

Tuning Receptors for the Encapsulation of Beryllium(2+) Cations.

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Supporting Information

Table S1 and **Figure S1**. Comparison of the binding energies of B3LYP/6-311++G(d,p) optimised L1chH_Be, L1chNH₂_Be, and L1chNHCH₃_Be using B3LYP, B3LYP-D3, M06-2X, and ωB97X-D functionals with the 6-311++G(d,p) basis set

Table S2. B3LYP/6-311++G(d,p) optimized geometry coordinates (Å) for the ligands **L1-L5** with their corresponding buttress groups.

Table S3. B3LYP/6-311++G(d,p) optimized geometry coordinates (Å) for the Be²⁺ complexes of **L1-L5** with their corresponding buttress groups.

Table S1. Comparison of the binding energies of B3LYP/6-311++G(d,p) optimised L1chH_Be, L1chNH₂_Be, and L1chNHCH₃_Be using B3LYP, B3LYP-D3, M06-2X, and ωB97X-D functionals with the 6-311++G(d,p) basis set.

	Binding Energy /kJ mol ⁻¹		
	L1chH_Be	L1chNH ₂ _Be	L1chNHCH ₃ _Be
B3LYP	-354.555	-383.712	-395.639
B3LYP-D3	-369.132	-412.553	-420.314
M06-2X	-336.011	-373.622	-377.439
ωB97X-D	-364.272	-403.539	-406.832

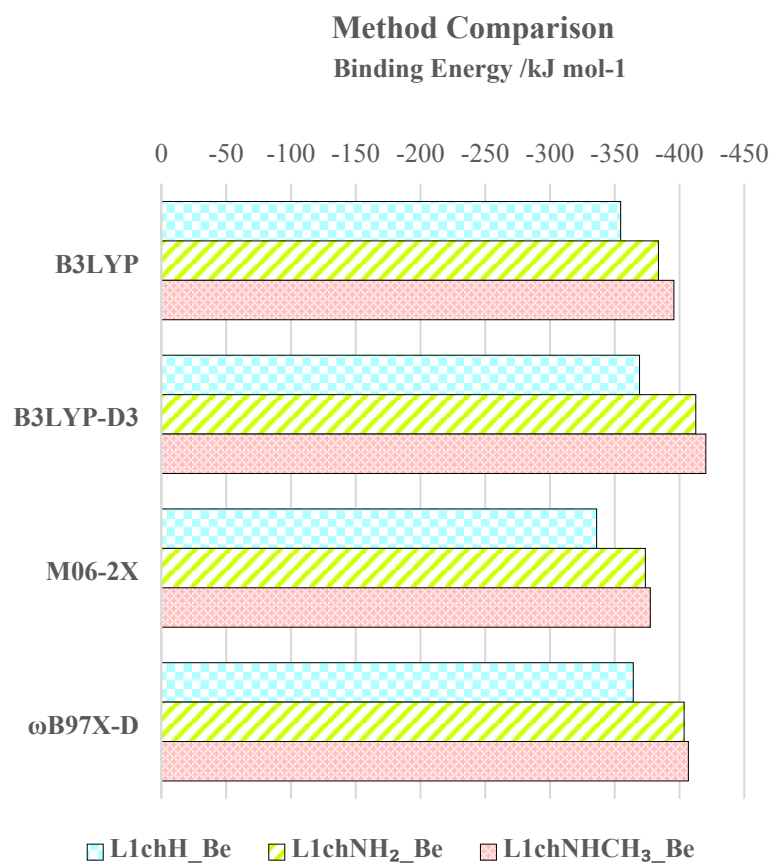


Figure S1. Comparison of the binding energies of B3LYP/6-311++G(d,p) optimised L1chH_Be, L1chNH₂_Be, and L1chNHCH₃_Be using B3LYP, B3LYP-D3, M06-2X, and ωB97X-D functionals with the 6-311++G(d,p) basis set.

Table S2. B3LYP/6-311++G(d,p) optimized geometry coordinates (Å) for the ligands **L1-L5** with their corresponding buttress groups.

