Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

Effects of the electronic structure of five-membered N-heterocyclic carbenes on insertion of silanes and boranes into the NHC C-N bond

Kalon J. Iversen, David J. D. Wilson and Jason L. Dutton**

david.wilson@latrobe.edu.au, j.dutton@latrobe.edu.au

Department of Chemistry, La Trobe Institute for Molecular Sciences, La Trobe University, Melbourne, Victoria, Australia

Table of Contents

Computational methods

All theoretical calculations were performed using the Gaussian 09 program.[1] Geometry optimisations were carried out using the M06-2X density functional[2] and def2-TZVP basis set.[3] Frequency calculations, performed at the same theory level, indicated that all optimised structures were minima on the potential energy surface. Transition state optimisations used the quadratic synchronous transit (QST) method.[4] All transition states were also confirmed using intrinsic reaction coordinate (IRC)[5] analysis. Thermodynamic corrections for energy values were taken from these calculations (standard T = 298.15 K and p = 1 atm). Geometry optimisations were also performed using other density functionals (B3LYP[6, 7] and PBE[8]) and basis sets (6-31G(d)[9, 10] and def2-SVP[11]), all of which produced comparable geometries. Single-point energies were calculated at the M06-2X/def2-TZVP geometries, including MP2, SOS-MP2[12] and SCS-MP2[13] energies. All reported ΔG values are SCS-MP2 energies with M06-2X/def2-TZVP thermochemical corrections. Molecular orbital (MO) analysis was carried out at the B3LYP/def2-TZVP level of theory at the M06-2X optimized geometries, as the results provided good agreement with previous studies. NBO analysis was carried out with NBO 5.9.[14]

References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, Revision D.1, 2009.
2. Y. Zhao and D. G. Truhlar, *Theor Chem Account*, 2008, **120**, 215-241.
3. A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Physics*, 1994, **100**, 5829-5835.
4. C. Peng, P. Y. Ayala, H. B. Schlegel and M. J. Frisch, *J. Comput. Chem.*, 1996, **17**, 49-56.
5. K. Fukui, *Account. Chem. Research.*, 1981, **14**, 363-368.
6. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.
7. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
8. M. Ernzerhof and J. P. Perdew, *J. Chem. Phys.*, 1998, **109**, 3313-3320.
9. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.
10. P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213-222.
11. A. Schäfer, H. Horn and R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571-2577.
12. Y. Jung, R. C. Lochan, A. D. Dutoi and M. Head-Gordon, *J. Chem. Phys.*, 2004, **121**, 9793-9802.
13. S. Grimme, *J. Chem. Phys.*, 2003, **118**, 9095-9102.
14. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales and F. Weinhold, NBO 5.9. see http://www.chem.wisc.edu/~nbo5, Theoretical Chemistry Institute, University of Wisconsin, Madison, WI2011.

Cartesian coordinates for starting NHC compounds (compounds 1-5)

NHC 1

E_e = -304.776887622 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.000000	0.000000	0.978473
N	0.000000	1.055682	0.122718
C	0.000000	0.674418	-1.204754
C	0.000000	-0.674418	-1.204754
N	0.000000	-1.055682	0.122718
C	0.000000	-2.433262	0.565404
C	0.000000	2.433262	0.565404
H	0.000000	-1.378756	-2.018578
H	0.000000	1.378756	-2.018578
H	0.888581	-2.952470	0.204413
H	-0.888581	2.952470	0.204413
H	0.000000	-2.427104	1.651401
H	0.000000	2.427104	1.651401
H	0.888581	2.952470	0.204413
H	-0.888581	-2.952470	0.204413

NHC 2

E_e = -305.971903732 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.000000	0.000000	1.016364
N	0.000000	1.068516	0.206579
C	-0.101795	0.757398	-1.221955
C	0.101795	-0.757398	-1.221955
N	0.000000	-1.068516	0.206579
C	0.135978	-2.428429	0.652805
C	-0.135978	2.428429	0.652805
H	1.104440	-2.845949	0.356759
H	-1.104440	2.845949	0.356759
H	0.059160	-2.439655	1.736723
H	-0.059160	2.439655	1.736723
H	0.650717	3.057707	0.227387
H	-0.650717	-3.057707	0.227387
H	1.086350	-1.047473	-1.603688
H	-0.655529	-1.292848	-1.797433
H	0.655529	1.292848	-1.797433
H	-1.086350	1.047473	-1.603688

NHC 3

E_e = -383.402962226 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.000029	1.563271	-0.000006
N	-1.053499	0.707316	0.000037
C	-0.676758	-0.630651	0.000024
C	0.676785	-0.630618	-0.000005
N	1.053470	0.707350	-0.000057
C	2.428313	1.152610	0.000032
C	-2.428340	1.152583	-0.000023
H	2.954082	0.795580	-0.887291
H	-2.954028	0.795796	0.887449
H	2.416970	2.238675	0.000039
H	-2.416981	2.238648	-0.000292
H	-2.954070	0.795336	-0.887279
H	2.953951	0.795577	0.887432
C	-1.660622	-1.745664	0.000018
H	-1.144719	-2.704296	0.000115
H	-2.305288	-1.712274	0.881286
H	-2.305148	-1.712369	-0.881354
C	1.660672	-1.745622	-0.000021
H	2.305403	-1.712162	0.881196
H	1.144770	-2.704255	0.000168
H	2.305136	-1.712374	-0.881444

NHC 4

E_e = -1223.97598149 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.000000	0.000000	1.939465
N	0.000000	1.062347	1.089843
C	0.000000	0.675208	-0.233169
C	0.000000	-0.675208	-0.233169
N	0.000000	-1.062347	1.089843
C	0.000000	-2.441162	1.534031
C	0.000000	2.441162	1.534031
H	0.887755	-2.959096	1.171413
H	-0.887755	2.959096	1.171413
H	0.000000	-2.421003	2.619552
H	0.000000	2.421003	2.619552
H	0.887755	2.959096	1.171413
H	-0.887755	-2.959096	1.171413
Cl	0.000000	-1.755806	-1.542050
Cl	0.000000	1.755806	-1.542050

NHC 5

E_e = -458.423106664 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.011259	0.000227	0.000005
N	1.168475	1.068800	0.000071
N	1.168772	-1.068551	0.000069
C	1.614764	-2.442189	-0.000115
C	1.614134	2.442522	-0.000093
H	1.251879	-2.962236	-0.888520
H	1.251134	2.962707	0.888169
H	2.700795	-2.435760	-0.000169
H	2.700163	2.436298	-0.000114
H	1.251179	2.962509	-0.888507
H	1.251893	-2.962448	0.888153
C	-1.347841	-1.422152	0.000126
C	-2.532670	-0.698959	-0.000092
C	-2.532849	0.698424	-0.000107
C	-1.348193	1.421867	0.000094
C	-0.165772	0.697535	0.000106
C	-0.165587	-0.697571	0.000119
H	-1.348709	-2.504261	0.000163
H	-3.476473	-1.227741	-0.000253
H	-3.476782	1.226978	-0.000277
H	-1.349268	2.503979	0.000116

Cartesian coordinates for reactant silane and boranes

H_2SiPh_2

E_e = -753.950242086 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.000000	0.000000	1.548782
H	-1.167494	0.267033	2.420418
H	1.167494	-0.267033	2.420418
C	0.267002	1.516048	0.487584
C	0.970985	1.447628	-0.717794
C	-0.217171	2.760249	0.897290
C	1.187966	2.583596	-1.484237
H	1.348331	0.492275	-1.067403
C	0.000000	3.900766	0.136606
H	-0.776449	2.840707	1.823149
C	0.703770	3.812770	-1.056178
H	1.734122	2.511313	-2.416294
H	-0.382818	4.856280	0.472204
H	0.873129	4.700004	-1.653175
C	-0.267002	-1.516048	0.487584
C	-0.970985	-1.447628	-0.717794
C	0.217171	-2.760249	0.897290
C	-1.187966	-2.583596	-1.484237
H	-1.348331	-0.492275	-1.067403
C	0.000000	-3.900766	0.136606
H	0.776449	-2.840707	1.823149
C	-0.703770	-3.812770	-1.056178
H	-1.734122	-2.511313	-2.416294
H	0.382818	-4.856280	0.472204
H	-0.873129	-4.700004	-1.653175

H_2BMe

E_e = -65.9220657636 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

B	-0.871069	-0.000011	-0.021386
H	-1.481158	-1.023097	0.008701
H	-1.481038	1.023160	0.008746
C	0.682092	0.000000	-0.016223
H	0.939623	-0.000023	1.055810
H	1.142719	-0.894210	-0.434484
H	1.142644	0.894225	-0.434502

H_1BMe_2

E_e = -105.248599578 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

B	0.000004	0.559534	-0.000034
H	-0.000049	1.755454	0.000024
C	1.368076	-0.192888	-0.013273
H	1.699356	-0.206848	1.035999
H	1.308854	-1.233737	-0.334321
H	2.157067	0.321346	-0.562785
C	-1.368051	-0.192926	0.013257
H	-2.156636	0.320919	0.563731
H	-1.700041	-0.205883	-1.035794
H	-1.308719	-1.234038	0.333416

BMe_3

E_e = -144.573890433 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

B	-0.001526	0.005872	-0.021205
C	1.295824	0.891022	-0.010571
H	1.592950	0.990451	1.042700
H	2.142663	0.415090	-0.509457
H	1.165982	1.901461	-0.398755
C	0.128575	-1.558504	0.012099
H	-0.703224	-2.061008	0.508995
H	0.094005	-1.884038	-1.037389
H	1.073101	-1.924990	0.416899
C	-1.425247	0.668943	-0.011142
H	-1.653878	0.885433	1.041980
H	-1.476234	1.624840	-0.534331
H	-2.222647	0.014639	-0.366939

Cartesian coordinates for optimized insertion pathway compounds H_2SiPh_2-NHC 1

H_2SiPh_2-NHC 1, A

E_e = -1058.72615285 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.089850	-0.213159	-0.024862
C	1.894429	-0.861709	-0.132605
C	2.621662	-1.166018	1.020094
C	2.524662	-1.048728	-1.363372
C	3.924408	-1.641931	0.951191
H	2.148427	-1.026153	1.987522
C	3.830499	-1.516384	-1.445770
H	1.973672	-0.824564	-2.270824
C	4.532740	-1.815295	-0.285890
H	4.466345	-1.881143	1.858320
H	4.300182	-1.651550	-2.412729
H	5.549283	-2.184413	-0.345208
C	-1.544667	-1.198639	0.155308
C	-2.149598	-1.805097	-0.947303
C	-2.183236	-1.319079	1.390187
C	-3.342003	-2.506099	-0.826845
H	-1.669387	-1.723404	-1.917956
C	-3.384284	-2.005897	1.521729
H	-1.721890	-0.868210	2.262780
C	-3.965342	-2.602965	0.411140
H	-3.786941	-2.977850	-1.694747
H	-3.864212	-2.082772	2.490057
H	-4.898094	-3.144636	0.509718
C	-0.219610	1.746353	-0.077460
C	-0.056271	3.936947	0.341157
C	-1.148022	3.749686	-0.434273
H	0.376208	4.833767	0.747132
H	-1.863153	4.448950	-0.829266
N	0.496264	2.695066	0.549091
N	-1.224214	2.399472	-0.684813
C	-2.280917	1.749011	-1.448447
H	-3.054783	1.378330	-0.777749
H	-2.701573	2.471265	-2.144241
H	-1.848749	0.911323	-1.990690
C	1.672061	2.433217	1.368587
H	2.264014	3.344003	1.422520
H	1.366980	2.119040	2.365078
H	2.259867	1.639458	0.913601
H	-0.033830	-0.197153	-1.580561
H	0.216311	-0.026067	1.520806

H_2SiPh_2-NHC 1, T1

E_e = -1058.70420902 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.000014	-0.065590	0.646516
C	1.598066	-0.951416	0.189932
C	2.431794	-1.396913	1.218103
C	1.968060	-1.245386	-1.124645
C	3.608075	-2.084778	0.946814
H	2.157414	-1.199076	2.248819
C	3.134573	-1.943352	-1.402927
H	1.337353	-0.909076	-1.939470
C	3.961579	-2.358190	-0.366535
H	4.245155	-2.409923	1.759902
H	3.400016	-2.164999	-2.429289
H	4.874814	-2.898255	-0.583074
C	-1.598098	-0.951341	0.190002
C	-1.968323	-1.245113	-1.124558
C	-2.431666	-1.396973	1.218245
C	-3.134899	-1.943010	-1.402743
H	-1.337744	-0.908697	-1.939440
C	-3.608006	-2.084777	0.947055
H	-2.157109	-1.199289	2.248942
C	-3.961738	-2.357988	-0.366272
H	-3.400526	-2.164493	-2.429093
H	-4.244956	-2.410021	1.760205
H	-4.875022	-2.898000	-0.582737
C	0.000035	1.770386	0.291400
C	0.670381	3.800253	-0.413060
C	-0.670161	3.800274	-0.413139
H	1.372001	4.565368	-0.693713
H	-1.371720	4.565407	-0.693892
N	1.089510	2.599849	0.148184
N	-1.089401	2.599892	0.148084
C	-2.447150	2.125529	0.048896
H	-2.689717	1.487809	0.896577
H	-3.115792	2.984056	0.045763
H	-2.582868	1.548062	-0.872032
C	2.447279	2.125474	0.049411
H	3.115907	2.984012	0.046150
H	2.689696	1.488016	0.897334
H	2.583196	1.547741	-0.871322
H	0.000073	0.786356	-1.055447
H	0.000039	-0.251001	2.144841

H_2SiPh_2-NHC 1, B

E_e = -1058.75214088 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.090443	-0.016144	0.986195
C	-0.960847	1.391125	0.357352
C	-0.729678	2.675070	0.860185
C	-1.956333	1.227033	-0.608931
C	-1.468675	3.762817	0.419109
H	0.040431	2.830182	1.609722
C	-2.697430	2.314738	-1.053038
H	-2.154426	0.243127	-1.016259
C	-2.456466	3.581402	-0.540084
H	-1.277792	4.748824	0.823689
H	-3.466460	2.171781	-1.801782
H	-3.037541	4.427395	-0.885478
C	1.873569	0.221459	0.468661
C	2.214039	1.040143	-0.610291
C	2.893868	-0.490027	1.106592
C	3.529921	1.138880	-1.043629
H	1.439445	1.603075	-1.119934
C	4.209602	-0.396507	0.676610
H	2.658345	-1.127349	1.953193
C	4.528042	0.418203	-0.402452
H	3.776963	1.777391	-1.882447
H	4.987458	-0.954033	1.183024
H	5.553982	0.494306	-0.739885
C	-0.549786	-1.685951	0.336227
C	-2.511754	-2.535172	-0.476891
C	-1.657220	-2.492056	-1.495154
H	-3.521781	-2.911772	-0.455915
H	-1.796104	-2.829480	-2.509529
N	-1.984134	-1.847287	0.636700
N	-0.489294	-1.778853	-1.136136
C	0.757882	-2.318528	-1.645573
H	0.968385	-3.311052	-1.218860
H	0.693219	-2.407238	-2.729775
H	1.584307	-1.651651	-1.404365
C	-2.260345	-2.397836	1.945685
H	-3.336598	-2.510900	2.072366
H	-1.779163	-3.377780	2.086981
H	-1.897239	-1.717925	2.716701
H	0.009055	-2.550744	0.771352
H	0.052982	-0.065903	2.470251

H_2SiPh_2-NHC 1, T2

E_e = -1058.70422682 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	-0.037371	-0.293264	-0.814344
C	0.540058	1.338616	-0.070890
C	1.580890	2.060634	-0.660705
C	-0.091431	1.897670	1.040204
C	1.982899	3.288964	-0.160073
H	2.086129	1.650704	-1.528845
C	0.323694	3.116149	1.565667
H	-0.925575	1.379824	1.500716
C	1.359826	3.815143	0.964916
H	2.782630	3.836403	-0.643629
H	-0.169826	3.523570	2.439204
H	1.677368	4.769669	1.365739
C	-1.915141	-0.272719	-0.456939
C	-2.793746	0.397556	-1.311793
C	-2.467121	-0.907389	0.658826
C	-4.159406	0.437994	-1.067337
H	-2.402104	0.897273	-2.193117
C	-3.832987	-0.873721	0.915714
H	-1.817873	-1.440563	1.348287
C	-4.682573	-0.199838	0.050244
H	-4.818022	0.963938	-1.747747
H	-4.234845	-1.373829	1.788574
H	-5.747621	-0.173629	0.243421
C	0.500197	-1.933730	-0.090862
C	2.748695	-0.829809	0.113654
C	2.237756	-1.310624	1.268548
N	2.020662	-0.961501	-1.028700
N	1.137242	-2.169351	1.073429
C	1.344785	-3.548188	1.510118
H	2.116822	-4.033711	0.905506
H	1.663184	-3.542617	2.551445
H	0.408297	-4.097407	1.432229
C	2.744719	-1.150590	-2.270832
H	2.038840	-1.115913	-3.101318
H	3.473678	-0.343884	-2.412700
H	3.282360	-2.102157	-2.306838
H	0.119099	-2.835363	-0.576173
H	-0.033634	-0.337277	-2.298209
H	2.672872	-1.215407	2.249599
H	3.719414	-0.344682	0.080813

H_2SiPh_2-NHC 1, C

E_e = -1058.73198802 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.111357	1.987550	-1.243455
C	0.868722	3.135422	0.587141
C	0.630237	2.117658	1.475997
H	1.346437	4.054214	0.876988
H	0.941628	2.303176	2.504150
H	-0.513318	2.143116	-2.241318
C	0.441505	4.330199	-1.455003
H	-0.133283	5.083105	-0.919040
H	1.479499	4.651271	-1.526901
H	0.032702	4.177960	-2.448393
C	-0.204553	0.080619	2.333862
H	0.512123	0.255263	3.140840
H	-1.215773	0.225598	2.720489
H	-0.116882	-0.958956	2.017834
N	0.390077	3.065648	-0.708936
N	0.053180	0.963062	1.202734
Si	-0.039845	0.176941	-0.610024
C	-1.736936	-0.591733	-0.261183
C	-2.017024	-1.876641	-0.730536
C	-2.758148	0.092629	0.399459
C	-3.255538	-2.468548	-0.527555
H	-1.249739	-2.424091	-1.268029
C	-4.011758	-0.479356	0.582983
H	-2.569721	1.092648	0.778012
C	-4.259777	-1.765816	0.126163
H	-3.442235	-3.472984	-0.887094
H	-4.794006	0.076492	1.085618
H	-5.232267	-2.218402	0.275220
C	1.531725	-0.878688	-0.269624
C	2.463678	-0.694736	0.756691
C	1.769412	-1.941580	-1.148426
C	3.564867	-1.528924	0.904666
H	2.341761	0.120833	1.459114
C	2.849987	-2.798661	-0.995469
H	1.095277	-2.090488	-1.984282
C	3.756269	-2.592421	0.034433
H	4.274225	-1.349092	1.703431
H	2.991941	-3.618827	-1.688403
H	4.608885	-3.249351	0.153405
H	-0.030073	-0.241464	-2.088755

H_2SiPh_2-NHC 1, T3

E_e = -1058.72120215 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.090787	2.064328	-0.997569
C	1.571217	2.907897	0.470866
C	1.286067	2.032114	1.460259
H	2.356262	3.637449	0.577496
H	1.865750	2.122895	2.375777
H	-0.729795	2.272122	-1.850660
C	1.240295	3.984985	-1.694024
H	1.340409	4.944565	-1.187864
H	2.195414	3.718980	-2.151581
H	0.481787	4.059027	-2.468938
C	0.120073	0.272904	2.623847
H	-0.705241	0.708331	3.193316
H	-0.147317	-0.755557	2.375796
H	1.005684	0.241945	3.266530
N	0.844077	2.961061	-0.736749
N	0.371238	1.026197	1.407949
Si	-0.019018	0.355724	-0.234210
C	-1.776965	-0.284818	-0.161380
C	-2.099589	-1.642562	-0.229855
C	-2.824042	0.625392	0.015635
C	-3.416870	-2.073258	-0.143257
H	-1.311899	-2.378043	-0.343709
C	-4.142987	0.201833	0.098959
H	-2.602522	1.683640	0.102039
C	-4.441854	-1.151181	0.015564
H	-3.643007	-3.130836	-0.198170
H	-4.936729	0.925936	0.234184
H	-5.469212	-1.486864	0.081565
C	1.229455	-1.097189	-0.228155
C	2.237939	-1.265204	0.721281
C	1.160372	-2.043356	-1.257299
C	3.130406	-2.330064	0.657571
H	2.349639	-0.543187	1.521760
C	2.027456	-3.123132	-1.317602
H	0.417729	-1.918824	-2.039542
C	3.020733	-3.268519	-0.356477
H	3.910453	-2.426294	1.402945
H	1.940882	-3.843735	-2.121452
H	3.709623	-4.102375	-0.405434
H	0.345630	0.518863	-1.853716

H_2SiPh_2-NHC 1, D

E_e = -1058.80661076 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.755009	-1.491882	-1.276933
C	2.064684	-2.585952	0.447017
C	1.298368	-2.224738	1.482717
H	0.040229	-2.305608	-1.488908
H	2.806495	-3.357308	0.599207
H	1.450559	-2.719145	2.434158
H	0.899651	-0.942822	-2.211734
C	2.700695	-2.813102	-1.855309
H	3.682754	-3.128040	-1.502577
H	2.118241	-3.707226	-2.122977
H	2.836465	-2.211007	-2.754290
C	-0.153462	-0.773678	2.766546
H	-0.468364	-1.617122	3.388004
H	0.625823	-0.221910	3.302989
H	-1.013437	-0.112891	2.642709
N	2.041927	-2.017814	-0.837862
N	0.300993	-1.239491	1.469320
Si	0.016794	-0.344812	0.020141
C	0.865303	1.322887	0.000414
C	0.242017	2.472539	0.493812
C	2.184256	1.431668	-0.452533
C	0.907529	3.690158	0.530738
H	-0.782010	2.419620	0.849599
C	2.851658	2.648162	-0.422682
H	2.695136	0.547997	-0.823039
C	2.213939	3.778968	0.069694
H	0.407814	4.569666	0.916960
H	3.871427	2.714764	-0.780682
H	2.734926	4.727848	0.095233
C	-1.824028	-0.113539	-0.209967
C	-2.721067	-1.007033	0.381867
C	-2.342266	0.895069	-1.026621
C	-4.088419	-0.894301	0.172125
H	-2.338764	-1.800222	1.016139
C	-3.708418	1.009274	-1.244829
H	-1.669615	1.605319	-1.496137
C	-4.583087	0.115234	-0.642460
H	-4.768753	-1.593674	0.641677
H	-4.091048	1.796419	-1.882136
H	-5.649339	0.205425	-0.807932

Cartesian coordinates for optimized insertion pathway compounds H_2SiPh_2-NHC 2

H_2SiPh_2-NHC 2, A

E_e = -1059.91946498 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	-0.000123	-0.192300	-0.000212
C	1.685486	-1.092701	-0.124186
C	2.300156	-1.626714	1.010096
C	2.329971	-1.261686	-1.349885
C	3.507241	-2.307330	0.928486
H	1.815396	-1.505098	1.974366
C	3.545446	-1.929190	-1.442924
H	1.862370	-0.866825	-2.245937
C	4.135492	-2.455730	-0.302050
H	3.959197	-2.723582	1.820744
H	4.029959	-2.044938	-2.405089
H	5.079465	-2.982323	-0.371063
C	-1.686053	-1.092152	0.123917
C	-2.301333	-1.625523	-1.010320
C	-2.330189	-1.261266	1.349788
C	-3.508696	-2.305620	-0.928532
H	-1.816795	-1.503864	-1.974698
C	-3.545905	-1.928308	1.443027
H	-1.862134	-0.866829	2.245790
C	-4.136580	-2.454179	0.302178
H	-3.961149	-2.721378	-1.820769
H	-4.030125	-2.044188	2.405324
H	-5.080769	-2.980369	0.371339
C	0.000500	1.824097	-0.000135
C	0.708051	4.012088	0.292228
C	-0.706137	4.012498	-0.291556
H	1.455869	4.356519	-0.428197
H	-0.797890	4.608913	-1.199066
N	0.915090	2.592517	0.580591
N	-0.913766	2.593138	-0.580601
C	-2.153912	2.136889	-1.168160
H	-2.976451	2.214048	-0.452499
H	-2.382369	2.749957	-2.040712
H	-2.044634	1.100872	-1.477761
C	2.154900	2.135430	1.168209
H	2.977566	2.212088	0.452652
H	2.383677	2.748364	2.040789
H	2.044821	1.099538	1.477911
H	-0.113542	-0.053378	-1.547695
H	0.113210	-0.053301	1.547291
H	-1.453756	4.356805	0.429146
H	0.799905	4.607963	1.200083

H_2SiPh_2-NHC 2, T1

E_e = -1059.91085739 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.120812	-0.167961	-0.582106
C	-1.329394	-1.273643	-0.075754
C	-1.793406	-2.238286	-0.973360
C	-1.978071	-1.164414	1.155129
C	-2.864588	-3.063765	-0.656217
H	-1.310882	-2.339284	-1.940030
C	-3.056255	-1.977962	1.476508
H	-1.630819	-0.423876	1.867694
C	-3.501509	-2.931280	0.570072
H	-3.206179	-3.806615	-1.366560
H	-3.547276	-1.872164	2.436231
H	-4.340775	-3.568701	0.819208
C	1.888561	-0.703377	-0.193718
C	2.339704	-0.910417	1.111426
C	2.779050	-0.943900	-1.240991
C	3.636677	-1.332221	1.363640
H	1.660682	-0.730375	1.938037
C	4.085584	-1.350016	-0.996534
H	2.443481	-0.809160	-2.263686
C	4.515424	-1.544607	0.307939
H	3.965990	-1.495234	2.382454
H	4.765768	-1.518539	-1.822210
H	5.530951	-1.866220	0.503231
C	-0.333232	1.658328	-0.401764
C	-1.712881	3.433235	0.184551
C	-0.298584	3.649501	0.707936
H	-2.469191	3.497749	0.969225
H	-0.223531	3.338942	1.760732
N	-1.611966	2.086614	-0.360375
N	0.480188	2.727141	-0.115610
C	1.848220	2.523640	0.294144
H	2.384801	1.940323	-0.450902
H	2.329696	3.495273	0.397877
H	1.890555	1.987044	1.252398
C	-2.743468	1.478173	-1.017339
H	-3.448212	1.054438	-0.297578
H	-3.259257	2.233268	-1.617454
H	-2.406833	0.680248	-1.675306
H	0.005656	0.633735	0.976748
H	0.119258	-0.440574	-2.074997
H	0.059493	4.672517	0.605023
H	-1.973281	4.138451	-0.612774

H_2SiPh_2-NHC 2, B

E_e = -1059.96914341 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.088738	0.122003	1.012305
C	-1.147007	1.329434	0.306779
C	-1.516636	2.456225	1.044316
C	-1.706726	1.156403	-0.962970
C	-2.415204	3.384445	0.534917
H	-1.100627	2.611517	2.034246
C	-2.604859	2.081833	-1.475456
H	-1.431707	0.286459	-1.548114
C	-2.960337	3.196760	-0.727097
H	-2.690837	4.251107	1.122520
H	-3.031959	1.933342	-2.459512
H	-3.663100	3.917058	-1.126995
C	1.835767	0.529056	0.481896
C	2.093155	1.141027	-0.746592
C	2.923647	0.147120	1.271063
C	3.395041	1.353649	-1.178794
H	1.264002	1.451150	-1.373491
C	4.227561	0.355606	0.843224
H	2.752390	-0.321158	2.235087
C	4.463866	0.957558	-0.385392
H	3.576670	1.829426	-2.134370
H	5.058916	0.053132	1.467546
H	5.479625	1.122721	-0.721920
C	-0.314327	-1.653344	0.448146
C	-1.930569	-3.085658	-0.317196
C	-1.163505	-2.617798	-1.543860
H	-2.991286	-3.257716	-0.502525
H	-1.801890	-2.002373	-2.182028
N	-1.729816	-1.966786	0.586842
N	-0.056294	-1.807131	-0.997438
C	1.253808	-2.366291	-1.277022
H	1.362656	-3.390326	-0.883936
H	1.420195	-2.385756	-2.354122
H	2.029438	-1.745449	-0.829461
C	-2.144087	-2.220972	1.946206
H	-3.206976	-2.462467	1.963549
H	-1.587124	-3.058090	2.400613
H	-1.989419	-1.332352	2.559849
H	0.295244	-2.397867	1.012362
H	0.046234	0.195550	2.495921
H	-0.779284	-3.447896	-2.139385
H	-1.488245	-4.010953	0.093058

