-0.547925	-1.064259	0.077284
6	-1.830565	0.676168	-0.268166
6	-1.830648	-0.675921	-0.268205
1	-2.617841	1.376400	-0.483417
1	-2.618024	-1.376033	-0.483485
6	-0.124821	-2.447500	0.213169
1	0.954066	-2.467385	0.338842
1	-0.592656	-2.911281	1.081999
1	-0.388724	-3.013931	-0.679737
6	-0.124466	2.447505	0.213161
1	-0.592248	2.911362	1.081979
1	0.954422	2.467235	0.338849
1	-0.388275	3.013962	-0.679756
6	3.424229	1.068874	0.416512
6	2.732447	-0.943031	-0.723701
6	4.738797	0.621565	0.399058
1	3.181730	2.006902	0.895751
6	4.049150	-1.384694	-0.726422
1	1.946414	-1.532468	-1.171622
6	5.057563	-0.604792	-0.173041
1	5.512779	1.230059	0.847214
1	4.285216	-2.342491	-1.170067
1	6.081828	-0.951651	-0.181615
6	-2.419462	0.290887	-0.155754
6	-3.424229	1.068870	0.416518
6	-2.732448	-0.943028	-0.723707
6	-4.738795	0.621563	0.399062
1	-3.181727	2.006895	0.895762
6	-4.049152	-1.384690	-0.726430
1	-1.946417	-1.532464	-1.171633
6	-5.057563	-0.604790	-0.173045
1	-5.512777	1.230055	0.847222
1	-4.285218	-2.342484	-1.170081
1	-6.081830	-0.951648	-0.181619

Mg–(NHC^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	0.000000	-2.134801	1.502096
6	0.000001	-0.116989	-0.138541
7	-1.070617	0.736114	-0.145609
7	1.070617	0.736115	-0.145615
6	-0.673546	2.069047	-0.139403
6	0.673546	2.069047	-0.139425
1	-1.364936	2.889470	-0.180699
1	1.364934	2.889471	-0.180747
6	2.419463	0.290889	-0.155754

E-L

E–(Nac^{R})

BERYLLIUM

Be–(Nac^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 2

7	0.000000	1.535270	-0.471596
7	0.000000	-1.535270	-0.471596
6	0.000000	1.293134	0.793400
6	0.000000	-1.293134	0.793400

6	0.000000	0.000000	1.389990
1	0.000000	2.125964	1.511352
1	0.000000	-2.125964	1.511352
1	0.000000	0.000000	2.473713
6	0.000000	2.914620	-0.883291
1	0.874485	3.099129	-1.513127
1	-0.874485	3.099129	-1.513127
1	0.000000	3.632839	-0.051404
6	0.000000	-2.914620	-0.883291
1	-0.874485	-3.099129	-1.513127
1	0.874485	-3.099129	-1.513127
1	0.000000	-3.632839	-0.051404
6	2.898641	-1.245560	0.720864
6	3.704173	0.603340	-0.595794
6	4.163738	-1.816495	0.684487
1	2.087707	-1.731373	1.246326
6	4.968854	0.030697	-0.619884
1	3.520830	1.520547	-1.138739
6	5.206900	-1.180239	0.021247
1	4.334789	-2.760335	1.185280
1	5.766236	0.525432	-1.158886
1	6.192245	-1.625772	-0.002463
6	-2.656068	-0.024606	-0.085605
6	-2.898641	-1.245560	-0.720865
6	-3.704173	0.603339	0.595795
6	-4.163739	-1.816495	-0.684487
1	-2.087707	-1.731372	-1.246327
6	-4.968854	0.030697	0.619885
1	-3.520829	1.520546	1.138739
6	-5.206900	-1.180239	-0.021247
1	-4.334789	-2.760335	-1.185280
1	-5.766235	0.525432	1.158887
1	-6.192245	-1.625772	0.002463

Be–(Nac^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 2:wq

4	0.000000	-0.372667	-0.000001
7	-1.349300	0.526363	-0.105449
7	1.349300	0.526363	0.105449
6	-1.211095	1.856484	-0.170529
6	1.211095	1.856484	0.170529
6	0.000000	2.515138	0.000000
1	-2.097766	2.447948	-0.376046
1	2.097766	2.447948	0.376046
1	0.000000	3.594398	0.000000
6	2.656068	-0.024606	0.085605

E-L

E–(Nac^{R})

MAGNESIUM

Mg–(Nac^{Me})

B3LYP/def2-TZVPP optimized geometry (Å).