L1chH_				L1chNH2_			
C	-0.67758	2.14381	1.77255	C	1.87302	0.98604	0.96774
C	0.46667	1.60046	1.18965	C	0.70793	1.95571	2.84369
H	-0.58633	2.88808	2.55707	C	-0.41193	1.21679	2.48521
C	0.29262	0.65084	0.18177	H	0.68251	2.60960	3.70884
H	1.45565	1.89843	1.51066	C	-0.33459	0.39026	1.35736
C	1.46317	-0.04131	-0.52395	H	-1.32842	1.27520	3.06101
H	1.14444	-0.17333	-1.55970	C	-1.57283	-0.42201	0.95959
C	3.00516	1.61321	-1.66121	H	-1.97900	-0.83215	1.88778
C	4.16328	2.38300	-1.67317	C	-3.99248	0.28115	0.75577
H	2.31342	1.64117	-2.49496	C	-4.97098	1.09625	0.17938
C	4.68428	1.46998	0.47066	H	-4.25254	-0.46843	1.49256
C	5.02676	2.31297	-0.58245	C	-3.24400	2.16100	-1.09258
H	4.38945	3.02188	-2.51924	C	-4.60795	2.04791	-0.75632
H	5.33248	1.38517	1.33827	H	-6.01110	0.98757	0.46637
H	5.94239	2.89039	-0.54692	H	-5.34332	2.69463	-1.21970
C	1.72866	-1.45148	-0.00023	C	-1.23973	-1.64033	0.10255
C	1.76708	-3.12994	1.72134	C	-0.96995	-2.80789	-1.96925
C	2.50854	-3.55928	-0.50591	C	-0.55923	-3.85238	0.14361
C	2.29442	-4.02041	0.78980	C	-0.58969	-3.93463	-1.26178
H	1.58179	-3.44284	2.74271	H	-1.00741	-2.83737	-3.05279
H	2.91445	-4.22240	-1.26466	H	-0.32469	-4.85678	-1.76525
H	2.53091	-5.04384	1.05405	C	-2.66742	0.46006	0.36219
C	2.73920	0.79483	-0.55750	C	-1.30260	-1.63407	-1.28763
C	1.47927	-1.82878	1.32184	H	-1.59130	-0.74013	-1.82179
H	1.06678	-1.11527	2.02342	N	0.77569	0.27533	0.62718
N	-0.91459	0.25546	-0.23463	N	-2.30216	1.38528	-0.53834
N	3.57122	0.72544	0.49144	N	-0.88448	-2.73188	0.80210
N	2.23444	-2.30945	-0.90021	C	1.86337	1.84526	2.07572
C	-1.93321	1.73363	1.34999	H	2.74986	2.41615	2.32343
H	-2.84017	2.12165	1.78728	C	3.11302	0.79902	0.16900
C	-3.33425	0.29479	-0.20885	C	4.27973	0.40592	0.83560
C	-3.33696	-0.40613	-1.43206	C	3.13153	1.04964	-1.25913
C	-4.59659	0.51740	0.48235	C	5.48838	0.18954	0.17168
C	-4.49046	-0.90253	-2.02244	H	4.23065	0.24210	1.90925
H	-2.38211	-0.55231	-1.92309	C	4.39201	0.79945	-1.90301
C	-5.76356	-0.02601	-0.16397	C	5.52363	0.38750	-1.21528
C	-5.71767	-0.70506	-1.36543	H	6.36934	-0.13247	0.71513
H	-4.44397	-1.42697	-2.97035	H	4.43665	0.96494	-2.97627
H	-6.71153	0.12588	0.34458	H	6.44866	0.22084	-1.76153
H	-6.63663	-1.08525	-1.80402	O	2.12087	1.49557	-1.91264
O	-4.71245	1.13829	1.59961	N	-0.14279	-4.92468	0.91388
C	-2.03699	0.76985	0.32252	H	-0.41487	-4.88073	1.88591
				N	-2.81945	3.05536	-2.05658
				H	-1.83140	3.26516	-2.04204
				H	-0.23351	-5.84336	0.50522
				H	-3.41020	3.85354	-2.23744