H_2SiPh_2-NHC 2, T2

E_e = -1059.91260035 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

C	-0.236956	2.057347	-0.950779
C	1.892134	2.365875	-0.134550
C	1.368943	1.821133	1.215671
H	-1.206612	2.500020	-1.190183
C	0.535165	4.360483	-0.751210
H	0.498925	4.681909	0.292744
H	1.352699	4.875164	-1.254888
H	-0.402645	4.614653	-1.238512
C	-0.564840	0.934344	2.297629
H	0.069303	0.434915	3.044985
H	-0.871082	1.895535	2.732518
H	-1.451045	0.320205	2.158600
N	0.739274	2.920316	-0.829053
N	0.127739	1.119635	1.038757
Si	-0.082603	0.158371	-0.622146
C	-1.815549	-0.513907	-0.298571
C	-2.052566	-1.872012	-0.522738
C	-2.904971	0.280276	0.064286
C	-3.320245	-2.419202	-0.379968
H	-1.227617	-2.512336	-0.819208
C	-4.180924	-0.254214	0.194588
H	-2.757797	1.336813	0.268831
C	-4.390114	-1.608552	-0.024609
H	-3.476144	-3.477058	-0.551812
H	-5.010891	0.384130	0.471944
H	-5.381778	-2.030227	0.081579
C	1.362396	-1.050087	-0.275266
C	1.696536	-1.475175	1.014938
C	2.102611	-1.580437	-1.333701
C	2.714250	-2.392258	1.239106
H	1.140594	-1.088850	1.861922
C	3.140254	-2.480633	-1.120527
H	1.850530	-1.284946	-2.346654
C	3.445509	-2.891835	0.168725
H	2.939919	-2.717108	2.247625
H	3.703122	-2.868876	-1.960740
H	4.245204	-3.601731	0.339856
H	-0.039132	-0.155131	-2.127198
H	2.163289	1.175880	1.619252
H	1.235258	2.653789	1.921296
H	2.657912	3.125819	0.006799
H	2.305551	1.553681	-0.734788

H_2SiPh_2-NHC 2, C

E_e = -1059.93458802 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.372404	-0.664143	1.188785
C	1.837963	-2.464170	0.688590
C	0.743488	-2.912381	-0.260046
H	2.156999	-3.294044	1.324124
H	1.130124	-3.791458	-0.783205
C	2.203849	-1.132703	2.738022
H	2.237493	-2.022823	3.366786
H	3.217150	-0.887667	2.414124
H	1.789934	-0.296611	3.294557
C	0.137856	-2.497764	-2.550124
H	1.050807	-2.965229	-2.936586
H	-0.644681	-3.267163	-2.522928
H	-0.172483	-1.728898	-3.252454
N	1.374882	-1.384062	1.563391
N	0.368017	-1.912415	-1.238572
Si	-0.242376	-0.313091	-0.830634
C	-1.985111	0.115832	-0.197267
C	-2.700025	1.113805	-0.864944
C	-2.610062	-0.501152	0.887766
C	-3.967311	1.501983	-0.451999
H	-2.249769	1.593280	-1.728604
C	-3.889907	-0.143412	1.293504
H	-2.090239	-1.288223	1.427462
C	-4.568048	0.868773	0.628093
H	-4.491905	2.290787	-0.977319
H	-4.357887	-0.649840	2.128994
H	-5.561455	1.159115	0.946469
C	1.030813	1.086439	-0.495388
C	2.324162	0.969003	-1.015957
C	0.726944	2.244841	0.224988
C	3.273684	1.964401	-0.827638
H	2.584336	0.088632	-1.596750
C	1.670231	3.248612	0.413678
H	-0.269411	2.370494	0.639094
C	2.948272	3.108817	-0.109341
H	4.265707	1.854367	-1.249290
H	1.406705	4.141067	0.968323
H	3.685356	3.888631	0.035437
H	-0.111597	-3.259091	0.339852
H	2.705991	-2.098230	0.130907
H	0.129868	0.115037	1.917781
H	-0.513286	0.065790	-2.275962

H_2SiPh_2-NHC 2, T3

E_e = -1059.91260017 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.236677	2.057468	-0.950907
C	1.892318	2.365765	-0.134248
C	1.368797	1.821333	1.215964
H	-1.206181	2.500310	-1.190618
C	0.535849	4.360511	-0.751687
H	0.499295	4.682245	0.292160
H	1.353685	4.874863	-1.255213
H	-0.401720	4.614755	-1.239413
C	-0.565142	0.934398	2.297619
H	0.068769	0.434669	3.044973
H	-0.871220	1.895567	2.732671
H	-1.451480	0.320499	2.158334
N	0.739662	2.920278	-0.829043
N	0.127637	1.119809	1.038876
Si	-0.082581	0.158504	-0.622030
C	-1.815543	-0.513745	-0.298516
C	-2.052422	-1.871965	-0.522118
C	-2.905088	0.280523	0.063797
C	-3.320101	-2.419171	-0.379378
H	-1.227378	-2.512380	-0.818121
C	-4.181025	-0.253997	0.194095
H	-2.758018	1.337149	0.267955
C	-4.390091	-1.608442	-0.024581
H	-3.475900	-3.477109	-0.550807
H	-5.011079	0.384410	0.471045
H	-5.381750	-2.030131	0.081598
C	1.362324	-1.050126	-0.275215
C	1.696989	-1.474808	1.014992
C	2.101921	-1.581080	-1.333788
C	2.714556	-2.392091	1.239029
H	1.141594	-1.088005	1.862107
C	3.139376	-2.481526	-1.120769
H	1.849484	-1.285864	-2.346730
C	3.445126	-2.892332	0.168494
H	2.940642	-2.716574	2.247573
H	3.701703	-2.870284	-1.961107
H	4.244681	-3.602412	0.339514
H	-0.039016	-0.155005	-2.127110
H	2.658194	3.125607	0.007110
H	2.163064	1.176184	1.619873
H	2.305717	1.553397	-0.734268
H	1.234963	2.654149	1.921380

H_2SiPh_2-NHC 2, D

E_e = -1060.02081835 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.782697	-1.456855	-1.291420
C	1.946409	-2.706478	0.406892
C	1.617570	-1.833823	1.606040
H	0.092626	-2.288799	-1.524934
H	2.899505	-3.200890	0.605363
H	1.590739	-2.476398	2.493595
H	0.924131	-0.894741	-2.219280
C	2.700602	-2.775574	-1.862125
H	3.687380	-3.103520	-1.532566
H	2.097346	-3.666927	-2.102598
H	2.817777	-2.190250	-2.774710
C	-0.059745	-0.507137	2.730044
H	-0.146928	-1.245026	3.533517
H	0.662069	0.258067	3.048564
H	-1.032434	-0.025045	2.611567
N	2.079203	-1.958600	-0.836045
N	0.332529	-1.157444	1.492089
Si	0.007050	-0.338194	0.004644
C	0.788327	1.366600	-0.060551
C	0.146687	2.481669	0.487440
C	2.073188	1.541749	-0.585919
C	0.758170	3.727389	0.505416
H	-0.851834	2.377814	0.900635
C	2.688312	2.786484	-0.572831
H	2.600339	0.687889	-0.999636
C	2.031121	3.880927	-0.027631
H	0.243207	4.578507	0.933151
H	3.681797	2.903371	-0.987660
H	2.509993	4.852071	-0.017650
C	-1.844080	-0.180028	-0.203347
C	-2.701432	-1.100678	0.405804
C	-2.408309	0.809585	-1.012352
C	-4.074840	-1.033612	0.217054
H	-2.281001	-1.875020	1.038848
C	-3.780939	0.878179	-1.209098
H	-1.767191	1.541801	-1.492155
C	-4.615690	-0.043242	-0.592144
H	-4.724407	-1.752633	0.700396
H	-4.199594	1.651408	-1.840839
H	-5.686869	0.010812	-0.740733
H	2.436839	-1.112907	1.755075
H	1.177401	-3.493483	0.307099

Cartesian coordinates for optimized insertion pathway compounds H_2SiPh_2-NHC 3

H_2SiPh_2-NHC 3, A

E_e = -1137.35399208 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	-0.674667	0.277771	-0.040833
C	-2.316532	-0.712544	-0.174705
C	-3.031621	-1.075446	0.968455
C	-2.841545	-1.085980	-1.412177
C	-4.226347	-1.778524	0.884411
H	-2.637890	-0.793441	1.940601
C	-4.028898	-1.801132	-1.509467
H	-2.305940	-0.803052	-2.312522
C	-4.725125	-2.146571	-0.358733
H	-4.770643	-2.039031	1.784246
H	-4.415063	-2.086039	-2.480821
H	-5.654502	-2.698371	-0.429975
C	-0.411643	2.161856	0.207450
C	-0.558402	3.061877	-0.849536
C	-0.035500	2.677570	1.447890
C	-0.342447	4.423019	-0.679283
H	-0.848416	2.681042	-1.824414
C	0.202587	4.035279	1.627289
H	0.066117	1.996228	2.286463
C	0.045933	4.911706	0.562143
H	-0.475832	5.104817	-1.510606
H	0.502866	4.411624	2.597880
H	0.221472	5.971732	0.699157
C	1.055976	-0.688351	-0.120269
C	2.718167	-2.134929	0.322780
C	3.239568	-1.129249	-0.425272
N	1.376329	-1.837553	0.492926
N	2.192552	-0.262049	-0.692170
C	2.316328	0.986992	-1.428908
H	2.579459	1.801880	-0.754211
H	3.082122	0.875059	-2.193168
H	1.359013	1.205821	-1.894971
C	0.450348	-2.647003	1.268238
H	0.618746	-3.698814	1.043320
H	0.597979	-2.470037	2.333435
H	-0.567706	-2.378846	1.000793
H	-0.597358	0.421312	-1.592893
H	-0.610891	0.013752	1.497564
C	3.341003	-3.359219	0.890066
H	3.183520	-3.421112	1.968320
H	2.927721	-4.263933	0.439471
H	4.412919	-3.353256	0.705120
C	4.621249	-0.893408	-0.919914
H	4.671014	-0.934742	-2.009831
H	4.992693	0.082937	-0.603636
H	5.293170	-1.652761	-0.525711

H_2SiPh_2-NHC 3, T1

E_e = -1137.33103608 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	-0.581094	-0.000075	0.694827
C	-1.447132	-1.590253	0.173273
C	-1.986004	-2.411709	1.165821
C	-1.638484	-1.964410	-1.158727
C	-2.665862	-3.580451	0.845632
H	-1.868732	-2.133792	2.207757
C	-2.326889	-3.123830	-1.486860
H	-1.228044	-1.342742	-1.946090
C	-2.836193	-3.938619	-0.483648
H	-3.065199	-4.208238	1.632439
H	-2.467734	-3.392920	-2.526370
H	-3.370084	-4.845571	-0.738526
C	-1.447690	1.589838	0.173544
C	-1.640458	1.963201	-1.158473
C	-1.985533	2.411835	1.166196
C	-2.329275	3.122391	-1.486556
H	-1.230842	1.341071	-1.945899
C	-2.665742	3.580381	0.846045
H	-1.867193	2.134486	2.208166
C	-2.837511	3.937753	-0.483269
H	-2.471283	3.390848	-2.526073
H	-3.064262	4.208627	1.632899
H	-3.371719	4.844529	-0.738105
C	1.277258	0.000345	0.477609
C	3.354474	-0.672345	-0.104293
C	3.354267	0.673291	-0.104732
N	2.112285	-1.088473	0.393034
N	2.111943	1.089396	0.392328
C	1.622283	2.436479	0.241915
H	0.894641	2.660050	1.019080
H	2.452475	3.133475	0.328889
H	1.136564	2.560500	-0.733401
C	1.623183	-2.435911	0.243999
H	1.138214	-2.561432	-0.731482
H	2.453523	-3.132542	0.332546
H	0.895017	-2.658613	1.020932
H	0.399266	0.000064	-0.941540
H	-0.875166	-0.000308	2.175857
C	4.433762	-1.641675	-0.424864
H	4.699190	-2.243581	0.447886
H	4.138085	-2.323923	-1.224421
H	5.326391	-1.111323	-0.749612
C	4.433298	1.642693	-0.425967
H	4.137633	2.324045	-1.226288
H	4.698254	2.245540	0.446275
H	5.326212	1.112323	-0.749904

H_2SiPh_2-NHC 3, B

E_e = -1137.38006806 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.566230	0.122631	1.110344
C	0.250517	1.815052	0.385995
C	1.175874	2.832123	0.640072
C	-0.845108	2.107815	-0.429528
C	1.017486	4.100679	0.101080
H	2.041449	2.629633	1.263818
C	-1.005861	3.376718	-0.971868
H	-1.578211	1.339854	-0.643234
C	-0.077007	4.373354	-0.708608
H	1.746517	4.873734	0.308918
H	-1.859741	3.587865	-1.603552
H	-0.204353	5.360849	-1.134488
C	2.199934	-0.536317	0.469396
C	2.772090	-0.029214	-0.699091
C	2.829522	-1.614508	1.098228
C	3.930589	-0.584126	-1.227092
H	2.302129	0.807166	-1.204729
C	3.985282	-2.175141	0.573415
H	2.411492	-2.024583	2.012315
C	4.536317	-1.659784	-0.593077
H	4.359736	-0.177815	-2.134319
H	4.459046	-3.010306	1.073830
H	5.439144	-2.093936	-1.003693
C	-0.836369	-1.081679	0.665942
C	-3.055336	-0.911833	0.087858
C	-2.397494	-1.305399	-1.006142
N	-2.132977	-0.543372	1.106153
N	-0.991527	-1.232615	-0.790175
C	-0.203801	-2.319859	-1.341860
H	-0.494547	-3.289787	-0.907272
H	-0.334138	-2.360765	-2.422277
H	0.852207	-2.150538	-1.136606
C	-2.474888	-0.905343	2.465823
H	-3.422569	-0.448095	2.746702
H	-2.550192	-1.997339	2.592372
H	-1.709259	-0.531491	3.145740
H	-0.690779	-2.091990	1.118255
H	0.651521	0.192875	2.591177
C	-4.507641	-0.671464	0.298414
H	-5.062958	-0.825598	-0.624327
H	-4.923210	-1.341078	1.054969
H	-4.676216	0.354398	0.637919
C	-2.909691	-1.633763	-2.362965
H	-2.714505	-2.675444	-2.628134
H	-3.983646	-1.470089	-2.422361
H	-2.421097	-1.006310	-3.113634

H_2SiPh_2-NHC 3, T2

E_e = -1137.32804861 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

Si	0.413961	-0.240961	0.958434
C	-0.081997	1.379463	0.132288
C	-0.916876	2.286412	0.788408
C	0.400765	1.734227	-1.128093
C	-1.265934	3.498081	0.208683
H	-1.298775	2.039598	1.774418
C	0.032804	2.931719	-1.728887
H	1.083149	1.069361	-1.647303
C	-0.799637	3.817846	-1.059928
H	-1.900951	4.193267	0.744347
H	0.406544	3.179094	-2.714767
H	-1.075870	4.758355	-1.520010
C	2.260943	-0.357966	0.449978
C	3.226429	0.399027	1.119621
C	2.700835	-1.163599	-0.602684
C	4.565354	0.359632	0.757803
H	2.924355	1.035030	1.947151
C	4.039528	-1.212707	-0.976839
H	1.983016	-1.767922	-1.151120
C	4.975532	-0.449105	-0.295308
H	5.291921	0.956672	1.295462
H	4.351657	-1.845955	-1.798568
H	6.019651	-0.483980	-0.580482
C	-0.259839	-1.877807	0.349704
C	-2.436400	-0.557819	0.279029
C	-2.054310	-1.131355	-0.894007
N	-1.610451	-0.713578	1.365482
N	-1.033302	-2.098032	-0.723341
C	-1.409260	-3.467056	-1.070663
H	-2.225182	-3.816432	-0.430095
H	-1.734436	-3.498866	-2.109147
H	-0.543674	-4.117081	-0.959323
C	-2.198412	-0.761861	2.688947
H	-2.666491	0.194769	2.950068
H	-2.951023	-1.549685	2.794058
H	-1.403220	-0.943333	3.412307
H	0.087093	-2.787953	0.844047
H	0.558199	-0.181191	2.436219
C	-3.700781	0.234042	0.426053
H	-4.221979	0.334815	-0.522109
H	-4.375441	-0.262503	1.126711
H	-3.489684	1.231663	0.817630
C	-2.680311	-0.977208	-2.244581
H	-3.458936	-1.719622	-2.443833
H	-3.121993	0.010810	-2.357655
H	-1.917708	-1.077992	-3.018216

H_2SiPh_2-NHC 3, C

E_e = -1137.34325828 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1			
C	-0.722182	-1.294872	-1.566512
C	-2.566661	-1.377960	-0.045871
C	-1.817936	-0.891840	1.018337
H	-0.338634	-1.747359	-2.477603
C	-2.624805	-2.624475	-2.145415
H	-3.089999	-3.421143	-1.570440
H	-3.390566	-2.084975	-2.699467
H	-1.903694	-3.039206	-2.841555
C	0.144518	-0.094387	2.136549
H	-0.443272	0.610142	2.728904
H	0.403545	-0.951675	2.765141
H	1.072372	0.404589	1.866646
N	-1.918469	-1.702312	-1.239441
N	-0.543639	-0.506386	0.917390
Si	0.349096	0.042736	-0.754896
C	2.014361	-0.696104	-0.214907
C	3.209927	-0.047389	-0.529823
C	2.101356	-1.925569	0.441358
C	4.440970	-0.584830	-0.179982
H	3.176842	0.895979	-1.064300
C	3.328656	-2.485977	0.772052
H	1.189659	-2.453799	0.701609
C	4.502840	-1.810893	0.469389
H	5.352912	-0.053184	-0.422194
H	3.370360	-3.447566	1.269333
H	5.461504	-2.239669	0.733557
C	-0.039870	1.890012	-0.384670
C	-1.040413	2.367439	0.466570
C	0.728096	2.851591	-1.050497
C	-1.259657	3.727057	0.652181
H	-1.680998	1.669448	0.991802
C	0.543001	4.212026	-0.847881
H	1.479131	2.522126	-1.759981
C	-0.458321	4.655587	0.004733
H	-2.056135	4.061455	1.305977
H	1.169116	4.926836	-1.367647
H	-0.619292	5.715788	0.155462
H	0.848194	0.413000	-2.164306
C	-4.052206	-1.613421	0.025312
H	-4.526297	-1.442802	-0.940500
H	-4.332385	-2.620141	0.354773
H	-4.514943	-0.904440	0.707522
C	-2.487752	-0.837528	2.372632
H	-2.713122	0.193712	2.658873
H	-3.407608	-1.410915	2.397472
H	-1.822808	-1.244444	3.132482

H_2SiPh_2-NHC 3, T3

E_e = -1137.33260721 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

C	-0.641164	-1.566505	-1.284823
C	-2.670336	-1.170988	-0.068454
C	-2.021768	-0.779686	1.068809
H	-0.145483	-2.162164	-2.044512
C	-2.702527	-2.340354	-2.265160
H	-3.478671	-2.981810	-1.853876
H	-3.159566	-1.603020	-2.927590
H	-2.007789	-2.942823	-2.844448
C	-0.041038	-0.375795	2.458058
H	-0.449310	0.503980	2.965918
H	-0.138727	-1.232690	3.130767
H	1.023792	-0.200463	2.307113
N	-1.953396	-1.688271	-1.194090
N	-0.649890	-0.641183	1.164547
Si	0.224546	-0.216852	-0.372376
C	2.006362	-0.734439	-0.131023
C	3.072650	0.164948	-0.194107
C	2.294955	-2.073542	0.149811
C	4.380822	-0.258203	0.000247
H	2.878175	1.213307	-0.389842
C	3.600818	-2.503419	0.343074
H	1.482998	-2.788615	0.231494
C	4.647186	-1.594535	0.265526
H	5.193223	0.455729	-0.053754
H	3.802627	-3.545418	0.558748
H	5.666809	-1.926042	0.417156
C	0.031958	1.682738	-0.332515
C	-0.691346	2.364660	0.647697
C	0.654141	2.458923	-1.317159
C	-0.786580	3.751783	0.654110
H	-1.205828	1.806895	1.419504
C	0.587589	3.844038	-1.307379
H	1.189114	1.959880	-2.118753
C	-0.138151	4.496687	-0.318518
H	-1.364676	4.250377	1.422599
H	1.088604	4.414917	-2.079518
H	-0.204209	5.577440	-0.313244
H	0.104419	-0.103908	-2.058179
C	-4.164682	-1.089732	-0.237820
H	-4.422889	-0.777112	-1.249619
H	-4.679493	-2.037045	-0.047237
H	-4.589782	-0.341352	0.423592
C	-2.824954	-0.455110	2.304660
H	-2.850095	0.620422	2.501674
H	-3.844708	-0.816890	2.237269
H	-2.372786	-0.930304	3.174599

H_2SiPh_2-NHC 3, D

E_e = -1137.41764511 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.077175	-0.060531	-1.602425
C	2.960497	-0.556959	-0.149546
C	2.254561	-0.977061	0.919258
H	1.141361	-1.037698	-2.105150
H	0.745050	0.667355	-2.347371
C	3.229217	0.956048	-2.074086
H	4.148908	1.330936	-1.628949
H	3.488037	0.259983	-2.885367
H	2.708005	1.804518	-2.520253
C	0.450026	-0.435601	2.511563
H	0.367280	-1.413289	2.994893
H	1.095662	0.199767	3.124971
H	-0.545042	0.013641	2.514286
N	2.371420	0.368794	-1.064369
N	0.931949	-0.521992	1.141878
Si	-0.103476	-0.040443	-0.147637
C	-0.785873	1.685359	0.118847
C	-2.077526	1.920324	0.594808
C	0.031201	2.792281	-0.138083
C	-2.542101	3.212957	0.804576
H	-2.734083	1.082256	0.803908
C	-0.429573	4.084915	0.063336
H	1.045692	2.632237	-0.490278
C	-1.719175	4.296562	0.535330
H	-3.546146	3.373236	1.177045
H	0.216179	4.928957	-0.144781
H	-2.080500	5.304844	0.694406
C	-1.539400	-1.234082	-0.326831
C	-1.497536	-2.477351	0.307095
C	-2.643819	-0.946946	-1.135155
C	-2.521767	-3.401681	0.146963
H	-0.646142	-2.723489	0.933588
C	-3.667880	-1.867809	-1.304956
H	-2.709248	0.013962	-1.636100
C	-3.607970	-3.097212	-0.661047
H	-2.471832	-4.359218	0.650174
H	-4.514206	-1.626987	-1.936016
H	-4.407135	-3.816317	-0.789310
C	2.738785	-1.982860	1.925892
H	2.808983	-1.541587	2.922801
H	2.035257	-2.817722	1.994548
H	3.714593	-2.387134	1.684083
C	4.344862	-1.037714	-0.489427
H	4.659875	-1.863121	0.138347
H	4.395243	-1.378270	-1.526101
H	5.087058	-0.244108	-0.375703

Cartesian coordinates for optimized insertion pathway compounds H_2SiPh_2-NHC 4

H_2SiPh_2-NHC 4, A

E_e = -1977.91887395 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

Si	-1.125747	0.054654	-0.021089
C	-2.240330	-1.491792	-0.220576
C	-2.768782	-2.146143	0.894041
C	-2.566159	-1.992347	-1.481465
C	-3.594905	-3.254002	0.759499
H	-2.527469	-1.770945	1.884319
C	-3.383332	-3.105997	-1.628784
H	-2.172715	-1.492451	-2.360426
C	-3.901054	-3.737815	-0.506105
H	-4.002984	-3.739328	1.637824
H	-3.620839	-3.479896	-2.617384
H	-4.543136	-4.603147	-0.615998
C	-1.688251	1.862534	0.253658
C	-2.145487	2.643462	-0.809666
C	-1.651448	2.449038	1.519017
C	-2.554148	3.956723	-0.622194
H	-2.183475	2.206035	-1.803129
C	-2.042802	3.767753	1.716912
H	-1.315336	1.854760	2.362426
C	-2.497819	4.523525	0.645126
H	-2.916137	4.539598	-1.460541
H	-1.999163	4.204841	2.707211
H	-2.810667	5.549287	0.796566
C	0.870642	-0.158493	-0.077846
C	2.944015	-0.895533	0.302143
C	3.042599	0.269642	-0.379351
N	1.600877	-1.140509	0.479347
N	1.755614	0.702188	-0.612760
C	1.398565	1.947098	-1.283121
H	1.416123	2.771482	-0.571615
H	2.109152	2.130819	-2.084967
H	0.396208	1.831808	-1.685727
C	1.063220	-2.303149	1.173458
H	1.481418	-3.206636	0.734070
H	1.324511	-2.252607	2.229174
H	-0.016447	-2.300918	1.060169
H	-1.039887	0.251139	-1.563318
H	-0.963836	-0.201167	1.506302
Cl	4.423307	1.105338	-0.882585
Cl	4.161550	-1.928668	0.855863

H_2SiPh_2-NHC 4, T1

E_e = -1977.89990154 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

Si	-1.024236	0.000058	0.688548
C	-1.864550	-1.598528	0.154752
C	-2.435417	-2.411630	1.136059
C	-2.006477	-1.985238	-1.179728
C	-3.100098	-3.585324	0.802747
H	-2.356424	-2.122827	2.178668
C	-2.679903	-3.149385	-1.521101
H	-1.570287	-1.369755	-1.958360
C	-3.222267	-3.955914	-0.528422
H	-3.525387	-4.207143	1.580584
H	-2.782617	-3.429253	-2.562137
H	-3.744030	-4.866955	-0.793326
C	-1.863695	1.599085	0.154720
C	-2.004901	1.986155	-1.179732
C	-2.434542	2.412265	1.135979
C	-2.677590	3.150725	-1.521116
H	-1.568753	1.370595	-1.958325
C	-3.098496	3.586366	0.802658
H	-2.356093	2.123204	2.178558
C	-3.219938	3.957316	-0.528478
H	-2.779737	3.430880	-2.562132
H	-3.523772	4.208235	1.580463
H	-3.741124	4.868685	-0.793389
C	0.854385	-0.000215	0.571930
C	2.918223	-0.671702	0.008664
C	2.918455	0.670626	0.008740
N	1.683714	-1.095744	0.490932
N	1.684088	1.095049	0.491056
C	1.199775	2.449588	0.355257
H	0.458238	2.646376	1.125482
H	2.032890	3.137072	0.472381
H	0.734889	2.587648	-0.626100
C	1.198800	-2.450010	0.354720
H	0.733329	-2.587339	-0.626468
H	2.031705	-3.137889	0.471025
H	0.457601	-2.646899	1.125252
H	-0.022710	-0.000301	-0.884168
H	-1.356055	0.000077	2.161855
Cl	4.198904	1.729686	-0.317246
Cl	4.198298	-1.731182	-0.317422