0 2

12	0.000000	0.000000	1.537311
7	0.000064	-1.516552	0.143035
7	-0.000064	1.516552	0.143035
6	0.000000	-1.253098	-1.146492

6	0.000000	1.253098	-1.146492
6	0.000000	0.000000	-1.766199
1	-0.000039	-2.109460	-1.825817
1	0.000039	2.109460	-1.825817
1	0.000000	0.000000	-2.845996
6	0.000090	-2.919696	0.539385
1	-0.878957	-3.150964	1.146423
1	-0.000434	-3.587233	-0.327053
1	0.879656	-3.151197	1.145572
6	-0.000090	2.919696	0.539385
1	0.878957	3.150964	1.146423
1	0.000434	3.587233	-0.327053
1	-0.879656	3.151197	1.145572

Mg–(Nac^{Ph})

B3LYP/def2-TZVPP optimized geometry (Å).

0 2

12	0.000000	0.000000	0.994113
7	-0.056504	1.519557	-0.428327
7	0.056504	-1.519557	-0.428327
6	-0.032409	1.254523	-1.724122
6	0.032409	-1.254523	-1.724122
6	0.000000	0.000000	-2.334339
1	-0.058517	2.105863	-2.404060
1	0.058517	-2.105863	-2.404060
1	0.000000	0.000000	-3.414427
6	0.000000	2.874166	-0.022547
6	-0.791574	3.299300	1.050225
6	0.859707	3.799893	-0.626492
6	-0.739613	4.614315	1.491881
1	-1.464964	2.595496	1.522815
6	0.903768	5.115424	-0.183347
1	1.516125	3.478986	-1.424197
6	0.104828	5.531481	0.875907
1	-1.366314	4.923290	2.318168
1	1.578810	5.814393	-0.659994
1	0.145800	6.555287	1.222078
6	0.000000	-2.874166	-0.022547
6	0.791574	-3.299300	1.050225
6	-0.859707	-3.799893	-0.626492
6	0.739613	-4.614315	1.491881
1	1.464964	-2.595496	1.522815
6	-0.903768	-5.115424	-0.183347
1	-1.516125	-3.478986	-1.424197
6	-0.104828	-5.531481	0.875907
1	1.366314	-4.923290	2.318168
1	-1.578810	-5.814393	-0.659994
1	-0.145800	-6.555287	1.222078

L

NHC^{R}

NHC^{H}

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

6	-0.000002	-1.271606	-0.000011
7	1.048172	-0.402784	-0.000085
7	-1.048172	-0.402782	-0.000086
6	0.675216	0.934854	0.000096
6	-0.675214	0.934856	0.000100
1	1.376997	1.748801	-0.000315

1	-1.376994	1.748804	-0.000336
1	1.999281	-0.723634	0.000362
1	-1.999282	-0.723629	0.000370

NHC^{Me}

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

6	-0.000001	-0.976908	-0.000965
7	1.060859	-0.121437	-0.000724
7	-1.060860	-0.121435	-0.000701
6	0.675797	1.210190	0.000424
6	-0.675796	1.210191	0.000431
6	-2.439624	-0.570696	0.000540
1	-2.965243	-0.214134	-0.886643
1	-2.432479	-1.656372	0.001258
1	-2.963491	-0.213771	0.888624
6	2.439624	-0.570697	0.000551
1	2.432482	-1.656372	0.001057
1	2.965316	-0.213956	-0.886517
1	2.963416	-0.213944	0.888749
1	1.374536	2.028088	-0.001244
1	-1.374533	2.028090	-0.001190