L1chNHCH3_

C	-1.92041	0.20243	1.38654
C	-1.05040	0.84503	3.53803
C	0.22936	0.58909	3.05231
H	-1.19270	1.19371	4.55527
C	0.36904	0.13590	1.73869
H	1.10243	0.74852	3.67443
C	1.76475	-0.03493	1.13819
H	2.47405	0.01406	1.96982
C	2.25394	-2.50408	1.32251
C	2.38726	-3.75831	0.72957
H	2.37464	-2.37239	2.39062
C	1.94519	-2.74211	-1.39536
C	2.23057	-3.89885	-0.64138
H	2.61553	-4.62777	1.33665
H	2.33122	-4.86563	-1.11543
C	2.10701	1.12530	0.19386
C	3.65890	2.44336	-1.05913
C	1.30339	2.88515	-1.09018
C	2.60093	3.20880	-1.53827
H	4.67003	2.67329	-1.37873
H	2.77411	4.02442	-2.22795
C	1.95471	-1.41311	0.49982
C	3.43064	1.38257	-0.18233
H	4.24638	0.77236	0.18592
N	-0.68631	-0.09325	0.94641
N	1.81021	-1.52963	-0.82149
N	1.09540	1.87085	-0.23149
C	-2.13855	0.67073	2.69064
H	-3.14517	0.89571	3.02231
C	-3.06080	0.03430	0.43390
C	-3.88256	-1.08883	0.54291
C	-3.31636	1.04658	-0.56987
C	-4.96323	-1.31123	-0.31603
H	-3.66375	-1.81734	1.32012
C	-4.42843	0.77360	-1.43363
C	-5.22061	-0.36042	-1.31032
H	-5.58014	-2.19663	-0.21254
H	-4.64715	1.50865	-2.20406
H	-6.05290	-0.50572	-1.99433
O	-2.62424	2.13051	-0.68316
N	0.17059	3.56106	-1.46333
H	-0.69935	3.08934	-1.22016
N	1.81290	-2.77079	-2.76092
H	1.42003	-1.92947	-3.15580
C	1.67687	-3.99687	-3.52796
H	1.52747	-3.73333	-4.57431
H	2.58361	-4.60478	-3.46203
H	0.82702	-4.60868	-3.19928
C	0.14774	4.53134	-2.54138
H	0.77571	5.39757	-2.31044
H	0.48710	4.11043	-3.49752
H	-0.87515	4.88536	-2.66715

L1chNHCOCH3_

C	-0.83520	-0.51758	2.25239
C	1.31299	-0.06483	3.24732
C	1.77741	0.31157	1.98922
H	1.97435	-0.03786	4.10654
C	0.88680	0.26364	0.91316
H	2.80454	0.62476	1.84396
C	1.39216	0.55423	-0.50602
H	2.39457	0.97272	-0.41717
C	2.72253	-1.14866	-1.86674
C	2.78765	-2.40741	-2.46333
H	3.58800	-0.49812	-1.84058
C	0.50451	-2.75912	-1.85692
C	1.67985	-3.24760	-2.44327
H	3.71306	-2.75057	-2.91167
H	1.74557	-4.25219	-2.83481
C	0.57131	1.61142	-1.23450
C	-1.38906	2.41346	-2.34565
C	0.51050	3.80325	-1.96662
C	-0.78938	3.66342	-2.45853
H	-2.39586	2.26740	-2.72006
H	-1.32821	4.49407	-2.88780
C	1.51658	-0.76442	-1.27631
C	-0.70950	1.36570	-1.73411
H	-1.14856	0.38623	-1.62143
N	-0.38927	-0.10123	1.05467
N	0.43786	-1.54547	-1.31265
N	1.16503	2.80667	-1.35898
C	0.00011	-0.50261	3.38094
H	-0.37744	-0.84113	4.33829
C	-2.24534	-0.98823	2.34336
C	-3.12456	-0.31545	3.19888
C	-2.69297	-2.14082	1.58778
C	-4.46668	-0.67634	3.32985
H	-2.74623	0.53214	3.76500
C	-4.08099	-2.46558	1.74056
C	-4.93421	-1.76177	2.57878
H	-5.12664	-0.12502	3.98983
H	-4.45155	-3.31817	1.17799
H	-5.97555	-2.06363	2.65507
O	-1.91383	-2.86652	0.85800
N	1.24368	5.00849	-1.99742
H	1.98583	5.04032	-1.30729
N	-0.67878	-3.50752	-1.68396
H	-1.20989	-3.24661	-0.83368
C	1.28248	6.06133	-2.88102
C	-1.26471	-4.44416	-2.49005
C	-0.67714	-4.73672	-3.85399
H	0.04323	-5.55631	-3.78194
H	-1.49010	-5.06506	-4.50053
H	-0.17596	-3.87762	-4.29929
C	0.38914	6.05534	-4.09708
H	0.82737	6.72558	-4.83465
H	0.26944	5.06032	-4.52606
H	-0.60133	6.43860	-3.83708
O	2.06264	6.98673	-2.66474
O	-2.28383	-5.02685	-2.11280