H_2SiPh_2-NHC 4, B

E_e = -1977.95563189 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	1.010613	0.270079	1.153055
C	0.771986	1.898588	0.277890
C	1.723352	2.903244	0.480762
C	-0.279614	2.151938	-0.605303
C	1.630261	4.122730	-0.173205
H	2.553629	2.731498	1.158955
C	-0.375137	3.371639	-1.262772
H	-1.031408	1.393413	-0.785184
C	0.577702	4.357237	-1.047823

H	2.376341	4.888344	-0.002047
H	-1.196438	3.551960	-1.944618
H	0.500423	5.307749	-1.560597
C	2.514670	-0.608476	0.474379
C	2.962959	-0.345373	-0.822238
C	3.168474	-1.598803	1.212799
C	4.023805	-1.055269	-1.367772
H	2.474734	0.422959	-1.411922
C	4.229520	-2.311049	0.671880
H	2.847624	-1.817487	2.226348
C	4.656431	-2.040370	-0.621762
H	4.358361	-0.838685	-2.374409
H	4.725915	-3.074207	1.257850
H	5.484822	-2.593566	-1.046022
C	-0.524088	-0.840146	0.937731
C	-2.714171	-0.528089	0.389713
C	-2.140421	-1.149623	-0.638842
N	-1.752988	-0.112043	1.329784
N	-0.740287	-1.216699	-0.480560
C	-0.112920	-2.479876	-0.842670
H	-0.483748	-3.303592	-0.215851
H	-0.323121	-2.700123	-1.887119
H	0.964743	-2.393607	-0.716296
C	-2.085458	-0.255598	2.735555
H	-2.991074	0.305549	2.955323
H	-2.233931	-1.309401	3.012331
H	-1.272452	0.155706	3.333005
H	-0.463882	-1.774110	1.538505
H	1.206642	0.476434	2.609632
Cl	-4.330491	-0.011194	0.519472
Cl	-2.866976	-1.604393	-2.109188

H_2SiPh_2-NHC 4, T2

E_e = -1977.90856603 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.775834	0.227546	1.250482
C	-0.347848	1.614076	0.692022
C	-0.512142	2.030622	-0.633029
C	-1.049955	2.305172	1.683244
C	-1.349737	3.086880	-0.954049
H	0.007448	1.510900	-1.428988
C	-1.900917	3.356441	1.366245
H	-0.931265	2.017553	2.721714
C	-2.050964	3.749596	0.045892
H	-1.462697	3.389201	-1.987453
H	-2.442199	3.868347	2.151812
H	-2.710201	4.570583	-0.206178
C	2.514725	0.180630	0.564893
C	2.944544	1.049016	-0.439332
C	3.418189	-0.774255	1.036244
C	4.224984	0.955099	-0.968153
H	2.270717	1.809340	-0.817487
C	4.697003	-0.880141	0.505928
H	3.127849	-1.448105	1.836509
C	5.100861	-0.016163	-0.502396
H	4.539347	1.638628	-1.746875
H	5.379506	-1.631787	0.882250
H	6.096973	-0.095538	-0.918877
C	0.100980	-1.527611	1.244744
C	-1.878040	-1.278743	0.160984
C	-1.098874	-1.002098	-0.931558
N	-1.177638	-1.906573	1.198945
N	0.227185	-0.986788	-0.818512
C	1.049688	-1.357963	-1.956454
H	0.726250	-2.288685	-2.431794
H	1.035961	-0.565201	-2.712199
H	2.077154	-1.469778	-1.611924
C	-1.554818	-3.289017	1.499647
H	-2.621801	-3.324373	1.705745
H	-1.329547	-3.933424	0.646008
H	-1.009559	-3.619959	2.380549
H	0.782761	-2.321067	1.557663
H	0.933121	0.494734	2.715655
Cl	-3.580961	-1.137498	0.255768
Cl	-1.861650	-0.670898	-2.455482

H_2SiPh_2-NHC 4, C

E_e = -1977.92662405 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.522779	-1.061438	-1.730632
C	-2.421707	-0.800847	-0.330512
C	-1.670621	-0.430596	0.777006
H	-0.176441	-1.581906	-2.619030
C	-2.607115	-2.032588	-2.432769
H	-3.130838	-2.818245	-1.894323
H	-3.334174	-1.378401	-2.907389
H	-1.940267	-2.454261	-3.176359
C	0.294110	-0.063481	2.085665
H	-0.112549	0.825966	2.568921
H	0.188109	-0.911358	2.765840
H	1.351798	0.101977	1.899108
N	-1.790697	-1.249063	-1.484794
N	-0.366511	-0.323975	0.810736
Si	0.765237	0.032589	-0.858556
C	2.157935	-1.066109	-0.193625
C	3.487511	-0.710181	-0.428565
C	1.917048	-2.268283	0.474112
C	4.537273	-1.505454	0.010146
H	3.706932	0.205118	-0.967598
C	2.959908	-3.082920	0.895356

H	0.894742	-2.570939	0.674943
C	4.274223	-2.697963	0.670686
H	5.560387	-1.200040	-0.170627
H	2.747731	-4.016146	1.402326
H	5.090361	-3.326248	1.004673
C	0.714863	1.903425	-0.467406
C	-0.232693	2.572810	0.312310
C	1.721374	2.684479	-1.047040
C	-0.175463	3.946565	0.510614
H	-1.048173	2.029656	0.773325
C	1.808319	4.051735	-0.827324
H	2.445898	2.211660	-1.700779
C	0.853841	4.689469	-0.047596
H	-0.936999	4.435561	1.105422
H	2.611453	4.621270	-1.278471
H	0.906165	5.758615	0.115232
H	1.419062	0.272385	-2.219417
Cl	-4.141977	-0.737038	-0.350744
Cl	-2.589330	-0.111278	2.231910

H_2SiPh_2-NHC 4, T3

E_e = -1977.91714359 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.224317	1.743651	-1.170787
C	-2.239676	1.190079	-0.063403
C	-1.608007	0.568023	0.974613
H	0.296485	2.440772	-1.818236
H	0.453185	0.359059	-2.153615
C	-2.267336	2.813111	-1.942036
H	-2.866441	2.243761	-2.651904
H	-2.922640	3.457734	-1.360586
H	-1.538376	3.412030	-2.480050
C	0.280738	-0.098183	2.349447
H	-0.107315	0.409937	3.232250
H	0.052195	-1.165302	2.431059
H	1.362951	0.024843	2.327321
N	-1.530898	1.913498	-1.053182
N	-0.261870	0.486808	1.130091
Si	0.623260	0.251536	-0.487208
C	0.311047	-1.607164	-0.587724
C	1.094517	-2.514989	0.131269
C	-0.764320	-2.115023	-1.321164
C	0.818023	-3.876485	0.114077
H	1.942647	-2.158950	0.708380
C	-1.060172	-3.470851	-1.322944
H	-1.375676	-1.441470	-1.914151
C	-0.264889	-4.356676	-0.608282
H	1.447442	-4.561747	0.668390
H	-1.904525	-3.838397	-1.892823
H	-0.485274	-5.416539	-0.619025
C	2.410731	0.676884	-0.191112
C	2.748794	1.787448	0.586128
C	3.441786	-0.082976	-0.746633
C	4.076433	2.130494	0.802373
H	1.959978	2.384578	1.033142
C	4.770869	0.255378	-0.533750
H	3.198482	-0.948634	-1.353485
C	5.088290	1.362971	0.241731
H	4.323144	2.993971	1.407321
H	5.559260	-0.342891	-0.972680
H	6.124835	1.626975	0.409978
Cl	-2.610439	-0.258644	2.134255
Cl	-3.940837	1.068201	-0.310111

H_2SiPh_2-NHC 4, D

E_e = -1978.00728274 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.630707	0.477418	1.676582
C	-2.571150	0.483353	0.269541
C	-2.041211	-0.130864	-0.800537
H	-0.966940	-0.387855	2.264061
H	-0.070337	1.132617	2.347938
C	-2.401140	2.157665	2.041199
H	-3.164597	2.731666	1.519686
H	-2.867608	1.646265	2.891943
H	-1.646800	2.848120	2.419510
C	-0.276404	-0.013851	-2.488846
H	-0.448332	-0.971965	-2.983861
H	-0.814746	0.763392	-3.035319
H	0.789058	0.213474	-2.536521
N	-1.760061	1.237050	1.121915
N	-0.689794	-0.045122	-1.091166
Si	0.467467	0.024055	0.207294
C	1.701628	1.387926	-0.123732
C	3.002978	1.139074	-0.563787
C	1.304795	2.719354	0.044130
C	3.882790	2.182521	-0.823745
H	3.336619	0.117040	-0.706916
C	2.180267	3.764124	-0.210803
H	0.291328	2.937074	0.367378
C	3.472494	3.495330	-0.644685
H	4.888012	1.970161	-1.165296
H	1.856159	4.788170	-0.074938
H	4.157587	4.309525	-0.844675
C	1.349374	-1.611321	0.402389
C	0.850429	-2.752946	-0.228716
C	2.482615	-1.744614	1.210512
C	1.465454	-3.987353	-0.063492
H	-0.032391	-2.675157	-0.855632
C	3.098523	-2.975841	1.381541

H	2.895960	-0.873673	1.709518
C	2.589629	-4.098976	0.741795
H	1.066274	-4.861733	-0.561658
H	3.975202	-3.060029	2.011288
H	3.069865	-5.060660	0.871618
Cl	-2.985753	-1.205183	-1.789922
Cl	-4.218485	0.193849	0.750418

Cartesian coordinates for optimized insertion pathway compounds H_2SiPh_2-NHC 5

H_2SiPh_2-NHC 5, A

E_e = -1212.36862300 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).
0 1

Si	-1.066557	0.033792	-0.016580
C	-2.123706	-1.558910	-0.159328
C	-2.683460	-2.154323	0.972932
C	-2.367886	-2.159013	-1.394979
C	-3.461820	-3.300191	0.879186
H	-2.504231	-1.703074	1.944449
C	-3.131966	-3.314770	-1.500092
H	-1.952536	-1.704563	-2.288522
C	-3.682998	-3.886146	-0.361041
H	-3.896768	-3.737649	1.769753
H	-3.302159	-3.768059	-2.469331
H	-4.284760	-4.783456	-0.438036
C	-1.687367	1.833996	0.180536
C	-2.193475	2.548043	-0.907181
C	-1.635839	2.482848	1.414265
C	-2.635264	3.857396	-0.772394
H	-2.240588	2.061471	-1.877132
C	-2.056771	3.799716	1.557952
H	-1.262413	1.939768	2.276403
C	-2.560648	4.488433	0.463287
H	-3.037237	4.387326	-1.627552
H	-1.998613	4.286917	2.523905
H	-2.898389	5.511680	0.572319
C	0.926231	-0.130629	-0.054383
C	3.015319	-0.851472	0.316966
C	3.091209	0.353484	-0.378824
N	1.667246	-1.105954	0.500762
N	1.782798	0.752757	-0.597731
C	1.398625	1.980290	-1.275110
H	1.388998	2.814803	-0.574324
H	2.111341	2.173879	-2.074763
H	0.405180	1.848595	-1.695021
C	1.152640	-2.280436	1.181658
H	1.399564	-3.174650	0.609538
H	1.597953	-2.345566	2.174153
H	0.074284	-2.192177	1.273634
H	-0.978784	0.171729	-1.567684
H	-0.918444	-0.148211	1.525402
C	4.153935	-1.552677	0.689319
C	4.312316	0.920490	-0.716915
C	5.372061	-0.991222	0.346950
C	5.449366	0.225215	-0.342318
H	4.092474	-2.491614	1.222850
H	6.285675	-1.501960	0.619405
H	6.421700	0.631068	-0.586935
H	4.376215	1.862301	-1.244532

H_2SiPh_2-NHC 5, T1

E_e = -1212.35432715 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	0.998007	0.000050	-0.644203
C	1.809068	1.616643	-0.106145
C	1.830030	2.067247	1.215589
C	2.468436	2.384630	-1.068411
C	2.470973	3.248717	1.561087
H	1.327612	1.485702	1.980467
C	3.106223	3.571962	-0.731872
H	2.479972	2.047808	-2.099453
C	3.106045	4.007104	0.585605
H	2.477783	3.578870	2.592576
H	3.604345	4.155011	-1.496507
H	3.604503	4.930307	0.853504
C	1.809449	-1.616374	-0.106222
C	2.468996	-2.384132	-1.068549
C	1.830521	-2.067081	1.215477
C	3.107090	-3.571326	-0.732103
H	2.480444	-2.047231	-2.099565
C	2.471742	-3.248428	1.560875
H	1.327980	-1.485713	1.980408
C	3.107006	-4.006583	0.585335
H	3.605362	-4.154181	-1.496788
H	2.478635	-3.578660	2.592340
H	3.605687	-4.929684	0.853166
C	-0.882786	-0.000144	-0.595140
C	-2.974844	0.698598	-0.124528
C	-2.974753	-0.699072	-0.124394
N	-1.710502	1.095882	-0.532904
N	-1.710359	-1.096269	-0.532698
C	-1.268147	-2.468791	-0.527820
H	-0.895228	-2.758091	0.458864
H	-2.106837	-3.105415	-0.804068
H	-0.469807	-2.602747	-1.253965
C	-1.268526	2.468486	-0.528428
H	-2.107303	3.104873	-0.804967
H	-0.895745	2.758176	0.458191
H	-0.470145	2.602346	-1.254545
H	1.386380	0.000147	-2.107480
H	0.002557	-0.000039	0.863116
C	-4.106124	1.418624	0.211665
C	-4.105942	-1.419170	0.211955
C	-5.248071	0.694995	0.547252
C	-5.247982	-0.695614	0.547393
H	-4.107724	2.499905	0.224595
H	-6.148860	1.227741	0.820542
H	-6.148701	-1.228421	0.820798
H	-4.107410	-2.500449	0.225106

H_2SiPh_2-NHC 5, B

E_e = -1212.40857217 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	1.008673	0.191745	1.122586
C	0.833918	1.845529	0.275123
C	1.833963	2.802425	0.476379
C	-0.217208	2.160294	-0.589586
C	1.788661	4.033922	-0.160420
H	2.665345	2.582943	1.139321
C	-0.265004	3.392248	-1.229009
H	-1.005909	1.440541	-0.767937
C	0.735695	4.329494	-1.016062
H	2.571691	4.761987	0.009789
H	-1.087720	3.619556	-1.895017
H	0.695528	5.289507	-1.515323
C	2.452267	-0.747397	0.390692
C	2.908831	-0.456934	-0.896903
C	3.044913	-1.810407	1.078343
C	3.915706	-1.211025	-1.484292
H	2.468062	0.367277	-1.447366
C	4.051025	-2.567630	0.495437
H	2.717268	-2.052937	2.084313
C	4.485312	-2.269289	-0.789808
H	4.256764	-0.972166	-2.483694
H	4.499572	-3.387525	1.042222
H	5.271009	-2.857808	-1.246525
C	-0.595495	-0.831273	0.953015
C	-2.802579	-0.363997	0.482999
C	-2.272944	-1.060252	-0.609557
N	-1.757328	-0.016835	1.342189
N	-0.882809	-1.175240	-0.452035
C	-0.266324	-2.391125	-0.944128
H	-0.680471	-3.279906	-0.446616
H	-0.436104	-2.477714	-2.016136
H	0.808101	-2.358769	-0.776872
C	-2.022436	0.101418	2.755747
H	-2.802293	0.842901	2.921965
H	-2.341655	-0.854874	3.194947
H	-1.124267	0.441873	3.270401
H	-0.567737	-1.762967	1.563521
H	1.275302	0.375636	2.571582
C	-4.153700	-0.102012	0.571319
C	-3.086922	-1.504891	-1.628918
C	-4.979647	-0.539844	-0.470748
C	-4.457065	-1.227793	-1.549935
H	-4.570130	0.420638	1.422192
H	-6.042286	-0.342792	-0.421747
H	-5.112417	-1.566738	-2.341084
H	-2.683921	-2.057343	-2.467344

H_2SiPh_2-NHC 5, T2

E_e = -1212.35072804 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

Si	-0.764978	0.043536	-1.045107
C	0.330394	1.533258	-0.698994
C	0.591210	2.034825	0.579256
C	0.867321	2.224204	-1.787346
C	1.353405	3.178005	0.764156
H	0.198382	1.518099	1.447576
C	1.652606	3.356225	-1.610343
H	0.662994	1.871369	-2.791772
C	1.893660	3.837347	-0.332682
H	1.534137	3.552025	1.764218
H	2.069121	3.865519	-2.470383
H	2.498277	4.724292	-0.189645
C	-2.509423	0.043873	-0.353430
C	-2.919912	0.939090	0.635413
C	-3.447272	-0.872248	-0.833090
C	-4.213276	0.909380	1.139966
H	-2.219612	1.672905	1.020502
C	-4.738400	-0.918621	-0.324248
H	-3.173889	-1.559657	-1.627913
C	-5.123038	-0.027329	0.667596
H	-4.512395	1.616319	1.903956
H	-5.446510	-1.643161	-0.707024
H	-6.129968	-0.056534	1.064192
C	-0.079641	-1.695656	-1.209926
C	1.994645	-1.377006	-0.243542
C	1.257399	-0.976907	0.901038
N	1.201874	-2.053894	-1.196691
N	-0.098652	-0.962290	0.798982
C	-0.854550	-1.177786	2.018689
H	-0.415227	-1.970610	2.632872
H	-0.908274	-0.264378	2.626380
H	-1.877929	-1.450619	1.766549
C	1.592412	-3.433782	-1.488265
H	1.591947	-4.029719	-0.572793
H	0.897069	-3.852057	-2.212111
H	2.591970	-3.443855	-1.917143
H	-0.758768	-2.499329	-1.502363
H	-1.049455	0.310421	-2.510386
C	3.379006	-1.315477	-0.290184
C	2.004837	-0.625687	2.039867
C	4.079187	-0.882415	0.820480
C	3.383075	-0.559812	1.985599
H	3.900637	-1.613673	-1.191145
H	5.157676	-0.814282	0.790700
H	3.930977	-0.238881	2.862746
H	1.484115	-0.351302	2.948395

H_2SiPh_2-NHC 5, C

E_e = -1212.36830005 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.371046	-1.328855	1.565862
C	2.442447	-1.030518	0.440052
C	1.815759	-0.480265	-0.717628
H	-0.140990	-1.897773	2.340482
C	2.278765	-2.517958	2.411139
H	2.851842	-3.256730	1.855589
H	2.939243	-1.973279	3.083697
H	1.499224	-3.003258	2.989018
C	-0.033043	0.111000	-2.115000
H	0.355631	1.091857	-2.406613
H	0.212797	-0.609899	-2.900832
H	-1.116285	0.196186	-2.059854
N	1.639139	-1.582641	1.474134
N	0.472498	-0.330096	-0.823337
Si	-0.669575	0.007998	0.666704
C	-2.183434	-0.939900	0.026617
C	-3.466483	-0.613354	0.472190
C	-2.061320	-2.028785	-0.840849
C	-4.583464	-1.322651	0.051673
H	-3.594421	0.203597	1.172653
C	-3.170157	-2.756449	-1.252807
H	-1.078512	-2.309852	-1.203955
C	-4.436779	-2.399406	-0.811790
H	-5.567703	-1.040172	0.404017
H	-3.046533	-3.600171	-1.920652
H	-5.304803	-2.960536	-1.134922
C	-0.566994	1.909493	0.415580
C	0.506129	2.584747	-0.170189
C	-1.616654	2.691870	0.906626
C	0.529245	3.971444	-0.269087
H	1.356929	2.028833	-0.547726
C	-1.623937	4.072833	0.778427
H	-2.442795	2.207609	1.416300
C	-0.543268	4.719210	0.191903
H	1.385289	4.466066	-0.711709
H	-2.463553	4.647660	1.149730
H	-0.534555	5.798476	0.104448
H	-1.247696	0.234978	2.089556
C	3.830726	-1.115388	0.545558
C	2.705362	-0.113878	-1.762945
C	4.656507	-0.702550	-0.476612
C	4.071355	-0.217081	-1.643532
H	4.276946	-1.509703	1.446784
H	5.729932	-0.768328	-0.372725
H	4.694998	0.092098	-2.473037
H	2.296761	0.278166	-2.680824

H_2SiPh_2-NHC 5, T3

E_e = -1212.36698576 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.465946	-1.670582	-1.176134
C	-2.558627	-1.026044	-0.238555
C	-1.942972	-0.324422	0.841497
H	0.042809	-2.325416	-1.879880
C	-2.469880	-2.551251	-2.193835
H	-3.166391	-3.245480	-1.726221
H	-3.014426	-1.900133	-2.879628
H	-1.722558	-3.107173	-2.750965
C	-0.086045	0.411782	2.207068
H	-0.314377	1.484029	2.205738
H	-0.504942	-0.039554	3.109370
H	0.997579	0.301057	2.248615
N	-1.779294	-1.761498	-1.176671
N	-0.574449	-0.272741	1.020472
Si	0.490835	-0.224633	-0.441358
C	2.149578	-0.993080	-0.051659
C	3.325038	-0.544024	-0.657284
C	2.234746	-2.066184	0.838203
C	4.544646	-1.151045	-0.389985
H	3.283923	0.294065	-1.345130
C	3.452337	-2.672198	1.117402
H	1.331445	-2.426948	1.320898
C	4.608836	-2.215264	0.499739
H	5.445629	-0.793667	-0.872686
H	3.500451	-3.500406	1.813348
H	5.560009	-2.687312	0.712015
C	0.710233	1.674746	-0.486554
C	-0.225557	2.459616	-1.166206
C	1.737522	2.340656	0.187551
C	-0.151695	3.845243	-1.166743
H	-1.027719	1.977370	-1.718212
C	1.830036	3.727819	0.178886
H	2.486981	1.770309	0.727219
C	0.882948	4.484455	-0.495267
H	-0.894383	4.427099	-1.698673
H	2.643278	4.218034	0.700377
H	0.951962	5.564910	-0.501982
H	0.322059	-0.214553	-2.068222
C	-3.944014	-1.020464	-0.379464
C	-2.817436	0.325702	1.733403
C	-4.767975	-0.367847	0.519076
C	-4.190333	0.301250	1.585092
H	-4.400718	-1.538183	-1.209082
H	-5.839867	-0.385268	0.381740
H	-4.808665	0.821852	2.304991
H	-2.400203	0.876709	2.561405

H_2SiPh_2-NHC 5, D

E_e = -1212.45761558 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.613830	0.275119	1.714823
C	-2.670629	0.329982	0.434483
C	-2.149461	-0.281529	-0.738070
H	-0.874300	-0.660665	2.231808
H	-0.046077	0.884192	2.422110
C	-2.421342	1.744385	2.399813
H	-3.188555	2.419636	2.022235
H	-2.872979	1.077342	3.148916
H	-1.655082	2.340637	2.894758
C	-0.350470	-0.517765	-2.380954
H	-0.433750	-1.582912	-2.623374
H	-0.933822	0.050028	-3.109887
H	0.697366	-0.234397	-2.495418
N	-1.804250	1.024653	1.305570
N	-0.782481	-0.212149	-1.028534
Si	0.430031	-0.006330	0.187790
C	1.513598	1.475463	-0.170793
C	2.727389	1.375008	-0.855316
C	1.082521	2.748102	0.219008
C	3.487489	2.502734	-1.138175
H	3.089541	0.402550	-1.172350
C	1.840656	3.876768	-0.055040
H	0.130855	2.855691	0.730225
C	3.045856	3.754540	-0.734701
H	4.424665	2.403942	-1.671326
H	1.491123	4.852778	0.257087
H	3.637721	4.634614	-0.952766
C	1.482393	-1.548070	0.318676
C	0.948391	-2.777896	-0.076290
C	2.762503	-1.536872	0.879031
C	1.669327	-3.954591	0.073460
H	-0.050147	-2.815193	-0.500925
C	3.486820	-2.710718	1.034995
H	3.202598	-0.598025	1.198795
C	2.941051	-3.920840	0.628688
H	1.239945	-4.897265	-0.241780
H	4.477298	-2.681638	1.471389
H	3.505553	-4.837321	0.745554
C	-3.034801	-0.910161	-1.610610
C	-4.040724	0.263786	0.665871
C	-4.908025	-0.360394	-0.225043
C	-4.402563	-0.948439	-1.365270
H	-4.452393	0.711779	1.558110
H	-5.968687	-0.381484	-0.013384
H	-5.058683	-1.439535	-2.071789
H	-2.652404	-1.375336	-2.507816

Cartesian coordinates for optimized insertion pathway compounds H_2BMe-NHC 1

H_2BMe-NHC 1, A

E_e = -370.775939198 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.871024	0.675349	-0.291540
C	1.871115	-0.675113	-0.291550
C	-0.192211	-0.000023	0.280139
H	2.651819	1.381457	-0.509694
H	2.651996	-1.381112	-0.509757
N	0.597201	-1.067515	0.056317
N	0.597056	1.067581	0.056330
C	0.147679	-2.443027	0.188427
H	0.865095	-3.091107	-0.309850
H	0.068631	-2.713245	1.240008
H	-0.830554	-2.546170	-0.273067
C	0.147370	2.443040	0.188422
H	-0.830874	2.546072	-0.273074
H	0.068291	2.713269	1.239999
H	0.864716	3.091190	-0.309864
C	-2.619639	-0.000155	-0.722506
H	-3.689178	-0.000172	-0.501551
H	-2.426416	0.877297	-1.349939
H	-2.426383	-0.877615	-1.349915
B	-1.753768	-0.000107	0.668478
H	-1.955110	0.997246	1.333709
H	-1.955012	-0.997467	1.333727

H_2BMe-NHC 1, T1

E_e = -370.721299439 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.013356	-1.672846	-0.075911
C	-1.930241	-0.705692	-0.071186
C	0.098518	0.299827	-0.034574
H	-1.145287	-2.741416	-0.061869
H	-3.004357	-0.781064	-0.050570
N	-1.298394	0.529876	-0.289941
N	0.260410	-1.106838	-0.292721
C	-1.892644	1.735478	0.228528
H	-1.525328	2.606253	-0.311477
H	-2.972550	1.679153	0.100604
H	-1.668157	1.870318	1.298225
C	1.399491	-1.769366	0.297007
H	1.490684	-1.533812	1.369523
H	1.275531	-2.845896	0.188511
H	2.319432	-1.481140	-0.205541
B	1.168330	1.395035	-0.074869
H	0.281141	0.477334	1.149845
H	0.743232	2.498572	0.069938
C	2.719630	1.136178	-0.123074
H	3.292990	2.061038	-0.086881
H	3.056521	0.510258	0.706631
H	2.991990	0.602490	-1.038687

H_2BMe-NHC 1, B

E_e = -370.742402361 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.243875	0.549217	-1.332028
C	0.983634	0.046255	-1.228754
C	0.154924	-0.028783	0.904622
H	-0.790860	0.854788	-2.207861
H	1.688786	-0.119138	-2.030083
N	1.309823	-0.329144	0.067754
N	-0.879269	0.580958	-0.042836
C	2.607552	0.068752	0.576645
H	2.807790	-0.451323	1.512660
H	3.376455	-0.215722	-0.141430
H	2.671883	1.151586	0.752522
C	-1.525393	1.839251	0.319419
H	-0.814043	2.665254	0.250784
H	-2.362074	2.018603	-0.356596
H	-1.906502	1.754636	1.334294
B	-1.205474	-0.812791	0.742401
H	0.393621	0.622142	1.744398
H	-2.023557	-0.585214	1.588501
C	-1.309590	-2.133380	-0.129385
H	-1.340719	-3.001622	0.533847
H	-2.226061	-2.162248	-0.724769
H	-0.464734	-2.278361	-0.805808