NHC^{Ph}

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

6	0.000000	-0.349883	-0.000167
6	0.673303	1.848826	-0.004793
1	1.366812	2.669603	-0.030186
6	-0.673315	1.848821	0.004693
1	-1.366830	2.669592	0.030144
7	1.064990	0.507524	-0.007563
7	-1.064993	0.507517	0.007457
6	2.419986	0.063718	-0.022786
6	2.738246	-1.155359	-0.619712
6	3.422966	0.837281	0.558630
6	4.056558	-1.591003	-0.633101
1	1.944172	-1.745481	-1.054662
6	4.742349	0.397103	0.529179
1	3.177550	1.767102	1.054800
6	5.065481	-0.817016	-0.065521
1	4.297281	-2.539173	-1.098085
1	5.515420	1.003240	0.985263
1	6.092598	-1.159235	-0.083978
6	-2.419986	0.063705	0.022769
6	-2.738195	-1.155423	0.619619
6	-3.423014	0.837316	-0.558500
6	-4.056505	-1.591068	0.633082
1	-1.944084	-1.745581	1.054452
6	-4.742394	0.397133	-0.528977
1	-3.177638	1.767178	-1.054613
6	-5.065476	-0.817035	0.065649
1	-4.297189	-2.539278	1.098007
1	-5.515504	1.003307	-0.984948
1	-6.092591	-1.159257	0.084162

L
Nac^{R}

Nac^{Me}

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

7	0.000000	1.535270	-0.471596
7	0.000000	-1.535270	-0.471596
6	0.000000	1.293134	0.793400
6	0.000000	-1.293134	0.793400
6	0.000000	0.000000	1.389990
1	0.000000	2.125964	1.511352
1	0.000000	-2.125964	1.511352

1	0.000000	0.000000	2.473713
6	0.000000	2.914620	-0.883291
1	0.874485	3.099129	-1.513127
1	-0.874485	3.099129	-1.513127
1	0.000000	3.632839	-0.051404
6	0.000000	-2.914620	-0.883291
1	-0.874485	-3.099129	-1.513127
1	0.874485	-3.099129	-1.513127
1	0.000000	-3.632839	-0.051404
1	3.598378	1.437399	1.298013
6	4.595639	-1.661670	-0.768516
1	2.543356	-1.697485	-1.414788
6	5.559605	-1.014896	0.007813
1	5.906962	0.610270	1.368033
1	4.866053	-2.545141	-1.336270
1	6.574486	-1.389041	0.055143
6	-2.892281	-0.040286	0.108423
6	-3.878177	0.587659	-0.689412
6	-3.294437	-1.192972	0.820871
6	-5.180503	0.107958	-0.738096
1	-3.598377	1.437397	-1.298015
6	-4.595639	-1.661669	0.768518
1	-2.543356	-1.697486	1.414788
6	-5.559605	-1.014895	-0.007811
1	-5.906963	0.610270	-1.368031
1	-4.866054	-2.545139	1.336273
1	-6.574487	-1.389039	-0.055139

Nac^{Ph}

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

7	1.580187	0.356177	-0.189605
7	-1.580186	0.356175	0.189600
6	1.273317	1.622775	-0.085615
6	-1.273317	1.622774	0.085616
6	0.000000	2.210936	0.000001
1	2.093034	2.359078	-0.099654
1	-2.093034	2.359076	0.099661
1	-0.000001	3.294917	0.000004
6	2.892281	-0.040284	-0.108425
6	3.878177	0.587660	0.689411
6	3.294438	-1.192972	-0.820871
6	5.180502	0.107958	0.738097

E_2

BERYLLIUM

Be_2

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

4	0.000000	0.000000	1.254733
4	0.000000	0.000000	-1.254733

MAGNESIUM

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Mg_2

B3LYP/def2-TZVPP optimized geometry (Å).

0 1

12	0.000000	0.000000	1.977120
12	0.000000	0.000000	-1.977120