L1chNHCONH2_

C	0.16308	0.10105	2.07678
C	2.54405	0.47149	2.03246
C	2.49506	0.37704	0.64325
H	3.48587	0.65657	2.53755
C	1.26180	0.13060	0.03802
H	3.38944	0.49851	0.04366
C	1.14757	0.09455	-1.48586
H	2.16135	0.11867	-1.89249
C	-0.83101	-1.40876	-2.11964
C	-1.28918	-2.66774	-2.49404
H	-1.52121	-0.59788	-1.93348
C	0.97802	-3.40593	-2.58627
C	-0.38428	-3.69785	-2.72154
H	-2.35211	-2.85648	-2.59111
H	-0.72893	-4.69446	-2.95748
C	0.40102	1.31791	-2.03253
C	-0.34248	2.70131	-3.83479
C	-0.98837	3.11049	-1.57131
C	-1.07742	3.45886	-2.92579
H	-0.38031	2.95042	-4.88927
H	-1.71487	4.26133	-3.26823
C	0.54380	-1.22291	-1.96621
C	0.41059	1.61480	-3.39962
H	0.97072	1.00633	-4.09919
N	0.13714	-0.03987	0.74133
N	1.42506	-2.20296	-2.20713
N	-0.25537	2.07317	-1.15798
C	1.36522	0.34938	2.75838
H	1.36296	0.45372	3.83676
C	-1.12815	-0.00904	2.81328
C	-1.32067	-1.07525	3.69612
C	-2.15216	0.99944	2.63908
C	-2.51001	-1.25139	4.40747
H	-0.51838	-1.79930	3.81593
C	-3.36155	0.77055	3.37454
C	-3.53244	-0.31200	4.22662
H	-2.63640	-2.09625	5.07482
H	-4.15605	1.50264	3.25687
H	-4.47130	-0.42521	4.76254
O	-1.99849	2.05341	1.91113
N	-1.69307	3.72784	-0.52399
H	-1.79349	3.14216	0.31752
N	2.00018	-4.35279	-2.77073
H	2.87911	-4.09770	-2.34020
C	-2.18095	5.01214	-0.40009
C	2.10764	-5.46288	-3.59287
O	-2.91202	5.31708	0.54518
O	3.10857	-6.17665	-3.52356
N	-1.84285	5.92327	-1.36886
H	-2.07246	6.87810	-1.13618
H	-0.99172	5.80246	-1.89824
N	1.07052	-5.73530	-4.43851
H	0.44715	-5.00044	-4.73838
H	1.26112	-6.45331	-5.12138

L2chH_

C	0.97947	-3.49814	7.24293
C	2.30540	-3.34876	6.73090
C	0.84677	-5.66844	6.18137
H	0.29821	-6.57735	5.95611
C	0.24974	-4.68954	6.95327
C	2.15760	-5.51783	5.67621
H	2.59072	-6.30939	5.07475
C	2.87981	-4.37815	5.94492
H	3.88762	-4.25270	5.56361
C	-1.16921	-4.89138	7.48144
O	-2.10258	-4.48952	6.74144
O	-1.27354	-5.47104	8.59226
N	0.38754	-2.52869	8.00675
C	2.37717	-1.19606	7.81310
C	1.04971	-1.42629	8.27380
C	2.99371	-2.14935	7.04982
H	4.00608	-2.00326	6.68733
H	2.88455	-0.27384	8.07136
C	0.38936	-0.34033	9.12471
C	0.01377	0.89146	8.30162
C	-0.00199	2.14950	8.91570
C	-0.36022	3.26495	8.16819
C	-0.68835	3.09477	6.82461
C	-0.63655	1.80876	6.29642
N	-0.29311	0.72775	7.00953
H	-0.37750	4.24884	8.62292
H	0.26399	2.24718	9.96192
H	-0.97070	3.93334	6.19998
H	-0.87838	1.63481	5.25175
C	-0.77530	-0.86184	9.96305
C	-0.51404	-1.45707	11.20277
C	-1.57409	-1.94085	11.96023
C	-2.86847	-1.81214	11.46092
C	-3.03402	-1.19783	10.22372
N	-2.01831	-0.72901	9.48674
H	-1.39465	-2.40455	12.92356
H	0.50497	-1.53769	11.56328
H	-3.72756	-2.17050	12.01466
H	-4.02764	-1.07161	9.80310
H	1.15361	-0.01021	9.83632