H_2BMe-NHC 1, T2

E_e = -370.734022201 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.242724	-0.606591	1.223488
C	0.951495	0.000119	1.205034
C	0.350304	0.270996	-0.994728
N	1.384252	0.341144	-0.081033
N	-0.922510	-0.610684	0.005969
C	2.681898	-0.209692	-0.455295
H	3.002032	0.223655	-1.400914
H	3.412832	0.053958	0.308219

H	2.641529	-1.300934	-0.545594
C	-1.718771	-1.782541	-0.325044
H	-1.174837	-2.704267	-0.112502
H	-2.651763	-1.771629	0.245804
H	-1.968772	-1.744355	-1.382500
B	-1.106501	0.797864	-0.713136
H	0.627275	-0.220550	-1.927336
H	-1.826514	0.631513	-1.663931
C	-1.395458	2.069139	0.206864
H	-1.419211	2.971733	-0.409035
H	-2.371382	1.997549	0.695833
H	-0.648301	2.234000	0.986675
H	-0.690492	-1.077166	2.087357
H	1.607457	0.155371	2.047141

H_2BMe-NHC 1, C

E_e = -370.770615993 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.086987	-1.250778	0.276081
C	0.256063	-1.486319	0.212909
C	-0.784678	0.999951	-0.395312
H	-1.815747	-1.992433	0.545538
H	0.599390	-2.488940	0.452968
N	1.167207	-0.590373	-0.122189
N	-1.570508	0.031033	-0.051822
C	2.560599	-0.961507	-0.187550
H	2.687238	-2.036879	-0.053958
H	2.968297	-0.671804	-1.160433
H	3.137348	-0.440994	0.581176
C	-3.023150	0.179619	0.009718
H	-3.294506	1.197909	-0.251297
H	-3.481104	-0.521189	-0.687375
H	-3.360168	-0.050041	1.019840
H	-1.307627	1.924656	-0.630101
B	0.814748	0.901807	-0.468271
H	1.160705	1.149527	-1.615214
C	1.490404	1.959327	0.567542
H	2.579318	1.983566	0.472114
H	1.145145	2.979367	0.372271
H	1.257577	1.731850	1.613575

H_2BMe-NHC 1, T3

E_e = -370.753449855 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.180890	-1.238123	-0.168555
C	-0.124916	-1.540057	-0.142827
C	0.717601	1.074585	-0.082787
H	1.947427	-1.990243	-0.255595
H	-0.402774	-2.588690	-0.171814
N	-1.148301	-0.628842	-0.142080
N	1.632552	0.116654	-0.164209
C	-2.456408	-1.099782	0.255600
H	-2.577036	-1.131694	1.347564
H	-3.223533	-0.439597	-0.147560
H	-2.634093	-2.103172	-0.136959
C	3.015382	0.333291	0.214591
H	3.266177	1.383515	0.082726
H	3.177071	0.048990	1.259261
H	3.667522	-0.269205	-0.417840
H	1.116773	2.081836	0.006719
B	-0.774057	0.811192	0.077262
H	-0.185938	1.043740	1.290843
C	-1.870089	1.940866	-0.151154
H	-1.453654	2.943845	-0.038003
H	-2.288190	1.866610	-1.159829
H	-2.703985	1.858740	0.548981

H_2BMe-NHC 1, D

E_e = -370.811407916 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	0.972062	2.012364	-0.463968
H	0.935625	1.444766	1.192655
C	0.733233	1.135244	0.146509
C	1.159321	-1.242027	-0.002107
C	-0.132602	-1.557618	0.110578
H	1.912167	-2.017295	0.044507
H	-0.452245	-2.579722	0.247137
N	-1.147539	-0.574492	0.016991
N	1.613980	0.042445	-0.242663
C	-2.496950	-1.099488	-0.064140
H	-2.603640	-1.750945	-0.935332
H	-2.740103	-1.682955	0.828327
H	-3.211377	-0.285274	-0.151955
C	3.016758	0.302659	-0.027562
H	3.245157	0.481111	1.034054
H	3.614039	-0.539053	-0.377797
H	3.313042	1.190273	-0.589000
B	-0.811142	0.785438	0.021719
C	-1.892478	1.934956	-0.029868
H	-2.387986	1.963287	-1.005390
H	-2.680429	1.799819	0.715047
H	-1.449379	2.918406	0.132371

Cartesian coordinates for optimized insertion pathway compounds H_2BMe-NHC 2

H_2BMe-NHC 2, A

E_e = -371.971495483 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-2.008461	-0.359371	0.217088
C	-1.136472	-1.609687	0.339044
C	0.187639	0.183880	-0.328853
H	-2.577062	-0.141588	1.121553
H	-1.002652	-1.922400	1.379764
N	0.134575	-1.147480	-0.206399
N	-1.015916	0.679600	-0.034993
C	1.270712	-2.036577	-0.221320
H	1.544705	-2.327093	0.797319
H	1.024890	-2.935761	-0.788808
H	2.108267	-1.527642	-0.688313
C	-1.427333	2.059044	-0.121592
H	-0.556340	2.673237	-0.324341
H	-2.158876	2.189850	-0.923957
H	-1.885001	2.367014	0.820863
C	2.329181	1.179767	0.750682
H	3.260650	1.726671	0.590733
H	1.759163	1.735551	1.502718
H	2.600824	0.220303	1.205260
B	1.523547	1.022698	-0.667193
H	1.213178	2.093275	-1.141047
H	2.154916	0.384196	-1.484597
H	-2.706745	-0.418223	-0.623467
H	-1.519862	-2.458060	-0.228269

H_2BMe-NHC 2, T1

E_e = -371.937585183 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.103906	-1.595438	-0.175119
C	2.058605	-0.419440	-0.094193
C	-0.170826	0.293593	-0.207922
H	1.425820	-2.457856	0.408027
H	2.487658	-0.360873	0.914168
N	1.191533	0.733432	-0.348036
N	-0.115191	-1.015151	0.373320
C	1.566964	1.902825	0.423813
H	1.436385	1.742918	1.504804
H	2.617348	2.128292	0.234779
H	0.979349	2.765339	0.119287
C	-1.277447	-1.856811	0.215741
H	-2.111989	-1.479999	0.801724
H	-1.590914	-1.929518	-0.839925
H	-1.037559	-2.859199	0.570151
C	-2.853140	0.927279	0.050260
H	-3.511919	1.757785	-0.199717
H	-3.226511	0.046696	-0.475607
H	-2.968835	0.720091	1.118270
B	-1.347539	1.255056	-0.294146
H	-0.631289	0.192834	-1.316694
H	-1.059895	2.305105	-0.781531
H	0.953445	-1.908727	-1.222172
H	2.873829	-0.478184	-0.817309

H_2BMe-NHC 2, B

E_e = -371.962992000 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.019457	-0.229489	1.379548
C	0.736537	1.057856	0.917935
C	0.126456	-0.016927	-1.015592
H	-0.769341	-0.030555	2.105618
H	0.048223	1.898375	0.930311
N	1.168716	0.790210	-0.450591
N	-0.531760	-0.793465	0.145387
C	2.464086	0.118366	-0.483200
H	2.730335	-0.097507	-1.517306
H	3.226352	0.778162	-0.068365
H	2.477517	-0.829017	0.078353
C	-0.635919	-2.242644	0.091142
H	0.333747	-2.705785	0.296483
H	-1.366317	-2.593272	0.822437
H	-0.974799	-2.532259	-0.900600
B	-1.427796	0.172109	-0.800785
H	0.485524	-0.679531	-1.797316
H	-2.071913	-0.526854	-1.533120
C	-2.158084	1.447470	-0.160670
H	-3.198795	1.494956	-0.483695
H	-2.178236	1.437683	0.933629
H	-1.689060	2.387890	-0.460682
H	1.589897	1.299403	1.549563
H	0.721957	-0.947252	1.810061

H_2BMe-NHC 2, T2

E_e = -371.948201475 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.934964	0.359287	1.193108
C	0.188213	-0.722682	1.204928
C	-0.482593	0.555737	-1.065406
H	-0.523224	1.323885	1.470793
H	-0.243315	-1.717908	1.371057
N	0.890032	-0.696859	-0.040765
N	-1.440487	0.440522	-0.165606
C	1.652747	-1.871804	-0.372673
H	1.967309	-1.812854	-1.413465
H	2.557984	-1.971387	0.243331
H	1.058405	-2.783031	-0.235156
C	-2.673710	-0.280575	-0.447209
H	-2.915768	-0.178888	-1.502291
H	-2.556283	-1.341884	-0.207379
H	-3.488056	0.131946	0.147295
H	-0.806601	0.283987	-2.070861
B	1.094278	0.688777	-0.717096
H	1.688591	0.528038	-1.758760
C	1.722103	1.899700	0.150624
H	1.374818	1.991877	1.183719
H	2.807877	1.780378	0.204771
H	1.542668	2.865419	-0.330976
H	0.828154	-0.493894	2.068956
H	-1.741537	0.106815	1.878809

H_2BMe-NHC 2, C

E_e = -371.966589942 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.085032	-1.287304	0.163303
C	0.380388	-1.283515	0.559304
C	-0.771068	1.042827	-0.353067
H	-1.708391	-1.718157	0.950251
H	0.696754	-2.330048	0.635604
N	1.154232	-0.587767	-0.428816
N	-1.585192	0.076963	-0.084199
C	2.566541	-0.863586	-0.308018
H	3.105879	-0.324125	-1.088727
H	2.990902	-0.553956	0.662105
H	2.767699	-1.933120	-0.432891
C	-3.033872	0.219786	-0.030250
H	-3.310414	1.238409	-0.288547
H	-3.490634	-0.474439	-0.736843
H	-3.389308	-0.017525	0.972903
H	-1.265138	2.005010	-0.491773
B	0.800798	0.904503	-0.502480
H	1.018588	1.372071	-1.614061
C	1.495524	1.868829	0.633886
H	1.117171	2.894583	0.605733
H	1.352166	1.499066	1.655086
H	2.572494	1.927753	0.461323
H	0.470917	-0.852737	1.576546
H	-1.230845	-1.861891	-0.754152

H_2BMe-NHC 2, T3

E_e = -371.964351842 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.204302	-1.255265	0.001090
C	-0.236442	-1.428921	-0.447960
C	0.709654	1.092518	-0.030800
H	1.882799	-1.822018	-0.642260
H	-0.486938	-2.489692	-0.337317
N	-1.122141	-0.618163	0.343408
N	1.616858	0.148691	-0.041841
C	-2.506311	-1.001429	0.194874
H	-3.128549	-0.414231	0.870145
H	-2.896243	-0.855454	-0.826224
H	-2.641440	-2.057405	0.451098
C	3.042585	0.390719	0.078036
H	3.236254	1.459191	0.024677
H	3.411370	0.006689	1.032349
H	3.575121	-0.115256	-0.728607
H	1.112439	2.103198	-0.072079
B	-0.788145	0.856349	0.300331
H	-0.365531	1.301809	1.432361
C	-1.857381	1.903261	-0.292569
H	-1.465695	2.923690	-0.307935
H	-2.141891	1.648361	-1.318295
H	-2.776605	1.926335	0.295855
H	-0.294954	-1.200739	-1.530207
H	1.319127	-1.615216	1.027803

H_2BMe-NHC 2, D

E_e = -372.027668000 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	0.902190	1.977363	-0.725661
H	0.996768	1.597256	0.983029
C	0.731464	1.168510	-0.006743
C	1.179981	-1.135904	0.387575
C	-0.183616	-1.601701	-0.081009
H	1.903129	-1.936140	0.215712

H	-0.515628	-2.429064	0.555878
N	-1.174610	-0.536448	-0.021459
N	1.599353	0.046283	-0.335373
C	-2.535173	-1.023871	-0.107829
H	-2.674842	-1.612366	-1.020601
H	-2.774536	-1.668325	0.743904
H	-3.237588	-0.194454	-0.124839
C	2.991759	0.355574	-0.095935
H	3.195191	0.565842	0.968433
H	3.622917	-0.477547	-0.409760
H	3.273307	1.237611	-0.672485
B	-0.810579	0.812290	0.022189
C	-1.881092	1.974912	0.100262
H	-2.426133	2.063736	-0.844860
H	-2.630332	1.809829	0.878015
H	-1.414269	2.942689	0.289999
H	-0.110078	-1.985421	-1.105175
H	1.149667	-0.946425	1.477358

Cartesian coordinates for optimized insertion pathway compounds H_2BMe-NHC 3

H_2BMe-NHC 3, A

E_e = -449.403400934 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.295005	0.676857	0.041387
C	-1.295150	-0.676641	0.041418
C	0.825548	-0.000128	-0.350986
N	0.015202	-1.065837	-0.198819
N	0.015431	1.065765	-0.198855
C	0.452160	-2.448145	-0.222041
H	0.315382	-2.900556	0.760448
H	-0.121812	-3.009715	-0.959012
H	1.504100	-2.462934	-0.487907
C	0.452705	2.447974	-0.222107
H	1.504668	2.462508	-0.487900
H	-0.121069	3.009640	-0.959159
H	0.315963	2.900462	0.760350
C	3.136580	-0.000091	0.900791
H	4.224386	-0.000135	0.801104
H	2.873445	0.878533	1.500931
H	2.873389	-0.878567	1.501121
B	2.426322	-0.000262	-0.572754
H	2.712074	0.987449	-1.219886
H	2.711986	-0.988195	-1.219585
C	-2.392073	-1.660267	0.234332
H	-2.544996	-2.269389	-0.659092
H	-2.179431	-2.335872	1.065132
H	-3.324671	-1.143690	0.451197
C	-2.391705	1.660731	0.234307
H	-2.179043	2.336100	1.065295
H	-2.544277	2.270083	-0.659017
H	-3.324490	1.144360	0.450860

H_2BMe-NHC 3, T1

E_e = -449.348250781 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.483529	0.315958	-0.047116
C	1.042046	-0.947432	-0.049128
C	-0.789187	0.402177	-0.039552
N	-0.360465	-0.946809	-0.283027
N	0.390195	1.183543	-0.285006
C	-1.148038	-1.995519	0.320997
H	-2.126054	-2.056516	-0.148015
H	-0.650743	-2.952518	0.178023
H	-1.284196	-1.826652	1.402597

C	0.412547	2.526589	0.237217
H	0.176242	2.549631	1.313848
H	1.398164	2.960999	0.083903
H	-0.315409	3.144707	-0.283948
B	-2.213432	0.964080	-0.089578
H	-1.042137	0.496993	1.141760
H	-2.278486	2.144862	0.054974
C	-3.532907	0.107083	-0.145172
H	-4.424540	0.732251	-0.151431
H	-3.552472	-0.524009	-1.038478
H	-3.616559	-0.567808	0.710174
C	1.801286	-2.225092	-0.033503
H	2.871974	-2.033005	-0.029813
H	1.568623	-2.831251	0.845065
H	1.564100	-2.821272	-0.919214
C	2.872903	0.842947	-0.022797
H	3.073266	1.440663	-0.916445
H	3.053280	1.478676	0.847012
H	3.590934	0.026444	0.008430

H_2BMe-NHC 3, B

E_e = -449.370819922 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.223313	0.992136	-0.153320
C	-1.019672	0.571134	0.098609
C	0.178141	-1.351059	-0.314247
N	-1.137553	-0.825324	0.021421
N	1.071991	-0.135568	-0.463837
C	-2.242290	-1.360663	-0.752166
H	-2.254754	-2.445046	-0.650227
H	-3.185567	-0.980591	-0.362336
H	-2.170215	-1.107985	-1.820665
C	1.913878	-0.013591	-1.649873
H	1.313336	0.275148	-2.516314
H	2.690769	0.730714	-1.473488
H	2.390617	-0.974000	-1.830856
B	1.389854	-1.237455	0.693776
H	0.174941	-1.983201	-1.200180
H	2.373448	-1.848508	0.383139
C	1.171516	-0.792370	2.202336
H	1.216683	-1.674118	2.846828
H	1.950067	-0.110204	2.554607
H	0.202164	-0.320020	2.377386
C	0.854195	2.331770	-0.031680
H	1.242681	2.689919	-0.988174
H	0.135570	3.064417	0.329413
H	1.689985	2.294156	0.673261
C	-2.200667	1.380474	0.509257
H	-2.970852	1.378872	-0.264762
H	-2.638899	0.962884	1.417921
H	-1.920803	2.414098	0.698979

H_2BMe-NHC 3, T2

E_e = -449.358840608 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.265034	0.919656	-0.116692
C	-0.981049	0.527715	0.218863
C	-0.076084	-1.542117	-0.264084
N	-1.229722	-0.829658	-0.085540
N	1.136708	-0.116062	-0.478345
C	-2.341605	-1.065224	-1.001176
H	-2.448876	-2.135952	-1.161415
H	-3.266194	-0.696948	-0.559886
H	-2.180309	-0.564521	-1.962686
C	2.135159	0.130505	-1.504709
H	1.700281	0.618778	-2.379517
H	2.946864	0.752630	-1.114050
H	2.558757	-0.825472	-1.803002
B	1.245395	-1.308985	0.561569
H	-0.122932	-2.246809	-1.094310
H	2.123593	-2.047366	0.190907
C	1.235660	-0.941786	2.118633
H	1.246256	-1.857251	2.715747
H	2.127389	-0.374878	2.403045
H	0.363930	-0.364233	2.437171
C	0.803793	2.313312	-0.076304
H	1.146372	2.626506	-1.064497
H	0.047741	3.022649	0.249495
H	1.658400	2.376200	0.602161
C	-2.093744	1.354570	0.774698
H	-1.727943	2.311277	1.138765
H	-2.870685	1.555330	0.032794
H	-2.561518	0.835241	1.613247

H_2BMe-NHC 3, C

E_e = -449.383347504 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.892196	0.657272	0.156275
C	-0.444124	0.936355	-0.042002
C	0.567060	-1.613561	-0.488453
N	-1.306123	-0.021243	-0.414582
N	1.361542	-0.604966	-0.294822
C	-2.662613	0.311530	-0.797402
H	-2.708965	1.138015	-1.509051
H	-3.100769	-0.567395	-1.264855
H	-3.282455	0.571951	0.068406
C	2.779631	-0.681874	-0.659600
H	2.981402	-1.668003	-1.065662
H	3.005596	0.080901	-1.403253

H	3.401741	-0.516778	0.217344
H	1.047581	-2.468235	-0.958930
B	-0.977460	-1.517060	-0.083272
H	-1.633487	-2.237265	-0.805764
C	-1.186025	-1.858906	1.494630
H	-2.228926	-1.710289	1.791802
H	-0.938341	-2.899758	1.723122
H	-0.570508	-1.227274	2.145375
C	1.915456	1.568019	0.767498
H	2.479000	1.056579	1.553016
H	2.642000	1.970665	0.054132
H	1.435266	2.412251	1.251246
C	-0.971657	2.337876	0.103203
H	-1.336467	2.695600	-0.860768
H	-1.814635	2.359980	0.796101
H	-0.218218	3.037551	0.445024

H_2BMe-NHC 3, T3

E_e = -449.367447563 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.199960	0.431260	-0.084615
C	-0.028293	1.108085	-0.040614
C	-0.061588	-1.673734	-0.110183
N	1.217953	0.492956	-0.037361
N	-1.206588	-1.018877	-0.053392
C	2.355683	1.221788	0.489490
H	3.257267	0.650771	0.279921
H	2.479886	2.199549	0.024744
H	2.296413	1.363776	1.578845
C	-2.401969	-1.682595	0.448814
H	-2.243659	-2.757410	0.409459
H	-2.590396	-1.389518	1.486222
H	-3.275365	-1.434167	-0.149756
H	-0.149613	-2.756751	-0.076853
B	1.298043	-1.007154	0.017088
H	0.945464	-1.508466	1.213986
C	2.633081	-1.751773	-0.442994
H	2.490458	-2.833594	-0.496989
H	2.937647	-1.410021	-1.436994
H	3.475034	-1.579123	0.229638
C	0.005512	2.611692	-0.074522
H	0.496549	2.997387	0.820184
H	0.585523	2.951430	-0.935777
H	-0.978429	3.059557	-0.123488
C	-2.556959	1.014098	-0.348815
H	-2.994608	0.567532	-1.247760
H	-3.257770	0.840268	0.471866
H	-2.517208	2.083067	-0.516787

H_2BMe-NHC 3, D

E_e = -449.424821857 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	-0.091356	-2.693352	0.021352
H	-0.316398	-1.760639	1.494607
C	-0.108422	-1.670979	0.408963
C	-1.177228	0.447180	-0.056152
C	-0.014503	1.116156	0.073592
N	1.225863	0.409782	-0.046186
N	-1.178006	-0.945334	-0.268007
C	2.378195	1.190985	-0.470928
H	2.171398	1.700105	-1.415362
H	2.662187	1.944429	0.266145
H	3.224050	0.527342	-0.624173
C	-2.436606	-1.657390	-0.204451
H	-2.819570	-1.744852	0.824578
H	-3.198847	-1.188671	-0.822002
H	-2.277217	-2.666694	-0.584518
B	1.284587	-0.976899	0.145389
C	2.624693	-1.811772	0.084336
H	2.922435	-1.980851	-0.956133
H	3.466302	-1.321784	0.577439
H	2.500223	-2.796825	0.537061
C	-2.520779	1.117248	-0.068934
H	-3.000762	0.976345	-1.040396
H	-3.189396	0.699721	0.686403
H	-2.447060	2.184854	0.097995
C	0.114507	2.578062	0.391495
H	0.753117	2.716285	1.268131
H	0.565354	3.146446	-0.425977
H	-0.841540	3.034562	0.619737

Cartesian coordinates for optimized insertion pathway compounds H_2BMe-NHC 4

H_2BMe-NHC 4, A

E_e = -1289.97003752 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.859344	0.674844	-0.028379
C	-0.859284	-0.674886	-0.028375
C	1.256370	0.000073	-0.351505
N	0.446361	-1.073203	-0.223713
N	0.446269	1.073276	-0.223699
C	0.878602	-2.461194	-0.241189
H	0.618396	-2.935019	0.704035
H	0.389602	-2.989437	-1.058172
H	1.953847	-2.465820	-0.382898
C	0.878388	2.461307	-0.241134
H	1.953636	2.466029	-0.382812
H	0.389364	2.989524	-1.058119
H	0.618113	2.935089	0.704091
C	3.536807	0.000020	0.950876
H	4.625812	0.000012	0.869475
H	3.263804	0.878474	1.546064
H	3.263785	-0.878477	1.545992
B	2.861789	0.000108	-0.537451
H	3.150649	0.988467	-1.178813
H	3.150649	-0.988167	-1.178944
Cl	-2.144909	1.757488	0.156688
Cl	-2.144752	-1.757647	0.156693

H_2BMe-NHC 4, T1

E_e = -1289.92256608 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.012748	0.526692	0.014913
C	-0.674752	-0.763737	0.017412
C	1.237372	0.427567	0.086429
N	0.703036	-0.890791	0.291398
N	0.121027	1.308105	0.292119
C	1.428354	-1.997590	-0.295816
H	0.818111	-2.895036	-0.232264
H	1.664847	-1.800829	-1.352294
H	2.350843	-2.170224	0.250745
C	0.221792	2.657034	-0.216318
H	0.951142	3.214149	0.366221
H	0.532308	2.665485	-1.271346
H	-0.746093	3.142663	-0.122707
C	3.947048	-0.083323	0.109823
H	3.966018	-0.672657	1.031061
H	3.948219	-0.798056	-0.715279
H	4.878485	0.477560	0.052131
B	2.695282	0.873086	0.083068
H	2.835472	2.046483	-0.056992
H	1.553607	0.517481	-1.097063
Cl	-2.575682	1.191102	0.001800
Cl	-1.711389	-2.109544	0.018739

H_2BMe-NHC 4, B

E_e = -1289.94495467 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.227945	0.662176	-0.243631
C	-0.918747	0.018880	-0.021878
C	0.647750	-1.621913	-0.165594
N	-0.782040	-1.363405	0.000764
N	1.307642	-0.258654	-0.400822
C	-1.669477	-2.126619	-0.866914
H	-1.518598	-3.186803	-0.672268
H	-2.702700	-1.878494	-0.632670
H	-1.481331	-1.923862	-1.929374
C	2.181162	-0.065396	-1.557510
H	1.592483	-0.033599	-2.476740
H	2.733359	0.865800	-1.437904
H	2.883666	-0.894292	-1.587808
B	1.723999	-1.176948	0.897903
H	0.850511	-2.317645	-0.975789
H	2.821789	-1.611597	0.700545
C	1.318089	-0.627807	2.327557
H	1.499717	-1.406470	3.072505
H	1.920162	0.234739	2.623251
H	0.265294	-0.349351	2.413059
Cl	0.545970	2.329089	-0.172831
Cl	-2.421494	0.747664	0.312943

H_2BMe-NHC 4, T2

E_e = -1289.93611234 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.291487	0.605627	-0.205557
C	-0.890855	0.014689	0.039478
C	0.415353	-1.837220	-0.140405
N	-0.881312	-1.368589	-0.149915
N	1.367941	-0.254252	-0.380392
C	-1.798656	-1.870066	-1.173585

H	-1.756078	-2.956738	-1.177448
H	-2.812129	-1.563051	-0.925548
H	-1.534775	-1.482276	-2.162937
C	2.392000	0.079235	-1.360858
H	1.949335	0.448397	-2.286676
H	3.066380	0.836528	-0.954964
H	2.966546	-0.821477	-1.562163
B	1.567459	-1.312264	0.801407
H	0.603167	-2.580119	-0.914584
H	2.593716	-1.902039	0.587172
C	1.307880	-0.804986	2.290247
H	1.400310	-1.642080	2.986374
H	2.052156	-0.063363	2.593109
H	0.321075	-0.364721	2.454211
Cl	0.546263	2.297363	-0.220032
Cl	-2.334302	0.813723	0.477246

H_2BMe-NHC 4, C

E_e = -1289.96605728 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.825479	0.181368	-0.005503
C	-0.474311	0.604880	-0.133172
C	0.206295	-2.048036	-0.442222
N	-1.478539	-0.218032	-0.378571
N	1.137806	-1.145383	-0.374186
C	-2.775214	0.273896	-0.806787
H	-2.683488	1.037696	-1.579029
H	-3.330268	-0.572763	-1.202831
H	-3.334952	0.696476	0.032285
C	2.526100	-1.432296	-0.758560
H	2.565691	-2.445256	-1.145247
H	2.848518	-0.721251	-1.516128
H	3.170512	-1.339006	0.112143
H	0.549091	-2.995398	-0.849815
B	-1.295023	-1.734870	0.026655
H	-2.068000	-2.394843	-0.628831
C	-1.450431	-1.964588	1.624216
H	-2.455758	-1.691841	1.957791
H	-1.297966	-3.011717	1.900585
H	-0.741541	-1.367201	2.207631
Cl	-0.793477	2.304941	0.010767
Cl	2.116471	1.185177	0.517447

H_2BMe-NHC 4, T3

E_e = -1289.95120614 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.924837	-0.204049	0.030987
C	-0.011498	0.786296	0.054600
C	0.746789	-1.859926	-0.141056
N	1.336296	0.599239	0.079236
N	-0.523869	-1.576400	0.089437
C	2.177428	1.505277	0.842684
H	3.198257	1.421229	0.475437
H	1.856163	2.537605	0.725869
H	2.173573	1.251327	1.910662
C	-1.441543	-2.543083	0.682775
H	-0.960565	-3.517618	0.675028
H	-1.667051	-2.257097	1.712362
H	-2.368945	-2.588654	0.117620
H	0.980729	-2.920954	-0.163180
B	1.860965	-0.817450	-0.104080
H	1.848952	-1.458671	1.051015
C	3.267309	-1.041580	-0.815610
H	3.508421	-2.102088	-0.915682
H	3.255430	-0.609669	-1.820051
H	4.093599	-0.577885	-0.274548
Cl	-0.581532	2.424055	-0.099467
Cl	-2.582719	0.040194	-0.375893

H_2BMe-NHC 4, D

E_e = -1290.00888543 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	0.960919	-2.858796	0.181813
H	0.424200	-1.947190	1.587834
C	0.643923	-1.865287	0.507563
C	-0.927850	-0.181859	-0.114612
C	-0.004857	0.789352	-0.042329
N	1.369486	0.479118	-0.119041
N	-0.552955	-1.510963	-0.257412
C	2.258592	1.527194	-0.608635
H	1.864762	1.956170	-1.530745
H	2.372555	2.328223	0.122113
H	3.232269	1.092530	-0.814311
C	-1.564090	-2.544470	-0.332046
H	-2.046037	-2.727499	0.637341
H	-2.328845	-2.285817	-1.059968
H	-1.078193	-3.464393	-0.655518
B	1.800165	-0.824124	0.201722
C	3.316790	-1.247422	0.202081
H	3.650667	-1.447523	-0.822026
H	3.983330	-0.485476	0.608725
H	3.473648	-2.168568	0.765110
Cl	-2.611336	0.183113	0.018391
Cl	-0.421656	2.433759	0.271848

Cartesian coordinates for optimized insertion pathway compounds H_2BMe-NHC 5

H_2BMe-NHC 5, A

E_e = -524.420718352 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.835818	-0.696519	-0.066353
C	0.836134	0.696456	-0.066197
C	-1.286820	0.000479	-0.346525
N	-0.482074	1.081340	-0.237637
N	-0.482537	-1.080775	-0.237963
C	-0.914016	2.464309	-0.248403
H	-0.639874	2.939546	0.693888
H	-0.436243	2.994237	-1.072938
H	-1.991280	2.484404	-0.374051
C	-0.915220	-2.463503	-0.248831
H	-1.992145	-2.483042	-0.377516
H	-0.435393	-2.994245	-1.071637
H	-0.644104	-2.938290	0.694569
C	-3.502213	-0.000685	1.035753
H	-4.593531	-0.000789	0.998343
H	-3.204018	-0.879954	1.617178
H	-3.204237	0.877608	1.618754
B	-2.890867	0.000744	-0.483383
H	-3.210624	-0.988402	-1.108487
H	-3.210550	0.991012	-1.106724
C	2.006208	1.423448	0.088507
C	2.005547	-1.424058	0.088267
C	3.177865	-0.699653	0.242066
C	3.178194	0.698476	0.242203
H	2.004911	-2.505715	0.089621
H	4.114023	-1.227031	0.366014
H	4.114596	1.225394	0.366260
H	2.006085	2.505105	0.089918

H_2BMe-NHC 5, T1

E_e = -524.377570854 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.956717	-0.668465	-0.122088
C	-0.739996	0.716820	-0.134499
C	1.289240	-0.308050	-0.006038
N	0.630727	0.935098	-0.305477
N	0.278237	-1.292918	-0.289266
C	1.218145	2.178965	0.120070
H	2.167610	2.342312	-0.382703
H	0.552207	2.995754	-0.149401
H	1.379671	2.203686	1.208017
C	0.478380	-2.661515	0.104468
H	0.654579	-2.754586	1.185996
H	-0.405951	-3.238286	-0.157346
H	1.329976	-3.086178	-0.422639
B	2.789693	-0.610223	0.009912
H	1.523155	-0.347366	1.174194
H	3.047107	-1.764911	0.148163
C	3.943404	0.459611	0.037331
H	3.772671	1.257383	0.761832
H	4.910566	0.011511	0.259056
H	4.020678	0.945020	-0.941386
C	-1.791163	1.601000	-0.025158
C	-2.227855	-1.187398	0.001758
C	-3.083572	1.075819	0.092110
C	-3.296997	-0.290309	0.105643
H	-1.633134	2.670953	-0.025167
H	-3.922248	1.752972	0.182984
H	-4.302213	-0.676857	0.207729
H	-2.403103	-2.254433	0.022736

H_2BMe-NHC 5, B

E_e = -524.394862141 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.354712	-0.647892	-0.173098
C	0.605405	0.711180	0.021625
C	-1.670314	0.535280	-0.325928
N	-0.567655	1.444272	-0.041160
N	-1.041183	-0.849310	-0.420462
C	-0.579292	2.731895	-0.697888
H	-1.527891	3.229194	-0.499592
H	0.214504	3.357617	-0.294177
H	-0.443078	2.646035	-1.784981
C	-1.389666	-1.714324	-1.544037
H	-0.850313	-1.406430	-2.442346
H	-1.138759	-2.746013	-1.299062
H	-2.462503	-1.649329	-1.706953
B	-2.144566	-0.514053	0.753765
H	-2.225249	0.806309	-1.223250
H	-3.152599	-1.107065	0.494790
C	-1.604388	-0.463959	2.242777
H	-2.361740	-0.010476	2.887459
H	-1.411676	-1.462837	2.642239
H	-0.691628	0.124695	2.358792
C	1.354483	-1.591421	-0.153112
C	1.906416	1.142929	0.239267
C	2.660366	-1.157253	0.076186
C	2.922959	0.192108	0.265442
H	1.135559	-2.639494	-0.312082
H	3.467359	-1.875995	0.108090
H	3.940922	0.516988	0.437737
H	2.127702	2.191070	0.388449

H_2BMe-NHC 5, T2

E_e = -524.384966797 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.609990	0.661591	0.150340
C	-0.222635	-0.626630	-0.255619
C	1.654376	0.999988	-0.079931
N	1.143287	-0.764784	-0.477484
N	0.426614	1.604673	0.004783
C	1.603153	-1.720389	-1.467677
H	2.627253	-1.474452	-1.738943
H	1.600450	-2.733440	-1.052907
H	0.972326	-1.695029	-2.358469
C	0.132900	2.709822	-0.905970
H	-0.069894	2.345022	-1.918379
H	-0.735947	3.256945	-0.547013
H	0.981908	3.389820	-0.921708
H	2.315289	1.461598	-0.812656
B	2.069559	-0.283031	0.732138
H	3.199477	-0.612231	0.477247
C	1.553622	-0.575330	2.215284
H	1.526801	-1.649526	2.419854
H	2.243141	-0.136898	2.941091
H	0.560063	-0.177796	2.436889
C	-1.926986	0.940153	0.476169
C	-1.186474	-1.618293	-0.397041
C	-2.873900	-0.068091	0.369516
C	-2.505741	-1.333737	-0.075109
H	-2.209437	1.933339	0.800454
H	-3.904911	0.136203	0.625220
H	-3.252632	-2.112307	-0.158436
H	-0.900943	-2.609806	-0.723805

H_2BMe-NHC 5, C

E_e = -524.412887322 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.752873	0.557845	-0.036958
C	-0.247269	-0.771821	-0.140811
C	1.430705	1.462757	-0.321188
N	1.052037	-1.014417	-0.382533
N	0.155874	1.654668	-0.211202
C	1.487223	-2.382264	-0.544560
H	0.912052	-2.899696	-1.318336
H	2.533140	-2.371635	-0.845411
H	1.404460	-2.958856	0.384823
C	-0.407696	3.005682	-0.253640
H	0.398049	3.707412	-0.442044
H	-1.148941	3.070849	-1.048092
H	-0.879017	3.238597	0.699761
H	1.999707	2.382154	-0.445419
B	2.157570	0.060697	-0.239618
H	2.937726	0.002573	-1.174919
C	2.963524	-0.017768	1.180621
H	3.484012	-0.976415	1.260476
H	3.725645	0.760831	1.277950
H	2.295789	0.060333	2.044898
C	-2.098170	0.806626	0.193043
C	-1.207919	-1.801936	0.004021
C	-3.006958	-0.228574	0.334002
C	-2.541164	-1.533195	0.233192
H	-2.458943	1.821823	0.267511
H	-4.049986	-0.016880	0.518517
H	-3.230936	-2.361136	0.341493
H	-0.882406	-2.829315	-0.053300

H_2BMe-NHC 5, T3

E_e = -524.405412505 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.831133	0.548749	-0.050326
C	0.289097	-0.767807	0.001356
C	-1.356116	1.497164	-0.041839
N	-1.065938	-0.991916	0.028594
N	-0.048232	1.682635	-0.047744
C	-1.517314	-2.358346	0.148645
H	-2.603302	-2.374391	0.145235
H	-1.169447	-2.974285	-0.687065
H	-1.170099	-2.827303	1.078057
C	0.525828	3.006234	0.134852
H	-0.284431	3.726453	0.202045
H	1.117232	3.042540	1.051984
H	1.164185	3.269465	-0.708640
H	-1.944340	2.410485	-0.030023
B	-2.032292	0.149754	0.152934
H	-2.028609	0.750965	1.342588
C	-3.558748	-0.051634	-0.271379
H	-3.631498	-0.466739	-1.281039
H	-4.100728	-0.724772	0.395152
H	-4.101087	0.896532	-0.266189
C	1.216444	-1.818080	0.015682
C	2.197496	0.750303	-0.095004
C	2.587937	-1.598113	-0.030789
C	3.092488	-0.317187	-0.088962
H	0.857938	-2.834173	0.068795
H	3.256801	-2.449233	-0.015656
H	4.156548	-0.131759	-0.122301
H	2.592016	1.754715	-0.136990

H_2BMe-NHC 5, D

E_e = -524.464192217 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	-2.009169	2.270958	-0.155525
H	-1.359758	1.797324	1.401404
C	-1.362112	1.531772	0.326527
C	0.827413	0.565171	-0.071234
C	0.308248	-0.753961	-0.030382
N	-1.091880	-0.953842	-0.115645
N	-0.035046	1.638982	-0.256973
C	-1.545411	-2.316098	-0.342752
H	-1.031851	-2.749785	-1.202842
H	-1.359348	-2.954031	0.525532
H	-2.612010	-2.310924	-0.544438
C	0.522748	2.969572	-0.247491
H	0.935401	3.248956	0.733394
H	1.310225	3.064603	-0.995241
H	-0.268127	3.674952	-0.498420
B	-1.989537	0.101713	0.125480
C	-3.551769	-0.103137	0.202711
H	-3.964243	-0.281031	-0.796098
H	-3.841926	-0.957764	0.817281
H	-4.053565	0.780420	0.599115
C	1.183572	-1.823651	0.082450
C	2.208051	0.733343	0.029567
C	2.560456	-1.634910	0.163251
C	3.068482	-0.353569	0.138150
H	0.796302	-2.831267	0.112171
H	3.215725	-2.491077	0.248417
H	4.134609	-0.181839	0.208385
H	2.625835	1.728761	0.023010

Cartesian coordinates for optimized insertion pathway compounds H_1BMe_2-NHC 1

H_1BMe_2-NHC 1, A

E_e = -410.089305023 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.298471	0.162630	0.023473
C	1.744205	1.385866	0.152195
C	0.070061	-0.087086	-0.127049
H	3.326356	-0.152202	0.037587
H	2.191271	2.352191	0.301665
N	0.380413	1.211116	0.060154
N	1.258311	-0.723855	-0.143723
C	-0.595192	2.282248	0.186148
H	-0.074440	3.182141	0.504860
H	-1.090003	2.456837	-0.766149
H	-1.341861	2.008521	0.927661
C	1.415142	-2.160472	-0.306667
H	0.760680	-2.679732	0.388287
H	1.150260	-2.454254	-1.319925
H	2.452782	-2.414481	-0.102135
C	-1.844253	-1.166153	1.299276
H	-2.791720	-1.711852	1.279904
H	-1.131025	-1.789692	1.849695
H	-2.013290	-0.269984	1.909208
B	-1.383237	-0.807663	-0.231944
H	-1.166899	-1.829454	-0.862328
C	-2.494273	0.091545	-1.017817
H	-2.911008	0.913222	-0.425721
H	-2.139748	0.516339	-1.963934
H	-3.341201	-0.551590	-1.271335

H_1BMe_2-NHC 1, T1

E_e = -410.038675520 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-2.151530	0.541326	-0.373621
C	-2.095946	-0.765814	-0.132053
C	0.031245	0.001893	-0.052007
H	-2.999646	1.161995	-0.608415
H	-2.876390	-1.507616	-0.168942
N	-0.789712	-1.121221	0.252077
N	-0.858804	1.100733	-0.221841
C	-0.307533	-2.453026	-0.013904
H	0.483835	-2.726028	0.679138
H	-1.127722	-3.158922	0.104313
H	0.082956	-2.533236	-1.040667

C	-0.761324	2.201879	0.728018
H	0.249826	2.599830	0.732424
H	-1.441194	2.994673	0.415287
H	-1.030772	1.890493	1.744139
B	1.549079	0.118192	-0.069185
H	0.576067	-0.253122	-1.172706
C	2.187033	1.489962	-0.547841
H	2.544240	2.049403	0.324200
H	3.066693	1.311879	-1.170873
H	1.501366	2.137141	-1.096585
C	2.510240	-1.069539	0.376715
H	3.548510	-0.733436	0.371920
H	2.282620	-1.419069	1.387110
H	2.460721	-1.941605	-0.277925

H_1BMe_2-NHC 1, B

E_e = -410.052000695 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.145412	0.182594	-0.347007
C	1.779611	-1.080308	-0.548205
C	-0.015946	0.005440	0.361257
H	3.109029	0.640393	-0.504012
H	2.365245	-1.906686	-0.916829
N	0.382118	-1.223173	-0.364389
N	1.017643	0.966430	-0.042312
C	-0.038754	-2.461176	0.258882
H	-1.117406	-2.585494	0.184521
H	0.432388	-3.297114	-0.257584
H	0.248003	-2.495949	1.321395
C	1.187899	2.070433	0.871659
H	1.405473	1.729703	1.896181
H	2.005716	2.705676	0.532348
H	0.278636	2.673703	0.893433
B	-1.506214	0.380226	-0.058141
H	0.094939	-0.191550	1.459427
C	-1.771616	1.596017	-1.001851
H	-2.672123	1.486738	-1.608473
H	-1.953832	2.461523	-0.347960
H	-0.916612	1.850992	-1.627224
C	-2.702260	-0.484559	0.474918
H	-2.948461	-1.215369	-0.306761
H	-2.497648	-1.043644	1.389008
H	-3.606682	0.112509	0.612224

H_1BMe_2-NHC 1, T2

E_e = -410.052411788 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.522513	-0.245035	1.030897
C	-0.458392	-1.053734	1.100592
C	-0.319294	0.540093	-0.754244
H	-2.355336	-0.217951	1.716052
H	-0.317184	-1.833347	1.836021
N	0.517655	-0.845413	0.124376
N	-1.548895	0.544312	-0.124349
C	1.182339	-2.035439	-0.391455
H	1.808845	-2.474589	0.390535
H	0.456275	-2.778357	-0.725380
H	1.823332	-1.759151	-1.223476
C	-2.749980	0.398200	-0.938954
H	-2.735993	1.135078	-1.739774
H	-2.825377	-0.607937	-1.366082
H	-3.624988	0.584229	-0.317158
H	-0.382201	0.419266	-1.837080
C	1.238582	1.476066	1.344577
H	2.051368	1.065554	1.952608
H	1.510451	2.511067	1.119487
H	0.346364	1.511422	1.972312
C	2.321868	0.739108	-1.030523
H	3.222515	0.282066	-0.608063
H	2.150804	0.279282	-2.009367
H	2.565906	1.788002	-1.217884
B	1.073647	0.657504	-0.021656

H_1BMe_2-NHC 1, C

E_e = -410.088612746 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.389391	1.243454	0.228475
C	0.089298	1.652792	0.126450
C	0.785332	-0.993825	-0.233725
H	2.214709	1.911613	0.392931
H	-0.110739	2.717365	0.215457
N	-0.931428	0.845352	-0.100374
N	1.701742	-0.092923	-0.073909
C	-2.254039	1.393981	-0.300464
H	-2.240303	2.480958	-0.208522
H	-2.631863	1.131788	-1.291159
H	-2.949627	0.987010	0.438070
C	3.125614	-0.375795	-0.249163
H	3.261436	-1.433360	-0.453560
H	3.511050	0.220947	-1.074755
H	3.652914	-0.104685	0.664673

H	1.171121	-1.965430	-0.537121
B	-0.781280	-0.723499	0.051046
C	-1.101171	-1.170695	1.587752
H	-2.146957	-0.973972	1.847118
H	-0.941018	-2.243346	1.738485
H	-0.480447	-0.641493	2.318449
C	-1.699980	-1.511513	-1.028266
H	-1.494300	-2.586230	-0.999685
H	-2.767194	-1.400903	-0.811761
H	-1.541243	-1.180165	-2.060214

H_1BMe_2-NHC 1, T3

E_e = -410.062469107 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.205988	-1.397775	-0.136776
C	-0.094625	-1.698804	-0.033013
C	0.718505	0.896424	-0.442879
H	1.973755	-2.153563	-0.096610
H	-0.368678	-2.736843	0.121041
N	-1.126185	-0.797808	-0.166249
N	1.652553	-0.068181	-0.379913
C	-2.438261	-1.222141	0.268666
H	-2.619771	-2.257886	-0.027617
H	-2.574029	-1.156976	1.357172
H	-3.199777	-0.601546	-0.202556
C	3.017760	0.232830	0.002011
H	3.276152	1.233419	-0.339975
H	3.148458	0.180037	1.088813
H	3.695842	-0.483351	-0.462948
H	1.110790	1.892227	-0.623651
B	-0.764072	0.652067	-0.261839
C	-1.868149	1.690814	-0.741697
H	-2.700077	1.772265	-0.036518
H	-1.457487	2.694518	-0.870400
H	-2.290539	1.382717	-1.702366
C	-0.115962	1.306831	1.374447
H	-0.038268	2.388296	1.447622
H	-1.061384	0.986368	1.820768
H	0.689264	0.812820	1.914995

H_1BMe_2-NHC 1, D

E_e = -410.119259984 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	1.016163	1.626634	-0.935003
C	0.721262	0.899161	-0.170226
C	0.901715	-1.507516	0.048278
C	-0.401900	-1.658320	0.296599
H	1.584141	-2.331526	0.209237
H	-0.804307	-2.591444	0.661493
N	-1.319903	-0.611549	0.049678
N	1.443874	-0.341349	-0.459365
C	-2.716218	-1.002940	0.097368
H	-2.922920	-1.780382	-0.642537
H	-2.973035	-1.395653	1.085038
H	-3.352045	-0.146983	-0.112520
C	2.886198	-0.253369	-0.499125
H	3.341220	-0.131599	0.492543
H	3.297753	-1.154053	-0.955766
H	3.175274	0.600864	-1.113219
B	-0.855438	0.677997	-0.244753
C	-1.826174	1.887736	-0.547088
H	-2.358234	1.737248	-1.491526
H	-2.591242	2.012368	0.223444
H	-1.286910	2.832516	-0.629480
C	1.072697	1.485416	1.209991
H	2.122289	1.777169	1.281016
H	0.469363	2.373274	1.411497
H	0.866410	0.750863	1.992575

Cartesian coordinates for optimized insertion pathway compounds H_1BMe_2-NHC 2

H_1BMe_2-NHC 2, A

E_e = -411.283039641 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.333656	0.108215	0.074589
C	1.674944	1.482345	-0.001682
C	0.026227	-0.159458	-0.068085
H	2.754372	-0.096290	1.064694
H	1.990432	2.156600	0.794397
N	0.263585	1.141145	0.131703
N	1.204836	-0.783503	-0.174962
C	-0.726182	2.191816	0.170447
H	-0.370940	2.979832	0.835721
H	-0.898440	2.614935	-0.822859
H	-1.658895	1.795644	0.554468
C	1.442583	-2.207673	-0.180571
H	0.510061	-2.724107	-0.377070
H	2.171921	-2.451943	-0.955156
H	1.840883	-2.528421	0.786696
C	-2.070042	-0.878145	1.363937
H	-3.044409	-1.373870	1.339870
H	-1.451450	-1.433541	2.076342
H	-2.237094	0.113965	1.798802
B	-1.448131	-0.855038	-0.149780
H	-1.262506	-1.994623	-0.528151
C	-2.405624	-0.102834	-1.242692
H	-2.862473	0.831376	-0.902710
H	-1.904497	0.112581	-2.193030
H	-3.236374	-0.771953	-1.482297
H	1.851523	1.973827	-0.963944
H	3.116213	-0.037921	-0.669706

H_1BMe_2-NHC 2, T1

E_e = -411.257384399 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-2.194196	0.596386	-0.207230
C	-1.997389	-0.894916	-0.399173
C	0.057004	0.007200	0.017231
H	-2.695845	0.789374	0.749075
H	-2.800247	-1.499510	0.021105
N	-0.743299	-1.114813	0.312717
N	-0.820684	1.098763	-0.166905
C	-0.190428	-2.436039	0.134510
H	0.611910	-2.618354	0.842760
H	-0.977388	-3.170053	0.305150
H	0.200360	-2.572512	-0.886745
C	-0.653665	2.238419	0.717693
H	-0.921978	1.987261	1.753202
H	0.371188	2.594980	0.697670
H	-1.304399	3.046779	0.381271
B	1.573198	0.115323	-0.103576
H	0.660987	-0.260083	-1.141218
C	2.201464	1.496360	-0.590110
H	2.592839	2.056878	0.266207
H	3.058389	1.307580	-1.241494
H	1.508429	2.146685	-1.125126
C	2.586398	-1.043584	0.329296
H	3.612211	-0.683201	0.232953
H	2.447426	-1.339473	1.372313
H	2.517687	-1.952056	-0.270385
H	-1.882517	-1.144252	-1.466728
H	-2.772296	1.062736	-1.006114

H_1BMe_2-NHC 2, B

E_e = -411.278972460 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.837424	0.647257	-0.592986
C	-0.520945	1.128962	-1.182678
C	-0.147744	-0.311338	0.686914
H	-2.605484	0.466732	-1.346488
H	-0.265949	0.574210	-2.082952
N	0.452645	0.810519	-0.112345
N	-1.428898	-0.588997	0.051170
C	0.908597	1.981451	0.629428
H	1.505935	1.665937	1.479054
H	1.525187	2.604287	-0.019472
H	0.053183	2.561706	0.988095
C	-2.403979	-1.142527	0.959653
H	-2.645015	-0.453289	1.787446
H	-3.324123	-1.369072	0.420203
H	-2.021964	-2.070273	1.385713
B	1.229057	-0.656342	-0.025914
H	-0.230639	-0.036636	1.744912
C	1.223614	-1.481914	-1.388317
H	1.870583	-1.027169	-2.145731
H	1.626099	-2.481473	-1.203273
H	0.230005	-1.615795	-1.819595
C	2.587449	-0.616406	0.816734
H	3.374534	-0.053106	0.305153
H	2.496008	-0.213013	1.828375
H	2.964025	-1.636804	0.925231
H	-2.225185	1.385172	0.133407
H	-0.496119	2.196737	-1.394769

H_1BMe_2-NHC 2, T2

E_e = -411.266941312 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.445560	-0.033612	-1.136865
C	0.454297	-1.224066	-0.961033
C	0.394738	0.882535	0.703030
H	2.422674	-0.373953	-1.474291
H	0.994691	-2.122432	-0.637220
N	-0.548706	-0.885403	0.003209
N	1.562845	0.622235	0.153546
C	-1.276546	-1.998409	0.558043
H	-0.591968	-2.781924	0.902812
H	-1.873047	-1.667466	1.405854
H	-1.961571	-2.455036	-0.170946
C	2.734098	0.292612	0.952915
H	2.673895	0.808905	1.907904
H	2.779150	-0.786176	1.130873
H	3.638201	0.606668	0.432587
H	0.453389	1.061994	1.778763
C	-1.432953	1.249880	-1.435237
H	-2.511771	1.165891	-1.597551
H	-1.199925	2.319083	-1.470389
H	-0.961985	0.792681	-2.310234
C	-2.202937	0.864206	1.101714
H	-3.140329	0.372369	0.824348
H	-1.949657	0.531253	2.114536
H	-2.420631	1.934823	1.161991
B	-1.047807	0.598424	0.004181
H	0.040516	-1.433417	-1.957855
H	1.050881	0.677923	-1.854775

H_1BMe_2-NHC 2, C

E_e = -411.283861488 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.411796	1.294800	-0.190055
C	0.009982	1.633350	0.278173
C	0.758337	-1.001133	0.096503
H	1.528244	1.524840	-1.251504
H	-0.164401	2.688103	0.036810
N	-0.952943	0.795731	-0.378898
N	1.710030	-0.137912	-0.012476
C	-2.290334	1.325152	-0.234555
H	-2.368080	2.317412	-0.691865
H	-3.002716	0.669514	-0.736685
H	-2.609270	1.416972	0.817596
C	3.127572	-0.475811	-0.005468
H	3.245706	-1.553816	0.062542
H	3.587390	-0.113103	-0.925608
H	3.615097	0.005289	0.842832
H	1.111641	-2.024351	0.237123
B	-0.805526	-0.694816	0.001606
C	-1.447530	-1.098187	1.463889
H	-2.538755	-1.045497	1.401288
H	-1.202494	-2.121361	1.765133
H	-1.139099	-0.438741	2.282023
C	-1.378925	-1.690125	-1.163669
H	-1.231502	-2.747744	-0.923464
H	-2.458098	-1.543656	-1.267345
H	-0.933942	-1.499341	-2.144253
H	-0.021158	1.556280	1.383506
H	2.164080	1.850271	0.374551

H_1BMe_2-NHC 2, T3

E_e = -411.274447893 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.289638	-1.343781	-0.423146
C	0.031303	-1.638094	0.275595
C	-0.682145	0.981610	-0.378023
H	-2.086924	-1.930934	0.035478
H	0.267578	-2.696349	0.118007
N	1.091894	-0.813473	-0.248550
N	-1.654669	0.070288	-0.330405
C	2.392491	-1.237712	0.213386
H	2.560252	-2.292105	-0.026991
H	3.171762	-0.653509	-0.274847
H	2.521621	-1.128358	1.304657
C	-3.010865	0.386363	0.061373
H	-3.206434	0.085866	1.096745
H	-3.171247	1.459647	-0.026042
H	-3.722463	-0.128852	-0.586392
H	-1.024657	2.010316	-0.443584
B	0.801621	0.643133	-0.283123
C	0.334646	1.298152	1.400530
H	0.486657	2.373410	1.455287
H	-0.556498	1.019380	1.960160
H	1.188545	0.787916	1.855244
C	1.923498	1.643021	-0.818830
H	1.541869	2.658918	-0.943645
H	2.780001	1.704184	-0.141238
H	2.303713	1.313447	-1.789368
H	-1.216211	-1.629279	-1.475647
H	-0.101988	-1.504417	1.365166

H_1BMe_2-NHC 2, D

E_e = -411.332162987 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	0.946020	1.448809	-1.214436
C	0.744208	0.866292	-0.305643
C	0.881737	-1.430424	0.424566
C	-0.561704	-1.750293	0.092700
H	1.472590	-2.343679	0.322848
H	-0.970080	-2.411007	0.865214
N	-1.382363	-0.550282	0.015952
N	1.406837	-0.430904	-0.479912
C	-2.801320	-0.837699	0.061803
H	-3.089562	-1.499210	-0.762040
H	-3.063419	-1.339251	0.998303
H	-3.380527	0.078861	-0.012376
C	2.852309	-0.368116	-0.449597
H	3.263800	-0.168294	0.552145
H	3.266928	-1.314870	-0.800887
H	3.195153	0.422985	-1.119108
B	-0.835015	0.717690	-0.201605
C	-1.749621	2.005714	-0.326568
H	-2.495373	1.896180	-1.118577
H	-2.303909	2.200176	0.596461
H	-1.169271	2.901656	-0.551210
C	1.267966	1.694586	0.886306
H	2.314804	1.975314	0.760739
H	0.692174	2.615417	0.990883
H	1.177607	1.144031	1.825575
H	0.954988	-1.117128	1.480871
H	-0.609605	-2.290504	-0.860074

Cartesian coordinates for optimized insertion pathway compounds H_1BMe_2-NHC 3

H_1BMe_2-NHC 3, A

E_e = -488.715678933 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.700192	-0.468579	-0.038234
C	1.438042	0.857845	0.043014
C	-0.543547	-0.217398	-0.092947
N	0.055862	0.982621	0.017475
N	0.468792	-1.104716	-0.110621
C	-0.662137	2.241234	0.118442
H	-0.034273	2.968454	0.627887
H	-0.929421	2.614276	-0.869579
H	-1.569458	2.081241	0.692614
C	0.287040	-2.544475	-0.194217
H	-0.580764	-2.827483	0.392495
H	0.125006	-2.850875	-1.227120
H	1.174347	-3.034361	0.199526
C	-2.716281	-0.623140	1.352210
H	-3.776204	-0.892444	1.334332
H	-2.213046	-1.357609	1.990621
H	-2.649534	0.340550	1.872743
B	-2.132746	-0.566087	-0.176304
H	-2.173924	-1.671043	-0.690107
C	-2.950156	0.485398	-1.124547
H	-3.198003	1.437426	-0.643583
H	-2.442606	0.721575	-2.066905
H	-3.906821	0.032541	-1.398473
C	2.991675	-1.205227	-0.053405
H	3.109791	-1.831508	0.833476
H	3.072872	-1.848348	-0.931573
H	3.820822	-0.501389	-0.075634
C	2.350831	2.026556	0.149750
H	2.163579	2.753782	-0.642369
H	2.240032	2.538305	1.108160
H	3.384796	1.698732	0.066623

H_1BMe_2-NHC 3, T1

E_e = -488.663383591 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.588412	0.656776	0.031106
C	-1.577259	-0.680467	0.029291
C	0.602632	0.012335	0.083690
N	-0.248583	-1.126557	0.258988
N	-0.274255	1.111358	0.267305

C	0.149971	-2.375429	-0.350419
H	0.964031	-2.842749	0.192705
H	-0.692415	-3.062426	-0.342136
H	0.467226	-2.217436	-1.394111
C	0.115841	2.453156	-0.074006
H	0.974704	2.757052	0.518762
H	0.367339	2.552974	-1.140455
H	-0.705509	3.129574	0.152175
B	2.135327	0.008473	0.053627
H	1.008093	-0.037972	-1.125585
C	3.014710	1.306980	-0.207578
H	3.309384	1.730700	0.760044
H	3.944326	1.023975	-0.706274
H	2.561895	2.105053	-0.788803
C	2.957297	-1.332833	0.295151
H	4.004309	-1.085200	0.479914
H	2.593001	-1.899509	1.154389
H	2.947487	-2.006021	-0.565111
C	-2.711680	-1.640853	-0.000565
H	-2.712239	-2.258351	-0.901503
H	-2.668929	-2.311711	0.861763
H	-3.659226	-1.107561	0.033865
C	-2.732173	1.605497	0.003514
H	-2.759530	2.210936	0.913785
H	-2.674407	2.288756	-0.846700
H	-3.671868	1.062975	-0.070020

H_1BMe_2-NHC 3, B

E_e = -488.679814452 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.559821	-0.499180	0.035136
C	1.360183	0.814499	0.176739
C	-0.643099	-0.113298	-0.468888
N	-0.035857	1.103767	0.109438
N	0.314133	-1.159998	-0.105914
C	-0.396024	2.323750	-0.584668
H	-1.469669	2.489706	-0.517280
H	0.100451	3.173424	-0.118220
H	-0.114405	2.284772	-1.649201
C	0.252535	-2.313306	-0.973443
H	0.463772	-2.056784	-2.024380
H	0.962088	-3.071735	-0.644983
H	-0.747572	-2.748442	-0.923247
B	-2.084462	-0.247575	0.193690
H	-0.651694	-0.004660	-1.581945
C	-2.231633	-1.156249	1.456014
H	-3.213262	-1.127181	1.928602
H	-1.995558	-2.193828	1.194168
H	-1.465557	-0.878708	2.186207
C	-3.294503	0.580211	-0.365274
H	-3.507426	1.394198	0.339232
H	-3.147278	1.019972	-1.352451
H	-4.203043	-0.028563	-0.378800
C	2.805583	-1.297991	0.176152
H	3.051055	-1.827295	-0.747548
H	3.650092	-0.661116	0.430348
H	2.688417	-2.048042	0.963470
C	2.316467	1.892531	0.543001
H	2.411320	2.643471	-0.244813
H	1.980507	2.405728	1.448707
H	3.306165	1.480764	0.730402

H_1BMe_2-NHC 3, T2

E_e = -488.677257265 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.404350	0.116874	0.234036
C	0.471882	1.027389	-0.109660
C	-0.325710	-1.316211	-0.279228
N	-0.765951	0.498654	-0.507802
N	1.022318	-1.206328	-0.082641
C	-1.496862	1.193517	-1.556821
H	-0.852403	1.417044	-2.409515
H	-2.318183	0.565561	-1.890199
H	-1.921808	2.128388	-1.177995
C	1.920416	-1.908349	-0.994247
H	1.534273	-2.910108	-1.170302
H	2.016027	-1.378231	-1.948761
H	2.905062	-2.002060	-0.539167
H	-0.596769	-1.963085	-1.115379
C	-1.256572	-0.168474	2.079442
H	-1.606744	-1.002007	2.694756
H	-0.231292	0.045601	2.389288
H	-1.869744	0.696781	2.353252
C	-2.928985	-0.938129	0.094554
H	-3.631227	-0.105148	0.202877
H	-3.023309	-1.311852	-0.930462
H	-3.290365	-1.734189	0.750965
B	-1.433863	-0.528637	0.525177
C	0.614799	2.513815	-0.042008
H	0.475698	2.965231	-1.026191
H	-0.137912	2.941605	0.625368
H	1.599989	2.802049	0.314334
C	2.760002	0.350135	0.816368
H	3.555914	0.202394	0.082212
H	2.853236	1.360044	1.207455
H	2.934379	-0.344522	1.640064

H_1BMe_2-NHC 3, C

E_e = -488.700876977 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.358723	0.299650	0.099345
C	0.290607	1.154807	-0.074138
C	-0.034246	-1.587977	-0.282684
N	-0.945520	0.686959	-0.309028
N	1.151373	-1.061065	-0.242040
C	-2.014497	1.595742	-0.671546
H	-1.682486	2.381616	-1.349414
H	-2.796843	1.031527	-1.172809
H	-2.461702	2.068955	0.211266
C	2.329932	-1.817380	-0.676270
H	2.010927	-2.804125	-0.996465
H	2.815410	-1.297122	-1.500441
H	3.035779	-1.914593	0.145585
H	-0.058587	-2.594163	-0.698384
B	-1.318611	-0.758148	0.211132
C	-1.400768	-0.775358	1.840276
H	-2.208926	-0.122746	2.188741
H	-1.616157	-1.776587	2.226531
H	-0.478088	-0.431793	2.320594
C	-2.658902	-1.349992	-0.479878
H	-2.765291	-2.409826	-0.226860
H	-3.568695	-0.860496	-0.119960
H	-2.659735	-1.282255	-1.573783
C	0.495083	2.646277	-0.058668
H	0.345642	3.052707	-1.060367
H	-0.229896	3.126638	0.600014
H	1.492987	2.926354	0.256767
C	2.741358	0.668422	0.549774
H	3.092724	-0.008467	1.333122
H	3.490160	0.658618	-0.249403
H	2.751119	1.660092	0.989819

H_1BMe_2-NHC 3, T3

E_e = -488.676620607 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

C	1.386648	0.332435	0.130947
C	0.373492	1.220732	0.031585
C	-0.147049	-1.484067	0.447095
N	-0.972874	0.859561	0.114188
N	1.117770	-1.078294	0.277807
C	-1.970654	1.759694	-0.430778
H	-1.883609	1.888170	-1.518888
H	-2.956582	1.347510	-0.225678
H	-1.934399	2.750656	0.024786
C	2.096336	-2.013329	-0.255327
H	1.747955	-3.026225	-0.063495
H	2.214964	-1.882586	-1.336919
H	3.068344	-1.885206	0.216749
H	-0.261115	-2.544448	0.650201
B	-1.341830	-0.573191	0.319058
C	-2.755907	-0.950132	0.954069
H	-3.598648	-0.725153	0.294933
H	-2.819333	-2.014495	1.192442
H	-2.917694	-0.397120	1.883368
C	-1.235807	-1.524277	-1.277825
H	-1.696660	-2.508843	-1.258198
H	-1.938287	-0.811175	-1.717566
H	-0.337340	-1.523592	-1.892834
C	2.842423	0.664829	0.282617
H	3.240129	0.199291	1.189736
H	3.445465	0.305600	-0.555828
H	3.014335	1.730598	0.372657
C	0.625387	2.698912	-0.087440
H	1.677794	2.945970	-0.145980
H	0.148681	3.094770	-0.985359
H	0.191674	3.224579	0.766955

H_1BMe_2-NHC 3, D

E_e = -488.733063119 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	-0.296217	-2.465010	-0.495663
C	-0.226457	-1.525437	0.062332
C	-1.074691	0.740467	-0.163090
C	0.141172	1.273638	0.073303
N	1.308582	0.467110	-0.118941
N	-1.192076	-0.605623	-0.544954
C	2.546051	1.179183	-0.404259
H	2.424262	1.833226	-1.271107
H	2.873500	1.789922	0.438903
H	3.329488	0.461544	-0.629242
C	-2.507514	-1.174262	-0.751511
H	-3.082060	-1.312599	0.174622
H	-3.100218	-0.562762	-1.428941
H	-2.383844	-2.153833	-1.214548
B	1.227171	-0.932061	-0.138710
C	2.479585	-1.877416	-0.334206
H	2.808828	-1.872730	-1.378772
H	3.342483	-1.582872	0.266754
H	2.240104	-2.912613	-0.084659
C	-0.516578	-1.820618	1.543156
H	-1.491565	-2.290613	1.688020
H	0.240191	-2.494849	1.950327
H	-0.491772	-0.894848	2.122887
C	-2.355323	1.521102	-0.085376
H	-2.823556	1.585896	-1.070018

H	-3.073619	1.042540	0.583634
H	-2.197918	2.535869	0.259712
C	0.397955	2.658274	0.593368
H	1.009157	2.615605	1.499263
H	0.934801	3.282853	-0.125083
H	-0.518646	3.175590	0.852439

Cartesian coordinates for optimized insertion pathway compounds H_1BMe_2-NHC 4

H_1BMe_2-NHC 4, A

E_e = -1329.28212732 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.226378	-0.589330	-0.043821
C	1.024712	0.744501	0.021126
C	-0.986644	-0.237198	-0.109102
N	-0.340261	0.943128	-0.011389
N	-0.019139	-1.178428	-0.114685
C	-1.003017	2.236006	0.088109
H	-0.308763	2.949594	0.522708
H	-1.318803	2.574943	-0.896114
H	-1.872881	2.127270	0.728283
C	-0.266318	-2.612965	-0.173978
H	-1.138002	-2.839661	0.430707
H	-0.456295	-2.917610	-1.201466
H	0.607456	-3.129591	0.213319
C	-3.140303	-0.592003	1.359691
H	-4.207349	-0.830278	1.354252
H	-2.648805	-1.352174	1.976484
H	-3.037343	0.360175	1.894323
B	-2.588957	-0.522870	-0.179407
H	-2.666677	-1.614288	-0.714426
C	-3.380310	0.575883	-1.090128
H	-3.578553	1.528945	-0.589539
H	-2.889457	0.803820	-2.042951
H	-4.360344	0.163907	-1.344334
Cl	2.165807	1.990078	0.118382
Cl	2.686511	-1.443782	-0.051504

H_1BMe_2-NHC 4, T1

E_e = -1329.23668655 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.115479	-0.673825	0.006769
C	1.125320	0.658875	0.003349
C	-1.043835	0.015459	0.107929
N	-0.170849	1.122843	0.258546
N	-0.192681	-1.131302	0.255580
C	-0.566547	2.471291	-0.065776
H	-1.408314	2.762526	0.555594
H	0.267176	3.136320	0.144094
H	-0.843526	2.571153	-1.122910
C	-0.599363	-2.381808	-0.356169
H	-0.975191	-2.205759	-1.374438

H	0.261903	-3.042316	-0.404780
H	-1.371579	-2.867538	0.228823
B	-2.571395	0.005487	0.043661
H	-1.501695	-0.044824	-1.108448
C	-3.386781	-1.341442	0.286227
H	-4.432296	-1.090330	0.473787
H	-3.383048	-2.018699	-0.570166
H	-3.024570	-1.903972	1.148754
C	-3.455294	1.305759	-0.196348
H	-3.761816	1.706625	0.776863
H	-3.009717	2.119945	-0.759929
H	-4.377716	1.022320	-0.707604
Cl	2.456931	-1.715201	0.013635
Cl	2.474140	1.689346	-0.002618

H_1BMe_2-NHC 4, B

E_e = -1329.25647743 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.099528	-0.581725	-0.077099
C	0.945819	0.737456	0.024804
C	-1.093438	-0.144942	-0.481651
N	-0.422769	1.088037	0.011621
N	-0.147420	-1.224052	-0.141340
C	-0.772087	2.282893	-0.738557
H	-1.822855	2.516313	-0.582315
H	-0.179070	3.120602	-0.378038
H	-0.590693	2.149242	-1.814767
C	-0.272477	-2.382932	-1.002311
H	-0.114094	-2.128427	-2.060441
H	0.447425	-3.142796	-0.705154
H	-1.275176	-2.796959	-0.888561
B	-2.502180	-0.220529	0.262723
H	-1.158314	-0.075730	-1.591768
C	-2.611181	-1.115662	1.535274
H	-3.572432	-1.067069	2.045481
H	-2.395043	-2.159244	1.281497
H	-1.815093	-0.836979	2.233027
C	-3.697473	0.658998	-0.239983
H	-3.812063	1.500867	0.454989
H	-3.591846	1.067912	-1.245344
H	-4.639104	0.107450	-0.176192
Cl	2.534041	-1.475840	0.118957
Cl	2.138219	1.892019	0.404522

H_1BMe_2-NHC 4, T2

E_e = -1329.25484784 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.083988	-0.329496	0.063251
C	0.292226	0.719100	-0.215672
C	-0.876630	-1.421610	-0.264786
N	-1.034775	0.419852	-0.499750
N	0.491308	-1.568692	-0.190988
C	-1.709109	1.198215	-1.532728
H	-1.078063	1.307335	-2.415507
H	-2.628397	0.687341	-1.803063
H	-1.963206	2.188501	-1.148165
C	1.163380	-2.387388	-1.200921
H	0.653623	-3.345595	-1.269548
H	1.157980	-1.890623	-2.176725
H	2.191709	-2.562092	-0.892119
H	-1.324429	-1.995844	-1.077023
C	-1.378191	-0.118290	2.143355
H	-0.307530	-0.077237	2.355167
H	-1.807323	0.843623	2.440264
H	-1.803831	-0.868500	2.815157
C	-3.340101	-0.620324	0.338432
H	-3.871476	0.324427	0.488945
H	-3.590582	-0.979944	-0.664674
H	-3.772465	-1.334978	1.043327
B	-1.769093	-0.470795	0.632624
Cl	0.797241	2.353242	-0.147953
Cl	2.695720	-0.243936	0.617978

H_1BMe_2-NHC 4, C

E_e = -1329.28363823 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.033937	-0.271919	-0.017378
C	0.216402	0.825871	-0.124858
C	-0.788626	-1.725480	-0.295867
N	-1.093596	0.735930	-0.286283
N	0.495575	-1.536970	-0.328191
C	-1.876322	1.887303	-0.700325
H	-1.362961	2.468255	-1.464955
H	-2.818578	1.529894	-1.105324
H	-2.090936	2.543186	0.148553
C	1.427131	-2.581315	-0.774319
H	0.843047	-3.432295	-1.109196
H	2.043980	-2.197253	-1.583810
H	2.068756	-2.871614	0.053969
H	-1.098447	-2.693211	-0.685377
B	-1.793150	-0.591206	0.256934

C	-1.785406	-0.609002	1.882094
H	-2.399030	0.210351	2.271012
H	-2.210153	-1.536880	2.276967
H	-0.785882	-0.497986	2.315157
C	-3.266989	-0.803557	-0.369197
H	-3.637901	-1.796326	-0.096185
H	-3.993459	-0.089234	0.027958
H	-3.303336	-0.738951	-1.462029
Cl	0.958639	2.394287	-0.061359
Cl	2.696423	-0.198171	0.404241

H_1BMe_2-NHC 4, T3

E_e = -1329.26102502 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.015654	-0.374778	-0.042405
C	-0.405371	0.823040	0.018386
C	1.031796	-1.480088	-0.461086
N	0.949275	1.008607	-0.046431
N	-0.271996	-1.583443	-0.162626
C	1.537422	2.140582	0.651194
H	1.140441	3.086149	0.283862
H	1.369507	2.095958	1.733679
H	2.609970	2.132860	0.468547
C	-0.803987	-2.791395	0.454198
H	-0.122737	-3.611698	0.239005
H	-0.885840	-2.666829	1.538049
H	-1.787147	-3.024802	0.053574
H	1.514770	-2.422422	-0.699314
B	1.811512	-0.185529	-0.384356
C	3.173391	0.041707	-1.175523
H	2.984336	0.575484	-2.109947
H	3.901143	0.629388	-0.610184
H	3.659419	-0.902797	-1.429732
C	2.223281	-1.100297	1.147584
H	2.643572	-0.184137	1.571799
H	1.458756	-1.456640	1.835966
H	3.017387	-1.833842	1.035805
Cl	-2.716255	-0.552016	-0.278618
Cl	-1.386530	2.256852	0.038617

H_1BMe_2-NHC 4, D

E_e = -1329.31821300 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	1.241539	-2.559599	-0.296487
C	0.827240	-1.662810	0.173563
C	-0.948554	-0.119530	-0.268129
C	-0.148140	0.944033	-0.094057
N	1.248604	0.810153	-0.226290
N	-0.416041	-1.362866	-0.552870
C	1.993680	2.008207	-0.600093
H	1.515048	2.500948	-1.447137
H	2.045728	2.718749	0.225151
H	3.001063	1.721289	-0.886486
C	-1.287739	-2.476234	-0.865244
H	-1.837259	-2.849624	0.006599
H	-2.009602	-2.190625	-1.627803
H	-0.671583	-3.282857	-1.261565
B	1.838978	-0.462578	-0.080156
C	3.393741	-0.697584	-0.184180
H	3.706895	-0.703896	-1.233961
H	3.982595	0.073465	0.315565
H	3.680762	-1.663795	0.233754
C	0.599219	-1.946124	1.663468
H	-0.061584	-2.801354	1.817393
H	1.548128	-2.160620	2.159312
H	0.153112	-1.076121	2.150882
Cl	-2.659530	0.008972	-0.045531
Cl	-0.746020	2.470803	0.442455

Cartesian coordinates for optimized insertion pathway compounds H_1BMe_2-NHC 5

H_1BMe_2-NHC 5, A

E_e = -563.732637024 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.205839	0.665619	-0.060843
C	-1.041535	-0.714955	0.019279
C	1.002665	0.228085	-0.098459
N	0.324726	-0.937037	0.006058
N	0.067098	1.204229	-0.126284
C	0.930570	-2.249942	0.127495
H	0.271962	-2.879599	0.723014
H	1.084362	-2.698979	-0.853079
H	1.885509	-2.151242	0.631408
C	0.307752	2.633087	-0.176373
H	1.376712	2.804983	-0.129466
H	-0.091590	3.044376	-1.104035
H	-0.185099	3.109452	0.671356
C	3.177496	0.366700	1.380316
H	4.257972	0.533711	1.374827
H	2.740865	1.129296	2.033324
H	3.015687	-0.599818	1.872767
B	2.617691	0.420582	-0.157390
H	2.790900	1.529513	-0.626548
C	3.332143	-0.673839	-1.139685
H	3.499527	-1.657882	-0.690758
H	2.803807	-0.836125	-2.085797
H	4.322911	-0.296480	-1.405593
C	-2.131824	-1.569789	0.091927
C	-2.461903	1.252964	-0.064525
C	-3.389022	-0.985956	0.086131
C	-3.552229	0.400667	0.010429
H	-2.012265	-2.643447	0.142672
H	-4.265140	-1.618281	0.137860
H	-4.551062	0.815544	0.008044
H	-2.585935	2.325875	-0.125614

H_1BMe_2-NHC 5, T1

E_e = -563.694497381 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.119531	-0.688550	0.045540
C	-1.127556	0.706599	-0.078334
C	1.050723	0.018317	0.016235
N	0.190446	1.129551	-0.286383
N	0.200570	-1.116704	-0.013226
C	0.587468	2.463080	0.089964
H	0.880670	2.504082	1.149664
H	1.420360	2.806980	-0.516551
H	-0.247603	3.141596	-0.065231
C	0.557597	-2.396674	-0.579134
H	0.719810	-3.163195	0.182835
H	-0.245589	-2.730863	-1.239719
H	1.470553	-2.295031	-1.163530
B	2.577055	-0.021244	0.067970
H	1.464833	0.220171	1.167445
C	3.296147	-1.350488	0.548626
H	3.776237	-1.834537	-0.308866
H	4.103345	-1.111931	1.245541
H	2.647771	-2.087870	1.021015
C	3.477274	1.245743	-0.256990
H	4.531784	0.964459	-0.260493
H	3.244948	1.679953	-1.232292
H	3.370299	2.045001	0.479520
C	-2.313671	1.408336	-0.050279
C	-2.289104	-1.408274	0.154341
C	-3.503928	0.682779	0.079029
C	-3.494474	-0.697650	0.169307
H	-2.338617	2.485668	-0.143736
H	-4.444856	1.215910	0.106002
H	-4.427732	-1.236596	0.262746
H	-2.274280	-2.486824	0.243233

H_1BMe_2-NHC 5, B

E_e = -563.709514238 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.083084	-0.675036	-0.019496
C	0.986928	0.713710	0.133562
C	-1.084521	-0.077665	-0.488603
N	-0.368645	1.083750	0.088085
N	-0.205035	-1.195948	-0.135297
C	-0.677381	2.372902	-0.491615
H	-1.741475	2.581099	-0.400987
H	-0.140357	3.152154	0.046380
H	-0.395456	2.417756	-1.553552
C	-0.404091	-2.416787	-0.874389
H	-0.117322	-2.313471	-1.931290
H	0.180848	-3.221236	-0.429863
H	-1.455259	-2.703881	-0.825740
B	-2.517768	-0.101435	0.212905
H	-1.119480	0.032507	-1.597685
C	-2.710161	-0.989877	1.481977
H	-3.603610	-0.757318	2.061665
H	-2.788734	-2.036407	1.159707
H	-1.826625	-0.956175	2.122746
C	-3.681417	0.793197	-0.337922

H	-3.859400	1.608480	0.374105
H	-3.515200	1.232051	-1.322354
H	-4.617393	0.226778	-0.356282
C	2.309364	-1.305332	-0.017299
C	2.112765	1.488945	0.300306
C	3.454318	-0.520419	0.165355
C	3.358795	0.849346	0.322174
H	2.390641	-2.375547	-0.155237
H	4.426037	-0.996183	0.172801
H	4.255618	1.440370	0.451455
H	2.045679	2.563687	0.405794

H_1BMe_2-NHC 5, T2

E_e = -563.703500466 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.974779	0.614614	0.169909
C	-0.461420	-0.612082	-0.282356
C	1.221619	1.208229	-0.140919
N	0.900166	-0.589033	-0.575148
N	-0.059243	1.673376	0.003196
C	1.387296	-1.471504	-1.622143
H	0.693380	-1.488897	-2.464576
H	2.358226	-1.123956	-1.964442
H	1.511994	-2.489374	-1.239655
C	-0.512161	2.741734	-0.886870
H	0.242966	3.524589	-0.915218
H	-0.692202	2.362851	-1.898515
H	-1.434601	3.169427	-0.500571
H	1.801858	1.753717	-0.886216
C	1.368185	-0.432269	2.100265
H	1.506442	-1.504686	2.272462
H	1.992987	0.083587	2.834464
H	0.329969	-0.197804	2.344819
C	3.392638	-0.263693	0.304952
H	3.665218	-1.323117	0.345271
H	3.725660	0.120936	-0.664392
H	3.994919	0.239743	1.065633
B	1.833231	-0.033100	0.619275
C	-2.296435	0.734800	0.564045
C	-1.311269	-1.705735	-0.398684
C	-3.125973	-0.374154	0.481138
C	-2.636733	-1.581099	-0.007499
H	-2.672144	1.683740	0.924616
H	-4.159063	-0.295514	0.791635
H	-3.291738	-2.440266	-0.068807
H	-0.932286	-2.652926	-0.760239

H_1BMe_2-NHC 5, C

E_e = -563.729793206 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.025385	0.561057	-0.000020
C	-0.513167	-0.770296	-0.000114
C	1.178160	1.455180	-0.000015
N	0.804764	-1.031031	-0.000274
N	-0.098361	1.655223	-0.000119
C	1.226519	-2.414770	-0.000380
H	0.870653	-2.950769	-0.887032
H	2.312809	-2.448655	-0.000432
H	0.870726	-2.950844	0.886263
C	-0.644656	3.014597	-0.000287
H	0.183674	3.715083	-0.000506
H	-1.255010	3.166297	-0.888811
H	-1.254803	3.166603	0.888331
H	1.763821	2.373395	-0.000053
B	1.924729	0.053778	0.000142
C	2.847833	-0.004114	1.348828
H	3.438676	-0.925082	1.370757
H	3.567494	0.820114	1.387540
H	2.261035	0.025769	2.271758
C	2.848494	-0.003960	-1.348108
H	3.568362	0.820106	-1.386350
H	3.439109	-0.925074	-1.370012
H	2.262075	0.026286	-2.271269
C	-1.493722	-1.794043	-0.000053
C	-2.389290	0.816574	0.000124
C	-2.844954	-1.518587	0.000064
C	-3.315415	-0.211992	0.000188
H	-3.545562	-2.344525	0.000118
H	-1.172660	-2.823995	-0.000135
H	-4.373372	0.005498	0.000296
H	-2.751999	1.833682	0.000211

H_1BMe_2-NHC 5, T3

E_e = -563.715542289 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.955757	0.576108	0.156949
C	-0.555818	-0.787496	0.067350
C	1.321001	1.272086	0.366301
N	0.774428	-1.154138	0.111495
N	0.025034	1.601523	0.289555
C	1.090366	-2.553199	-0.060545
H	0.736765	-2.940339	-1.023890
H	2.168399	-2.682441	-0.017672
H	0.646427	-3.170191	0.728142

C	-0.380742	2.981528	0.095488
H	0.505170	3.610053	0.129933
H	-0.871959	3.110408	-0.872698
H	-1.067362	3.301882	0.880320
H	1.989401	2.107742	0.540725
B	1.851351	-0.125668	0.193695
C	3.297494	-0.529875	0.728075
H	3.842626	-1.175166	0.033897
H	3.922352	0.350221	0.895780
H	3.226502	-1.065308	1.678682
C	2.143484	0.714992	-1.442092
H	3.048197	1.315502	-1.499380
H	2.334496	-0.264968	-1.886427
H	1.326841	1.179800	-1.991397
C	-2.296627	0.914588	0.106263
C	-1.577304	-1.734172	-0.067262
C	-2.920234	-1.376325	-0.111338
C	-3.290873	-0.052615	-0.025075
H	-2.591174	1.951749	0.171639
H	-4.329927	0.243486	-0.062547
H	-3.669129	-2.150279	-0.220453
H	-1.320549	-2.779230	-0.145176
C	1.629377	-1.685246	0.225625
C	2.940598	-1.232357	0.337673
C	3.206994	0.110830	0.172706
H	2.399315	2.046549	-0.212969
H	4.218109	0.486794	0.258835
H	3.734697	-1.934374	0.552540
H	1.431547	-2.738398	0.360309

H_1BMe_2-NHC 5, D

E_e = -563.772789867 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

H	-2.227233	1.697677	-0.593955
C	-1.501781	1.135869	0.004294
C	0.851287	0.562901	-0.223511
C	0.582195	-0.818949	-0.051701
N	-0.747089	-1.287222	-0.188187
N	-0.183263	1.427049	-0.555609
C	-0.924636	-2.726703	-0.290420
H	-0.272236	-3.136924	-1.063546
H	-0.696413	-3.229281	0.653241
H	-1.954789	-2.944485	-0.554455
C	0.131252	2.827479	-0.717563
H	0.502087	3.298748	0.203039
H	0.885055	2.960106	-1.494711
H	-0.773582	3.348869	-1.028418
B	-1.838076	-0.400567	-0.141019
C	-3.337251	-0.893540	-0.178009
H	-3.585127	-1.313291	-1.158293
H	-3.539276	-1.678048	0.555244
H	-4.037389	-0.077732	0.006062
C	-1.640987	1.582962	1.469480
H	-1.498557	2.659921	1.577409
H	-2.632582	1.336658	1.854782
H	-0.898894	1.076716	2.091557
C	2.170971	0.997511	-0.097740

Cartesian coordinates for optimized insertion pathway compounds BMe_3-NHC 1

BMe_3-NHC 1, A

E_e = -449.400691936 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.337695	-0.754982	-0.022613
C	2.399673	0.590200	-0.032003
C	0.220537	0.016925	-0.054008
H	3.113272	-1.499176	-0.007145
H	3.240648	1.259475	-0.026192
N	1.099462	1.044444	-0.050187
N	1.002168	-1.086641	-0.032747
C	0.769557	2.461483	0.000231
H	1.702803	3.019131	0.019663
H	0.187727	2.747710	-0.869798
H	0.198447	2.678777	0.899092
C	0.533559	-2.463250	0.010696
H	-0.267448	-2.551806	0.737852
H	0.165979	-2.773061	-0.964339
H	1.369630	-3.092185	0.307828
C	-1.822949	-0.190969	1.581858
H	-2.913636	-0.205189	1.678227
H	-1.461711	-1.133160	2.010418
H	-1.460381	0.611754	2.234369
B	-1.432159	0.041715	0.005930
C	-2.054122	1.464840	-0.514520
H	-1.868726	2.328738	0.129569
H	-1.759211	1.738278	-1.534977
H	-3.141186	1.344210	-0.538769
C	-2.043635	-1.143757	-0.955081
H	-3.096375	-0.914492	-1.143675
H	-1.567640	-1.205507	-1.941697
H	-2.034695	-2.149624	-0.526901

BMe_3-NHC 1, T1

E_e = -449.337861207 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.213730	-0.682604	-0.100634
C	2.228528	0.650448	-0.081334
C	0.035151	0.010990	-0.117371
H	3.027169	-1.383984	-0.039678
H	3.056105	1.334654	-0.010244
N	0.926161	1.102158	-0.312262
N	0.898947	-1.109996	-0.359864
C	0.568817	2.491282	-0.270290
H	1.448350	3.074984	-0.539962
H	-0.214706	2.704218	-0.996393
H	0.228959	2.824526	0.717851
C	0.524113	-2.462988	-0.025280
H	0.132709	-2.550092	0.995594
H	-0.219164	-2.849413	-0.717533
H	1.412104	-3.088825	-0.101848
C	-0.429029	-0.001101	1.612718
H	-1.264896	-0.604919	1.966111
H	0.495125	-0.414744	2.016158
H	-0.555940	1.022905	1.949832
B	-1.492984	0.010115	-0.205017
C	-2.382453	1.320136	-0.084001
H	-1.913737	2.216583	0.312544
H	-2.776401	1.561924	-1.078026
H	-3.258963	1.102884	0.533855
C	-2.313246	-1.322526	-0.511052
H	-3.385687	-1.119553	-0.523597
H	-2.046382	-1.719402	-1.495200
H	-2.149144	-2.129275	0.203975

BMe_3-NHC 1, B

E_e = -449.370106531 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.500068	0.940919	-0.899364
C	0.371866	0.791703	-1.589521
C	0.195201	-0.413374	0.448374
H	2.359186	1.532532	-1.179998
H	0.078295	1.226150	-2.529397
N	-0.548440	-0.043260	-0.864208
N	1.475285	0.298789	0.319200
C	-1.177220	-1.080481	-1.679883
H	-1.897011	-1.638625	-1.088901
H	-1.704983	-0.595742	-2.501600
H	-0.425654	-1.758100	-2.089970
C	2.694079	-0.257356	0.862378
H	2.996046	-1.200320	0.390632
H	3.493813	0.468810	0.719292
H	2.583165	-0.423136	1.933866
B	-1.129756	0.448103	0.600405
C	-1.037203	2.017825	0.859267
H	-1.778439	2.566341	0.269620
H	-1.264248	2.222146	1.909463
H	-0.058509	2.452336	0.652474
C	-2.505950	-0.255653	1.021399
H	-3.342686	0.124629	0.426168
H	-2.540949	-1.346156	0.966994
H	-2.728551	0.005360	2.059625
C	0.337574	-1.888045	0.718940
H	0.939197	-2.401229	-0.037170
H	0.818946	-2.031177	1.686856
H	-0.637246	-2.366268	0.775531

BMe_3-NHC 1, T2

E_e = -449.364234075 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.385594	-1.362686	0.110395
C	0.291568	-1.530079	0.860531
C	0.311433	0.643360	-0.310779
H	2.180218	-2.078488	-0.032276
H	0.071633	-2.391897	1.473185
N	-0.622227	-0.472813	0.788519
N	1.500451	-0.090637	-0.451342
C	2.799554	0.540168	-0.259965
H	3.000387	0.785052	0.788510
H	3.564910	-0.154714	-0.603548
H	2.869788	1.444841	-0.860409
B	-1.079397	-0.018164	-0.683002
C	-1.148518	-1.187178	-1.777471
H	-1.862538	-1.961901	-1.478398
H	-1.511918	-0.778331	-2.724631
H	-0.198173	-1.682265	-1.984701
C	-2.381638	0.927597	-0.649364
H	-3.291913	0.319973	-0.640565
H	-2.459456	1.622083	0.191273
H	-2.424687	1.530339	-1.561340
C	0.457936	2.061073	0.152121
H	1.133529	2.178845	1.002322
H	0.847942	2.661820	-0.673783
H	-0.515030	2.473090	0.405745
C	-1.324606	-0.090080	2.005478
H	-2.389425	-0.312873	1.923879
H	-0.899026	-0.615154	2.861540
H	-1.214757	0.981498	2.182294

BMe_3-NHC 1, C

E_e = -449.400245572 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.840797	-1.787122	0.130170
C	0.512684	-1.843091	0.007833
C	-0.857757	0.581941	-0.070551
H	-1.458311	-2.657774	0.243468
H	0.975523	-2.826345	0.013620
N	1.297519	-0.786250	-0.142870
N	-1.503975	-0.545845	-0.009946
C	2.714666	-0.970835	-0.357362
H	2.977347	-2.028918	-0.312768
H	3.015662	-0.579940	-1.332345
H	3.288280	-0.436797	0.404980
C	-2.966717	-0.618473	-0.105517
H	-3.316722	-0.016343	-0.940426
H	-3.255670	-1.651555	-0.267104
H	-3.419573	-0.256474	0.816995
B	0.757125	0.669458	0.114787
C	1.039711	1.121065	1.661947
H	2.113786	1.196181	1.861243
H	0.618009	2.105560	1.891029
H	0.625213	0.411524	2.385914
C	1.406039	1.711611	-0.953590
H	1.008247	2.724437	-0.843143
H	2.486408	1.801096	-0.802262
H	1.250644	1.413836	-1.996625
C	-1.637633	1.844316	-0.256594
H	-1.834778	2.005788	-1.322120
H	-2.592977	1.850455	0.268072
H	-1.042699	2.686164	0.089231

BMe_3-NHC 1, T3

E_e = -449.372952979 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.643691	-1.819637	-0.175422
C	0.691338	-1.804588	-0.149075
C	-0.774718	0.562109	-0.281716
H	-1.196677	-2.744889	-0.166121
H	1.217363	-2.750908	-0.092194
N	1.458816	-0.665236	-0.252040
N	-1.423281	-0.636777	-0.302669
C	2.856995	-0.785430	0.098104
H	3.254065	-1.735546	-0.265636
H	3.428492	0.014901	-0.369790
H	3.036006	-0.741404	1.181890
C	-2.804399	-0.762552	0.130168
H	-3.428544	-0.003810	-0.334517
H	-3.176638	-1.738056	-0.177432
H	-2.899042	-0.685330	1.220426
B	0.743938	0.641733	-0.171777
C	0.017268	0.942644	1.559162
H	0.983230	0.650800	1.977594
H	-0.161594	1.997380	1.748072
H	-0.745594	0.327112	2.033195
C	1.602771	1.940737	-0.505051
H	1.030211	2.867712	-0.516918
H	2.409578	2.080535	0.220207
H	2.075001	1.834129	-1.486252
C	-1.643703	1.774937	-0.456292
H	-2.170758	1.690491	-1.409566
H	-2.391344	1.874579	0.333076
H	-1.043354	2.678400	-0.473450

BMe_3-NHC 1, D

E_e = -449.426572849 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.740600	0.586274	0.130230
C	0.430911	-1.809332	-0.080570
C	-0.887151	-1.730127	0.116933
H	0.927952	-2.768564	-0.023185
H	-1.478463	-2.605125	0.341288
N	-1.572956	-0.503067	-0.016503
N	1.211582	-0.713675	-0.397158
C	-3.015904	-0.646620	-0.100326
H	-3.292788	-1.241934	-0.973885
H	-3.398115	-1.151789	0.790565
H	-3.492696	0.324685	-0.176280
C	2.642118	-0.938681	-0.457053
H	3.137161	-0.823591	0.515903
H	2.825410	-1.950945	-0.814380
H	3.109155	-0.253136	-1.162857
B	-0.849939	0.696686	-0.105179
C	-1.508495	2.113661	-0.325099
H	-1.168063	2.531051	-1.277991
H	-2.596233	2.139039	-0.328026
H	-1.165389	2.815086	0.441498
C	0.978837	0.680304	1.650733
H	2.044433	0.668444	1.894652
H	0.565003	1.612827	2.041450
H	0.494508	-0.151064	2.167524
C	1.490746	1.718997	-0.567222
H	1.399516	1.640273	-1.652955
H	1.085939	2.682512	-0.258570
H	2.552011	1.719141	-0.308968

Cartesian coordinates for optimized insertion pathway compounds BMe_3-NHC 2

BMe_3-NHC 2, A

E_e = -450.593146785 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.335467	-0.819167	-0.082015
C	2.401763	0.689220	0.095891
C	0.166804	0.038882	-0.019837
H	2.913426	-1.369379	0.660434
H	2.721064	0.975605	1.103446
N	1.007679	1.078586	-0.107797
N	0.909039	-1.074368	0.077562
C	0.699072	2.491220	-0.035452
H	1.510302	3.036101	-0.518890
H	-0.226433	2.706639	-0.550381
H	0.621630	2.827841	1.001916
C	0.468076	-2.447525	-0.003567
H	-0.580676	-2.520795	0.246633
H	0.625134	-2.841717	-1.011976
H	1.050112	-3.044415	0.701002
C	-1.927657	-0.624968	1.450118
H	-3.014306	-0.757685	1.449279
H	-1.498367	-1.590284	1.731621
H	-1.701858	0.061420	2.273823
B	-1.490037	0.021165	0.001517
C	-2.198473	1.491543	-0.089697
H	-1.932382	2.189460	0.710627
H	-2.070543	2.005494	-1.049153
H	-3.274815	1.318534	0.010151
C	-1.999882	-0.836434	-1.303899
H	-3.094163	-0.806607	-1.316047
H	-1.671788	-0.377894	-2.243869
H	-1.724877	-1.892490	-1.358017
H	3.050259	1.183521	-0.626682
H	2.660415	-1.135325	-1.079108

BMe_3-NHC 2, T1

E_e = -450.552093564 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	2.175402	-0.765325	0.081681
C	2.175398	0.765298	0.081724
C	-0.005970	0.000001	-0.195933
H	2.318130	-1.160822	1.098164
H	2.318074	1.160740	1.098238
N	0.858979	1.099348	-0.441974

N	0.858958	-1.099361	-0.441978
C	0.482198	2.476149	-0.283111
H	1.332787	3.090074	-0.584113
H	-0.356939	2.727067	-0.925239
H	0.229580	2.747630	0.754025
C	0.482160	-2.476152	-0.283056
H	0.229537	-2.747583	0.754092
H	-0.356977	-2.727094	-0.925173
H	1.332743	-3.090100	-0.584029
C	-0.500922	0.000019	1.549378
H	-1.538073	-0.000061	1.893198
H	-0.032457	-0.899011	1.941381
H	-0.032607	0.899142	1.941347
B	-1.533923	0.000006	-0.152551
C	-2.395881	1.345413	-0.216264
H	-2.007372	2.180259	0.364721
H	-2.479838	1.689092	-1.252329
H	-3.413853	1.157600	0.131655
C	-2.395884	-1.345398	-0.216320
H	-3.413902	-1.157566	0.131453
H	-2.479700	-1.689142	-1.252373
H	-2.007451	-2.180211	0.364768
H	2.951695	1.195071	-0.553927
H	2.951672	-1.195056	-0.554032

BMe_3-NHC 2, B

E_e = -450.587145017 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.754891	0.662581	-0.904451
C	-0.402622	1.032644	-1.488823
C	-0.149468	-0.218097	0.568586
H	-2.496281	0.421694	-1.668540
H	-0.150531	0.395670	-2.334728
N	0.530508	0.764831	-0.369144
N	-1.409636	-0.509956	-0.130321
C	1.129886	1.978740	0.176809
H	1.803991	1.735911	0.990953
H	1.706478	2.463976	-0.610722
H	0.361517	2.669348	0.536045
C	-2.475781	-1.069873	0.661153
H	-2.883501	-0.376248	1.413202
H	-3.291514	-1.365475	-0.000302
H	-2.121104	-1.964309	1.174699
B	1.195277	-0.736184	-0.111469
C	1.130784	-1.710419	-1.371749
H	1.815148	-1.392909	-2.165867
H	1.457351	-2.709786	-1.071035
H	0.133221	-1.816669	-1.800026
C	2.584314	-0.706891	0.685716
H	3.393108	-0.300923	0.069182
H	2.593352	-0.163369	1.633299
H	2.870055	-1.735626	0.921312
C	-0.308837	0.260398	1.993534
H	-0.984762	1.117515	2.082250
H	-0.719769	-0.550067	2.596304
H	0.648462	0.526647	2.435964
H	-0.325700	2.077538	-1.786391
H	-2.152314	1.489380	-0.286650

BMe_3-NHC 2, T2

E_e = -450.577798573 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.245963	1.340190	0.612495
C	0.299254	1.685238	-0.567530
C	0.380324	-0.806740	0.362004
H	0.771093	1.577799	1.557643
H	-0.219026	2.620171	-0.317085
N	-0.599907	0.586148	-0.764765
N	1.505316	-0.088404	0.541868
C	-1.249139	0.536953	-2.051113
H	-1.746342	-0.421120	-2.185749
H	-2.009247	1.322533	-2.162083
H	-0.520302	0.664354	-2.859121
C	2.745187	-0.451498	-0.134941
H	2.668243	-0.308572	-1.219754
H	3.548698	0.174088	0.247756
H	2.999881	-1.489479	0.062434
B	-1.100299	-0.148010	0.536906
C	-1.464965	0.779353	1.830966
H	-2.505850	0.625938	2.126951
H	-0.858100	0.539619	2.710222
H	-1.356361	1.854589	1.656128
C	-2.305513	-1.182042	0.237311
H	-3.236133	-0.623502	0.095185
H	-2.196500	-1.833779	-0.632948
H	-2.466761	-1.830729	1.104452
C	0.571349	-2.188155	-0.193188
H	1.076136	-2.189446	-1.161565
H	1.197669	-2.755927	0.500636
H	-0.376433	-2.704951	-0.285767
H	0.876282	1.863568	-1.483228
H	2.181921	1.890890	0.545612

BMe_3-NHC 2, C

E_e = -450.598345702 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.869303	-1.809235	-0.118519
C	0.563380	-1.761150	0.361580
C	-0.839866	0.608120	0.056582
H	-0.912917	-2.147246	-1.156561
H	0.996841	-2.752736	0.187997
N	1.285201	-0.753236	-0.360170
N	-1.523226	-0.490610	-0.051755
C	2.713092	-0.935063	-0.219245
H	3.024120	-1.897846	-0.638820
H	3.242580	-0.149817	-0.759490
H	3.053776	-0.903307	0.829493
C	-2.981945	-0.559837	-0.113026
H	-3.396839	0.345635	-0.543529
H	-3.258621	-1.407161	-0.737839
H	-3.394808	-0.712008	0.886040
B	0.775950	0.668633	-0.030669
C	1.345029	1.252005	1.398535
H	2.414186	1.460981	1.296502
H	0.879575	2.190603	1.712455
H	1.237093	0.548456	2.231379
C	1.101034	1.708249	-1.256191
H	0.790511	2.737783	-1.055436
H	2.182772	1.741590	-1.413675
H	0.652345	1.397055	-2.204600
C	-1.604984	1.887708	0.192944
H	-2.029845	2.164750	-0.776792
H	-2.421790	1.810709	0.912219
H	-0.932336	2.683335	0.496590
H	0.568633	-1.604776	1.458911
H	-1.467479	-2.487030	0.496022

BMe_3-NHC 2, T3

E_e = -450.584229569 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.658928	-1.810943	0.154018
C	0.770647	-1.786871	-0.343065
C	-0.755217	0.555770	-0.317667
H	-1.174554	-2.692489	-0.233138
H	0.764277	-1.835752	-1.446676
N	1.465918	-0.627158	0.151555
N	-1.407023	-0.631794	-0.261454
C	2.890668	-0.704141	-0.067484
H	3.291627	-1.624702	0.369069
H	3.166879	-0.700560	-1.134560
H	3.397840	0.134421	0.406985
C	-2.825359	-0.707679	0.042919
H	-3.397030	-0.015924	-0.570435
H	-3.175704	-1.716751	-0.169434
H	-3.025947	-0.490371	1.099816
B	0.747096	0.666132	-0.005751
C	-0.131849	1.157377	1.564165
H	0.787500	1.002986	2.128126
H	-0.411938	2.207682	1.591743
H	-0.909100	0.544845	2.022785
C	1.613620	1.946602	-0.421705
H	1.037278	2.865214	-0.535358
H	2.381673	2.157303	0.327854
H	2.138880	1.772772	-1.365580
C	-1.599380	1.739256	-0.698508
H	-2.050276	1.549751	-1.675299
H	-2.406962	1.924296	0.013276
H	-0.992868	2.635681	-0.768165
H	1.262831	-2.700374	0.009784
H	-0.657363	-1.872254	1.251222

BMe_3-NHC 2, D

E_e = -450.639902105 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.765686	0.634861	-0.030487
C	0.489242	-1.750147	0.371159
C	-0.943672	-1.803640	-0.107032
H	0.955771	-2.720581	0.188030
H	-1.507914	-2.505810	0.516975
N	-1.574042	-0.496608	-0.029950
N	1.235819	-0.734652	-0.340360
C	-3.018278	-0.567403	-0.121537
H	-3.313834	-1.115123	-1.022040
H	-3.439698	-1.093582	0.740895
H	-3.452260	0.427335	-0.170107
C	2.663111	-0.944824	-0.182823
H	2.985821	-0.968113	0.869519
H	2.936942	-1.897965	-0.638509
H	3.224239	-0.161974	-0.690577
B	-0.834991	0.686663	0.051409
C	-1.574453	2.084931	0.180230
H	-2.071347	2.346857	-0.759614
H	-2.350926	2.070226	0.948685
H	-0.897566	2.905596	0.416456
C	1.365669	1.178331	1.280873
H	2.441129	1.347213	1.184205
H	0.909453	2.131657	1.550232
H	1.204905	0.489542	2.113600
C	1.176452	1.555691	-1.188921
H	0.760063	1.192263	-2.129971
H	0.826793	2.575120	-1.021921
H	2.262585	1.600844	-1.296003
H	0.504756	-1.588675	1.463913
H	-0.978931	-2.176113	-1.137429

Cartesian coordinates for optimized insertion pathway compounds BMe_3-NHC 3

BMe_3-NHC 3, A

E_e = -528.026339245 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.784466	-0.679079	-0.001300
C	1.817871	0.672299	-0.011691
C	-0.360828	0.047370	-0.019406
N	0.493643	1.094092	-0.026890
N	0.445770	-1.036611	-0.001385
C	0.116772	2.499648	-0.004143
H	0.989969	3.096217	-0.251835
H	-0.663143	2.686465	-0.731705
H	-0.242919	2.782088	0.983630
C	0.018696	-2.424712	-0.008235
H	-1.016669	-2.481370	0.297236
H	0.122863	-2.847613	-1.007968
H	0.634877	-2.990287	0.688954
C	-2.459980	-0.611425	1.466057
H	-3.547378	-0.739633	1.476755
H	-2.034940	-1.576864	1.758645
H	-2.221857	0.085032	2.278073
B	-2.017961	-0.003318	0.003185
C	-2.732109	1.461218	-0.149160
H	-2.492198	2.188447	0.632629
H	-2.580545	1.944688	-1.121023
H	-3.809847	1.285852	-0.071834
C	-2.527802	-0.910389	-1.268476
H	-3.621601	-0.870481	-1.296762
H	-2.181567	-0.503144	-2.225660
H	-2.267098	-1.972100	-1.268049
C	2.976842	1.604565	-0.009316
H	3.001417	2.223641	-0.908205
H	2.959628	2.268200	0.857120
H	3.903019	1.035149	0.026914
C	2.878484	-1.685526	0.010441
H	2.892320	-2.254067	0.942675
H	2.772598	-2.396734	-0.810796
H	3.842511	-1.193083	-0.095427

BMe_3-NHC 3, T1

E_e = -527.963377066 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.672238	-0.672343	-0.088442
C	1.676767	0.666138	-0.077706
C	-0.519560	0.009613	-0.125791
N	0.361057	1.103967	-0.326210
N	0.349065	-1.106980	-0.362616
C	-0.031799	2.483465	-0.277762
H	0.814947	3.099961	-0.573035
H	-0.840330	2.665980	-0.983707
H	-0.358671	2.812171	0.717357
C	-0.047692	-2.449466	-0.010212
H	-0.405532	-2.527890	1.024603
H	-0.827918	-2.809118	-0.674108
H	0.808340	-3.110766	-0.122485
C	-0.980452	-0.000049	1.607941
H	-1.814560	-0.603886	1.965847
H	-0.054723	-0.411530	2.009507
H	-1.108752	1.024448	1.942735
B	-2.050100	0.001553	-0.206379
C	-2.952707	1.302969	-0.070095
H	-2.498126	2.198528	0.343779
H	-3.344912	1.555913	-1.062154
H	-3.830030	1.065073	0.539063
C	-2.876752	-1.327617	-0.517749
H	-3.945621	-1.109926	-0.559305
H	-2.592272	-1.744633	-1.488153
H	-2.742533	-2.123933	0.215396
C	2.807661	-1.628763	-0.021220
H	2.729771	-2.310005	0.829831
H	2.858504	-2.238900	-0.927656
H	3.748076	-1.089523	0.070806
C	2.810162	1.623713	0.001555
H	2.932986	2.173733	-0.936008
H	2.665284	2.358329	0.797231
H	3.738514	1.093341	0.201022

BMe_3-NHC 3, B

E_e = -527.997181199 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.549193	-0.197273	0.071493
C	-0.683398	-1.122806	-0.351988
C	0.480010	0.932185	-0.065592
N	0.630945	-0.537126	-0.498693
N	-0.942731	1.038336	0.285811
C	1.321360	-0.883747	-1.739108

H	2.275746	-0.370063	-1.786338
H	1.513504	-1.956341	-1.747735
H	0.713677	-0.617650	-2.607466
C	-1.673442	2.251991	-0.008019
H	-1.816290	2.438884	-1.081002
H	-2.653744	2.196211	0.462811
H	-1.155774	3.105762	0.426950
B	1.406734	0.019527	0.846351
C	0.846537	-0.564847	2.222364
H	1.068665	-1.631505	2.330721
H	1.344818	-0.062276	3.056247
H	-0.227296	-0.430353	2.363766
C	3.001817	0.086603	0.709807
H	3.449399	-0.908755	0.798325
H	3.403698	0.540354	-0.198626
H	3.398017	0.672388	1.544124
C	0.956834	1.956882	-1.062060
H	0.387912	1.937519	-1.996303
H	0.860961	2.952908	-0.629963
H	2.010161	1.814118	-1.289577
C	-0.833672	-2.589011	-0.545164
H	-1.830444	-2.913834	-0.254670
H	-0.679755	-2.889798	-1.584579
H	-0.107943	-3.132377	0.067735
C	-2.987503	-0.382250	0.413057
H	-3.178283	-0.034665	1.430995
H	-3.632432	0.186143	-0.259919
H	-3.271865	-1.429146	0.344179

BMe_3-NHC 3, T2

E_e = -527.988246948 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.491904	-0.141797	-0.177488
C	0.687285	-1.087490	0.340867
C	-0.476037	1.099828	-0.054642
N	-0.643100	-0.683744	0.527075
N	0.899539	1.139855	-0.220353
C	-1.361303	-1.186803	1.684403
H	-1.723171	-2.205725	1.513701
H	-0.729576	-1.177224	2.575051
H	-2.226763	-0.555004	1.869510
C	1.694324	2.197330	0.393466
H	1.836032	2.042413	1.469387
H	2.671442	2.221884	-0.084860
H	1.221390	3.162346	0.229330
B	-1.331703	-0.033557	-0.765354
C	-0.847521	-0.637573	-2.177049
H	-1.014554	-1.719662	-2.218647
H	-1.441279	-0.203083	-2.986202
H	0.201816	-0.461187	-2.422878
C	-2.936470	0.064082	-0.654991
H	-3.311060	0.755221	-1.415824
H	-3.387856	-0.908533	-0.876977
H	-3.357836	0.394139	0.297254
C	-1.081907	2.161134	0.813744
H	-2.105776	1.898862	1.063936
H	-0.524204	2.352058	1.732245
H	-1.125004	3.094795	0.245426
C	2.898572	-0.301884	-0.656467
H	3.137629	-1.350659	-0.813465
H	3.026706	0.213397	-1.610619
H	3.630433	0.105940	0.044807
C	1.045773	-2.507574	0.638701
H	0.450101	-3.191292	0.027871
H	2.098967	-2.700586	0.452184
H	0.848280	-2.748614	1.685224

BMe_3-NHC 3, C

E_e = -528.011862767 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.438490	0.313051	0.088494
C	0.544801	1.322495	-0.156640
C	-0.260950	-1.361629	-0.086195
N	-0.758622	1.055758	-0.363976
N	0.998349	-1.025842	-0.133863
C	-1.658929	2.098390	-0.808822
H	-1.161717	2.829933	-1.443760
H	-2.464324	1.651953	-1.388520
H	-2.116788	2.630312	0.035198
C	2.032109	-1.989882	-0.540064
H	1.655216	-2.611047	-1.347497
H	2.906423	-1.454819	-0.892248
H	2.313654	-2.625432	0.300092
B	-1.349100	-0.229593	0.324551
C	-1.356303	-0.080193	1.952869
H	-2.028635	0.727496	2.262484
H	-1.717397	-0.992006	2.440534
H	-0.368600	0.142546	2.370512
C	-2.826335	-0.587246	-0.244872
H	-3.224808	-1.491434	0.223409
H	-3.542625	0.204041	-0.005168
H	-2.864276	-0.740782	-1.329888
C	-0.643104	-2.769030	-0.421171
H	-0.679993	-2.907653	-1.507492
H	0.047898	-3.508427	-0.014615
H	-1.639237	-2.970825	-0.037666
C	2.851200	0.488102	0.570486
H	3.153340	-0.358874	1.189357
H	3.597784	0.595241	-0.224331
H	2.927974	1.365175	1.209501

C	1.021871	2.748279	-0.223813
H	0.970383	3.115828	-1.250279
H	0.393769	3.396642	0.389330
H	2.052266	2.846663	0.101532

BMe_3-NHC 3, T3

E_e = -527.985281489 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.365552	-0.667143	-0.121820
C	1.364350	0.678694	-0.072696
C	-1.052590	-0.779330	-0.293190
N	0.186115	1.424172	-0.074375
N	0.131590	-1.415515	-0.104372
C	0.219570	2.769745	0.463229
H	0.930562	3.412230	-0.059541
H	-0.763781	3.219980	0.347081
H	0.471908	2.793430	1.532712
C	0.188814	-2.696237	0.586567
H	-0.772478	-3.195288	0.535823
H	0.928985	-3.353335	0.134838
H	0.456034	-2.552533	1.640302
B	-1.126987	0.740976	-0.239387
C	-1.756650	0.096032	1.401860
H	-1.509438	1.055485	1.861486
H	-2.834710	-0.041579	1.392493
H	-1.274950	-0.683610	1.990653
C	-2.327148	1.598611	-0.856759
H	-3.182644	0.999950	-1.171198
H	-2.716758	2.337721	-0.151092
H	-1.976832	2.151072	-1.733162
C	-2.242220	-1.646515	-0.614747
H	-1.974561	-2.312703	-1.437074
H	-2.568569	-2.261788	0.224898
H	-3.085383	-1.035153	-0.920982
C	2.568711	-1.528657	-0.383180
H	2.853528	-2.137940	0.478907
H	2.359131	-2.214338	-1.209610
H	3.434464	-0.943024	-0.670221
C	2.633269	1.485251	-0.109055
H	2.649626	2.127561	-0.993382
H	2.693244	2.137157	0.763921
H	3.523666	0.868513	-0.109931

BMe_3-NHC 3, D

E_e = -528.038916804 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.271667	0.312008	0.230200
C	-0.481796	-1.330326	-0.172286
C	-1.455848	-0.421546	0.025449
N	-1.154590	0.964102	-0.152437
N	0.816646	-0.899313	-0.497364
C	-2.277123	1.800912	-0.555706
H	-2.770915	1.372791	-1.430858
H	-3.020311	1.905855	0.236806
H	-1.919954	2.789064	-0.823859
C	1.826945	-1.904108	-0.766720
H	2.281752	-2.327649	0.140271
H	1.402982	-2.720396	-1.344259
H	2.622445	-1.472803	-1.370508
B	0.162622	1.433280	-0.041450
C	0.568589	2.957969	-0.137258
H	1.120437	3.151816	-1.062503
H	-0.253817	3.669095	-0.087771
H	1.258060	3.206938	0.674549
C	1.398425	0.040149	1.739859
H	2.154940	-0.723613	1.942511
H	1.698573	0.949488	2.265843
H	0.446672	-0.295734	2.156271
C	2.628598	0.768687	-0.305192
H	2.605428	0.895333	-1.390148
H	2.895916	1.726196	0.140347
H	3.425380	0.065070	-0.055087
C	-0.705272	-2.812611	-0.062599
H	-0.619567	-3.297247	-1.037546
H	0.034379	-3.273802	0.595562
H	-1.690367	-3.048176	0.322056
C	-2.849582	-0.716927	0.500198
H	-3.089150	-0.102537	1.372596
H	-3.605433	-0.502205	-0.259372
H	-2.972573	-1.752646	0.795294

Cartesian coordinates for optimized insertion pathway compounds BMe_3-NHC 4

BMe_3-NHC 4, A

E_e = -1368.59251802 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.330382	-0.669532	-0.013622
C	1.363316	0.677275	-0.011296
C	-0.799821	0.054485	-0.052268
N	0.051648	1.108414	-0.048767
N	0.003901	-1.037176	-0.047088
C	-0.304413	2.521290	-0.095340
H	0.486590	3.055891	-0.614281
H	-1.235795	2.629770	-0.632218
H	-0.412401	2.919105	0.912243
C	-0.410741	-2.432317	-0.081562
H	-1.473125	-2.470695	-0.271099
H	0.129196	-2.940564	-0.878484
H	-0.184947	-2.907582	0.872182
C	-2.838461	-0.848578	1.374444
H	-3.927495	-0.950993	1.416094
H	-2.434814	-1.859459	1.474387
H	-2.545517	-0.305951	2.280252
B	-2.461165	-0.001257	0.016872
C	-3.164497	1.466893	0.174321
H	-2.793384	2.076637	1.004888
H	-3.158895	2.084403	-0.730342
H	-4.220242	1.277467	0.391350
C	-3.020062	-0.675029	-1.369690
H	-4.113822	-0.686220	-1.322321
H	-2.755961	-0.075159	-2.247620
H	-2.717858	-1.701882	-1.595585
Cl	2.706173	1.705595	0.034437
Cl	2.608018	-1.776424	0.023049

BMe_3-NHC 4, T1

E_e = -1368.53731183 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.230892	-0.671392	-0.088933
C	1.235048	0.662266	-0.073994
C	-0.938870	0.009168	-0.147150
N	-0.063407	1.110828	-0.336917
N	-0.074956	-1.114884	-0.379858
C	-0.449733	2.496101	-0.330669
H	0.403675	3.093178	-0.643140
H	-1.256758	2.648535	-1.043667
H	-0.773440	2.848283	0.654950
C	-0.477464	-2.462701	-0.044060
H	-0.876506	-2.534884	0.973806
H	-1.227736	-2.816159	-0.744141
H	0.390894	-3.111705	-0.120048
C	-1.420243	0.000626	1.602268
H	-2.295452	-0.539309	1.964205
H	-0.529997	-0.481463	2.003684
H	-1.470019	1.032483	1.934743
B	-2.467897	0.000719	-0.178347
C	-3.359190	1.312244	-0.060869
H	-2.897243	2.209097	0.341747
H	-3.751553	1.556655	-1.054619
H	-4.235575	1.089175	0.554513
C	-3.302286	-1.327930	-0.474481
H	-4.371871	-1.111121	-0.458726
H	-3.068860	-1.717249	-1.469814
H	-3.133118	-2.143958	0.228002
Cl	2.566920	1.708670	0.035985
Cl	2.567942	-1.714967	-0.006867

BMe_3-NHC 4, B

E_e = -1368.57236303 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.183948	0.358564	0.031588
C	-0.558029	-0.753882	-0.349059
C	1.032077	0.950493	-0.044253
N	0.845320	-0.537378	-0.476189
N	-0.339061	1.442342	0.198989
C	1.462564	-1.061605	-1.694576
H	2.531002	-0.874250	-1.664936
H	1.297815	-2.137407	-1.730376
H	1.024263	-0.597778	-2.580523
C	-0.771075	2.716277	-0.358964
H	-0.814567	2.719650	-1.454007
H	-1.763247	2.937235	0.028470
H	-0.099685	3.502939	-0.023310
B	1.647776	-0.137019	0.932736
C	0.874938	-0.560786	2.261672
H	0.745372	-1.645744	2.321849
H	1.474676	-0.274057	3.129535
H	-0.106838	-0.101207	2.389273
C	3.213646	-0.455646	0.894474
H	3.396951	-1.518005	1.081257
H	3.759072	-0.188883	-0.012670
H	3.697703	0.084938	1.712806
C	1.832903	1.794939	-0.997564
H	1.346487	1.935596	-1.965761
H	1.994254	2.776342	-0.551642
H	2.814241	1.357285	-1.158762
Cl	-2.839497	0.472567	0.424957
Cl	-1.189835	-2.328827	-0.466392

BMe_3-NHC 4, T2

E_e = -1368.56679320 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.116026	0.412771	-0.088165
C	0.566970	-0.744959	0.305385
C	-1.085952	1.053363	-0.001250
N	-0.815641	-0.721648	0.442552
N	0.240086	1.500661	-0.079092
C	-1.419782	-1.449086	1.549746
H	-1.628906	-2.481173	1.260902
H	-0.763820	-1.442455	2.420405
H	-2.360368	-0.969764	1.812334
C	0.693578	2.646416	0.708417
H	0.759451	2.414482	1.776397
H	1.679003	2.935128	0.351455
H	0.017047	3.483331	0.557123
B	-1.589405	-0.178459	-0.870941
C	-0.878229	-0.526986	-2.265669
H	-0.731192	-1.607286	-2.367878
H	-1.528906	-0.224326	-3.090448
H	0.089379	-0.050277	-2.435948
C	-3.161106	-0.512200	-0.849982
H	-3.331590	-1.522101	-1.234779
H	-3.675503	-0.451332	0.111566
H	-3.685739	0.165815	-1.529738
C	-1.983459	1.821141	0.919434
H	-1.546721	2.013645	1.900687
H	-2.203716	2.785464	0.453468
H	-2.931591	1.305404	1.037878
Cl	1.417241	-2.217237	0.511621
Cl	2.743395	0.622055	-0.563411

BMe_3-NHC 4, C

E_e = -1368.59568052 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.941481	0.607900	-0.042709
C	-0.797597	-0.739223	-0.190872
C	1.395077	0.979640	-0.111695
N	0.392816	-1.311560	-0.318935
N	0.184147	1.444906	-0.256964
C	0.525571	-2.651075	-0.861375
H	-0.242140	-2.854640	-1.605667
H	1.499725	-2.741830	-1.334793
H	0.454355	-3.408063	-0.073876
C	-0.098159	2.804350	-0.746924
H	0.691379	3.115053	-1.422495
H	-1.043933	2.796972	-1.277563
H	-0.165107	3.496970	0.091310
B	1.592493	-0.556497	0.396603
C	1.417723	-0.579404	2.015114
H	1.495326	-1.606079	2.387114
H	2.204420	-0.003607	2.513395
H	0.457355	-0.181615	2.358171
C	3.018693	-1.162060	-0.071224
H	3.843478	-0.658872	0.440110
H	3.103108	-2.216654	0.205416
H	3.213291	-1.092237	-1.147418
C	2.547576	1.878368	-0.425294
H	2.692526	1.950040	-1.508637
H	2.409733	2.888262	-0.037887
H	3.456049	1.458505	-0.003793
Cl	-2.231209	-1.724081	-0.188592
Cl	-2.384979	1.375604	0.487108

BMe_3-NHC 4, T3

E_e = -1368.57157497 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.927028	-0.677359	0.066988
C	0.964044	0.662380	0.055931
C	-1.434839	-0.729682	-0.292332
N	-0.162610	1.438977	0.064205
N	-0.305950	-1.374208	0.112088
C	-0.133140	2.707759	0.769373
H	0.659345	3.353816	0.392365
H	-1.083160	3.215096	0.613306
H	0.016941	2.578072	1.847930
C	-0.376410	-2.658605	0.800115
H	-1.138839	-2.628147	1.581776
H	-0.612641	-3.467394	0.106959
H	0.582250	-2.870231	1.262648
B	-1.473566	0.792696	-0.304598
C	-2.337229	0.242176	1.229110
H	-2.168277	1.230021	1.663929
H	-3.401666	0.090881	1.075845
H	-1.939771	-0.488015	1.931350
C	-2.513994	1.657683	-1.144551
H	-3.418713	1.111504	-1.415708
H	-2.840672	2.550608	-0.605166
H	-2.046724	2.000720	-2.070992
C	-2.565005	-1.617898	-0.726804
H	-2.213437	-2.230308	-1.560218
H	-2.898098	-2.293351	0.063667
H	-3.415193	-1.029937	-1.059675
Cl	2.299455	-1.658295	-0.316986
Cl	2.487820	1.478358	-0.158665

BMe_3-NHC 4, D

E_e = -1368.62491623 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.555842	-0.475797	0.281760
C	-0.766656	-0.701477	-0.282184
C	-0.999686	0.610218	-0.134196
N	0.057399	1.530051	-0.256896
N	0.513345	-1.159719	-0.534998
C	-0.303215	2.873938	-0.702005
H	-0.990758	2.812839	-1.545905
H	-0.786595	3.441875	0.093550
H	0.591694	3.396951	-1.022067
C	0.701217	-2.551405	-0.899366
H	0.721860	-3.221350	-0.031079
H	-0.106942	-2.866975	-1.553400
H	1.633185	-2.660419	-1.448644
B	1.377849	1.093005	-0.014529
C	2.620103	2.061522	-0.026775
H	3.241817	1.874282	-0.908154
H	2.383220	3.123432	-0.004344
H	3.258820	1.850935	0.835460
C	1.371050	-0.780805	1.776112
H	1.474854	-1.851700	1.971187
H	2.127104	-0.258453	2.366377
H	0.387205	-0.461671	2.125975
C	2.939650	-0.943092	-0.162807
H	3.083177	-0.803603	-1.236587
H	3.704263	-0.366594	0.356472
H	3.107523	-1.994884	0.076383
Cl	-2.031248	-1.856266	-0.010137
Cl	-2.523146	1.230935	0.388810

Cartesian coordinates for optimized insertion pathway compounds BMe_3-NHC 5

BMe_3-NHC 5, A

E_e = -603.042940512 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.346297	-0.677974	-0.016053
C	1.368924	0.711360	-0.010869
C	-0.791409	0.049074	-0.043139
N	0.043539	1.116731	-0.042819
N	0.013880	-1.042646	-0.042934
C	-0.318345	2.523367	-0.084158
H	0.469334	3.057902	-0.611655
H	-1.251214	2.644987	-0.616185
H	-0.418688	2.926536	0.923048
C	-0.381308	-2.438264	-0.071800
H	-1.448217	-2.509282	-0.223206
H	0.138152	-2.934260	-0.892234
H	-0.111995	-2.917225	0.870331
C	-2.822394	-0.857585	1.382310
H	-3.909758	-0.980200	1.410889
H	-2.398440	-1.858099	1.499810
H	-2.551222	-0.297685	2.284244
B	-2.443552	-0.017659	0.018516
C	-3.171646	1.440853	0.154582
H	-2.819062	2.063353	0.983824
H	-3.162853	2.050505	-0.755425
H	-4.227420	1.238622	0.360304
C	-2.985703	-0.713331	-1.366176
H	-4.079094	-0.746845	-1.320589
H	-2.731839	-0.112089	-2.246145
H	-2.659406	-1.733871	-1.585554
C	2.564477	1.415408	0.020527
C	2.512642	-1.429264	0.004219
C	3.732266	0.669430	0.041829
C	3.707547	-0.728867	0.032896
H	2.591992	2.496095	0.037155
H	4.684926	1.180874	0.069576
H	4.641330	-1.274313	0.051952
H	2.491217	-2.510546	0.002548

BMe$_3$-NHC 5, T1

E_e = -602.996315416 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.242956	-0.701679	-0.171261
C	1.244573	0.700909	-0.144291
C	-0.934869	0.003684	-0.135131
N	-0.064352	1.110155	-0.331206
N	-0.069319	-1.107428	-0.402238
C	-0.438478	2.489537	-0.455836
H	0.392095	3.024885	-0.916144
H	-1.305623	2.584362	-1.105364
H	-0.661985	2.965123	0.506674
C	-0.448925	-2.484593	-0.232290
H	-0.718904	-2.722327	0.804784
H	-1.281436	-2.737322	-0.881417
H	0.396727	-3.107953	-0.515806
C	-1.372655	-0.025677	1.610281
H	-1.299222	0.998450	1.962824
H	-2.296799	-0.470095	1.984024
H	-0.539158	-0.619851	1.981017
B	-2.462930	0.004392	-0.113845
C	-3.323256	1.336173	0.025904
H	-3.719991	1.608315	-0.958724
H	-4.196151	1.135719	0.653187
H	-2.823899	2.212392	0.431507
C	-3.329201	-1.316473	-0.342676
H	-3.039784	-2.172019	0.266570
H	-4.383434	-1.119012	-0.139355
H	-3.263143	-1.637502	-1.386941
C	2.413719	1.413985	0.009241
C	2.414072	-1.412768	-0.023906
C	3.605330	-0.691245	0.130756
C	3.605905	0.691091	0.143113
H	2.415710	2.495316	0.039516
H	4.537249	1.226245	0.271240
H	4.536040	-1.229377	0.250322
H	2.427034	-2.494056	-0.028006

BMe$_3$-NHC 5, B

E_e = -603.028168074 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.095187	0.663407	-0.229978
C	-0.775449	-0.694595	-0.210596
C	1.222829	0.560939	-0.442134
N	0.645436	-0.846897	-0.329050
N	0.034364	1.421949	-0.470672
C	1.095953	-1.911648	-1.220537
H	2.179257	-1.906329	-1.279940
H	0.780744	-2.870009	-0.810075
H	0.665987	-1.786477	-2.216035
C	0.169857	2.732491	0.124476
H	1.036163	3.235775	-0.303355
H	-0.708654	3.332975	-0.107429
H	0.295862	2.679731	1.212741
B	1.607326	-0.213356	0.890959
C	0.836615	0.062127	2.260214
H	0.693575	-0.867775	2.819465
H	1.449036	0.710953	2.893355
H	-0.142713	0.534413	2.166599
C	3.024044	-0.943838	1.018805
H	2.915098	-1.956976	1.419135
H	3.621001	-1.015034	0.107370
H	3.632889	-0.395814	1.743123
C	2.114990	0.823805	-1.625823
H	1.586673	0.669013	-2.569998
H	2.427984	1.868481	-1.590620
H	3.019037	0.218588	-1.608204
C	-2.408845	1.059847	-0.036547
C	-1.725918	-1.672594	-0.061317
C	-3.056641	-1.274773	0.104425
C	-3.380838	0.071103	0.124888
H	-2.681166	2.106425	-0.021703
H	-4.411580	0.368444	0.268698
H	-3.827324	-2.022049	0.232539
H	-1.455550	-2.720547	-0.047672

BMe$_3$-NHC 5, T2

E_e = -603.015278235 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-1.038593	0.610649	0.229121
C	-0.714299	-0.634903	-0.330308
C	1.265831	0.858281	0.050364
N	0.649814	-0.817278	-0.534649
N	0.048983	1.502790	0.241231
C	1.086850	-1.623819	-1.658535
H	0.370664	-1.550510	-2.478775
H	2.054173	-1.266951	-2.009301
H	1.201745	-2.672631	-1.370126
C	-0.213155	2.799205	-0.376766
H	0.631928	3.464163	-0.216220
H	-0.412799	2.712881	-1.450073
H	-1.082780	3.243208	0.100586
C	0.874000	-0.875383	2.175858
H	1.587910	-0.689459	2.983350
H	-0.031904	-0.316427	2.417572
H	0.619311	-1.939380	2.225962
C	3.047245	-1.129991	0.631698

H	3.049789	-2.189396	0.906641
H	3.529109	-1.057922	-0.346061
H	3.708571	-0.629273	1.345159
B	1.560467	-0.526343	0.766517
C	-2.349081	0.911171	0.566815
C	-1.721426	-1.546921	-0.617563
C	-3.344153	-0.021891	0.310730
C	-3.033840	-1.236900	-0.289027
H	-2.593891	1.863373	1.018700
H	-4.368555	0.204407	0.574862
H	-3.817106	-1.957373	-0.484212
H	-1.475886	-2.503344	-1.061616
C	2.261172	1.546449	-0.831182
H	1.827448	1.981130	-1.732761
H	2.736840	2.349609	-0.261009
H	3.048209	0.851339	-1.108568

BMe_3-NHC 5, C

E_e = -603.042099419 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	-0.988333	0.673610	-0.042182
C	-0.886924	-0.733924	-0.187354
C	1.383536	0.947458	-0.024516
N	0.316948	-1.315419	-0.388014
N	0.200007	1.471280	-0.173199
C	0.328124	-2.744614	-0.607014
H	-0.336130	-3.023131	-1.429481
H	1.334115	-3.056549	-0.870621
H	0.017388	-3.307451	0.283628
C	-0.001832	2.893226	-0.480743
H	0.880851	3.291210	-0.966265
H	-0.844101	2.982213	-1.160249
H	-0.208341	3.459993	0.427547
B	1.598121	-0.639353	0.195573
C	1.742435	-0.879284	1.811030
H	1.878159	-1.947587	2.008174
H	2.609678	-0.371546	2.245717
H	0.857922	-0.557812	2.370940
C	2.933451	-1.124289	-0.605330
H	3.822965	-0.544650	-0.346774
H	3.184470	-2.157797	-0.352561
H	2.816843	-1.075944	-1.693404
C	2.577762	1.845217	-0.021947
H	2.948385	1.964484	-1.045377
H	2.391280	2.830199	0.401964
H	3.368761	1.360437	0.544328
C	-2.204620	1.291481	0.205349
C	-2.105025	-1.447571	-0.131398
C	-3.311443	-0.815916	0.098120
C	-3.377104	0.557493	0.285793
H	-2.250318	2.361275	0.351661
H	-4.316249	1.052348	0.486743
H	-4.215107	-1.411093	0.143657
H	-2.090034	-2.520182	-0.247863

BMe_3-NHC 5, T3

E_e = -603.024247403 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	0.979781	-0.685374	-0.046371
C	0.976897	0.730799	0.010333
C	-1.424138	-0.770266	-0.256431
N	-0.214770	1.419452	0.101734
N	-0.250509	-1.399369	0.010653
C	-0.145075	2.849103	0.296505
H	0.286008	3.369685	-0.567693
H	-1.146099	3.241739	0.455765
H	0.460501	3.101117	1.172895
C	-0.193797	-2.803153	0.381616
H	-1.164405	-3.132616	0.737724
H	0.102139	-3.437699	-0.458568
H	0.528657	-2.937236	1.186806
B	-1.516373	0.744076	-0.165548
C	-2.268625	0.065917	1.401830
H	-2.062984	1.017103	1.896764
H	-3.341592	-0.081295	1.306003
H	-1.819557	-0.724036	2.001184
C	-2.667123	1.608314	-0.858782
H	-3.515802	1.017147	-1.203725
H	-3.076319	2.363777	-0.182361
H	-2.268877	2.142867	-1.725720
C	-2.567905	-1.641800	-0.695341
H	-2.235292	-2.261292	-1.531019
H	-2.926746	-2.309265	0.089755
H	-3.406051	-1.034859	-1.022919
C	2.174553	-1.374891	-0.156758
C	2.216624	1.375219	-0.024434
C	3.410328	0.666816	-0.116556
C	3.398481	-0.709257	-0.188376
H	2.166668	-2.453470	-0.222751
H	4.317489	-1.273630	-0.264636
H	4.346795	1.209347	-0.132519
H	2.254283	2.453082	0.022646

BMe_3-NHC 5, D

E_e = -603.077783480 (Hartrees)
M06-2X/def2-TZVP optimized geometry (Å).

0 1

C	1.531893	-0.624641	0.178596
C	-0.873398	-0.674539	-0.208396
C	-0.985796	0.730013	-0.083653
N	0.178024	1.521707	-0.213861
N	0.367607	-1.236107	-0.503975
C	-0.030924	2.942753	-0.449404
H	-0.786188	3.084136	-1.223600
H	-0.361772	3.463195	0.453508
H	0.894337	3.393981	-0.791358
C	0.383947	-2.672494	-0.687514
H	0.181335	-3.233774	0.235719
H	-0.368866	-2.950006	-1.424724
H	1.347485	-2.984228	-1.077526
B	1.453182	0.958468	-0.020053
C	2.762848	1.837128	0.057553
H	3.298977	1.803915	-0.897092
H	2.596217	2.884463	0.303902
H	3.453432	1.433561	0.801313
C	1.516709	-0.941730	1.686165
H	1.607851	-2.017622	1.858548
H	2.352736	-0.454201	2.192630
H	0.589141	-0.597573	2.149390
C	2.831322	-1.155995	-0.431918
H	2.812275	-1.077091	-1.521173
H	3.681333	-0.583729	-0.063864
H	3.013639	-2.197540	-0.161921
C	-2.033564	-1.437975	-0.069001
C	-2.228130	1.301068	0.152902
C	-3.374254	0.522134	0.272424
C	-3.271534	-0.848731	0.160075
H	-2.314362	2.373558	0.250733
H	-4.329699	0.995401	0.453955
H	-4.148223	-1.476137	0.255072
H	-1.979702	-2.513795	-0.135363

Table S1. Activation barriers for T1 (hydride migration), NBO partial charges on carbenic carbon of adduct A, and ^{31}P chemical shifts of NHC-PPh adducts for NHC compounds 1-5.

Insertion compound	NHC compound	Activation barrier [a] / kJ mol^{-1}	Partial charge [b] / e	^{31}P NMR chemical shift of NHC-PPh adduct [c] / ppm
Ph_2SiH_2	1	61.5	0.165	-61.2
	2	28.2	0.266	-10.4
	3	71.4	0.167	-53.5
	4	58.8	0.185	-
	5	50.6	0.220	-34.6
H_2BMe	1	145.2	0.366	-61.2
	2	90.0	0.452	-10.4
	3	156.1	0.370	-53.5
	4	129.0	0.383	-
	5	116.9	0.419	-34.6
$HBMe_2$	1	133.8	0.364	-61.2
	2	73.5	0.456	-10.4
	3	149.7	0.371	-53.5
	4	132.5	0.383	-
	5	105.4	0.419	-34.6
BMe_3	1	167.8	0.366	-61.2
	2	113.6	0.458	-10.4
	3	173.3	0.368	-53.5
	4	152.8	0.381	-
	5	125.2	0.418	-34.6

[a] Difference between adduct A and transition state T1. SCS-MP2/def2-TZVP//M06-2X/def2-TZVP calculated ΔG values. Units of kJ/mol.
[b] Charge on carbenic carbon (adduct A). B3LYP/def2-TZVP//M06-2X/def2-TZVP values.
[c] Values reproduced from O. Back, M. Henry-Ellinger, C. D. Martin, D. Martin, G. Bertrand, *Angew. Chem. Int. Ed.* **2013**, *52*, 2939-2943.

Table S2. Correlation (r^2) between calculated NBO charges and T1 barrier height; ΔE_e refers to electronic energies (T1 barrier height), ΔG refers to Gibb's free energies (M06-2X/def2-TZVP thermochemical corrections employed for all ΔG results).

	Ph_2SiH_2		BH_2Me		$BHMe_2$		BMe_3	
	ΔE_e	ΔG	ΔE_e	ΔG	ΔE_e	ΔG	ΔE_e	ΔG
B3LYP/SVP	0.923	0.859	0.946	0.858	0.956	0.848	0.833	0.741
B3LYP/TZVP	0.989	0.917	0.958	0.911	0.505	0.533	0.944	0.914
M06-2X/SVP	0.972	0.908	0.951	0.895	0.977	0.906	0.926	0.873
M06-2X/TZVP	0.985	0.907	0.953	0.895	0.973	0.940	0.937	0.902
BP86/SVP	0.928	0.852	0.950	0.896	0.849	0.712	0.840	0.772
BP86/TZVP	0.959	0.857	0.919	0.817	0.962	0.907	0.902	0.821
M06-L/SVP	0.962	0.896	0.917	0.830	0.980	0.911	0.945	0.884
M06-L/TZVP	0.974	0.899	0.903	0.798	0.816	0.822	0.796	0.727
B3LYP-D3BJ/SVP	0.936	0.857	0.931	0.850	0.885	0.826	0.601	0.517
B3LYP-D3BJ/TZVP	0.959	0.856	0.872	0.785	0.861	0.853	0.679	0.597