L2chNH2_			
C	2.37704	0.59776	0.08509
C	3.00515	1.30150	1.15917
C	4.53327	0.33079	-0.97592
H	5.14819	-0.03840	-1.79037
C	3.17155	0.10250	-0.99411
C	5.15300	1.03309	0.08493
H	6.22599	1.18887	0.06277
C	4.40744	1.51195	1.13663
H	4.87654	2.04716	1.95546
C	2.52464	-0.67544	-2.14080
O	2.27365	-0.01975	-3.18418
O	2.32703	-1.90261	-1.94946
N	1.03389	0.37165	0.06154
C	0.82304	1.48579	2.17379
C	0.28401	0.77751	1.06306
C	2.16862	1.74974	2.21195
H	2.60355	2.29253	3.04500
H	0.17143	1.81019	2.97633
C	-1.21080	0.44854	1.05727
C	-2.00988	1.08781	-0.07888
C	-1.58968	1.07944	-1.40611
C	-2.41607	1.67853	-2.36046
C	-3.61717	2.25086	-1.97810
C	-3.96246	2.21141	-0.61430
N	-3.17111	1.64603	0.30762
H	-2.11820	1.69545	-3.40333
H	-0.64547	0.62781	-1.66923
H	-4.27668	2.71852	-2.69957
C	-1.44829	-1.06493	1.14060
C	-2.06936	-1.61146	2.26345
C	-2.24532	-2.99853	2.30848
C	-1.79013	-3.78677	1.26579
C	-1.16324	-3.14513	0.17852
N	-1.02541	-1.81637	0.11965
H	-2.72854	-3.45863	3.16349
H	-2.40301	-0.97953	3.07668
H	-1.90110	-4.86453	1.28281
H	-1.63175	0.87312	1.96839
N	-5.17169	2.71777	-0.16619
H	-5.20942	2.90802	0.82547
H	-5.60257	3.43304	-0.73379
N	-0.68816	-3.85434	-0.91221
H	-0.49127	-4.83326	-0.76125
H	0.03224	-3.37096	-1.43627

L2chNHCH3_			
C	-2.71902	0.09359	0.93605
C	-3.14239	-0.86699	1.90643
C	-5.03932	0.55834	0.42979
H	-5.79268	1.10082	-0.13230
C	-3.70178	0.81319	0.19259
C	-5.45457	-0.39318	1.38833
H	-6.51396	-0.56424	1.54450
C	-4.52452	-1.09611	2.11854
H	-4.83204	-1.82788	2.85797
C	-3.29510	1.85181	-0.85068
O	-3.17652	3.03491	-0.44233
O	-3.15051	1.43401	-2.02749
N	-1.39478	0.34446	0.69828
C	-0.81353	-1.28113	2.36907
C	-0.48090	-0.31271	1.37876
C	-2.12993	-1.55288	2.62561
H	-2.41142	-2.28401	3.37655
H	-0.02365	-1.79011	2.90903
C	1.00051	-0.04807	1.10743
C	1.64948	-1.13846	0.25625
C	0.94071	-1.88966	-0.67173
C	1.63703	-2.85917	-1.40687
C	2.98844	-3.04053	-1.20077
C	3.63248	-2.22788	-0.23643
N	2.96634	-1.31026	0.47879
H	1.11501	-3.46663	-2.13828
H	-0.11677	-1.72703	-0.82816
H	3.55092	-3.78257	-1.75559
C	1.27659	1.35669	0.57307
C	1.41735	2.40972	1.47258
C	1.65241	3.69118	0.96050
C	1.75167	3.87613	-0.40387
C	1.61084	2.74587	-1.24287
N	1.37315	1.51905	-0.75472
H	1.76171	4.53627	1.63157
H	1.34326	2.23936	2.53959
H	1.94069	4.85494	-0.82950
H	1.50223	-0.10802	2.07771
N	4.98248	-2.34961	-0.02198
H	5.42292	-3.16866	-0.41007
N	1.74892	2.87594	-2.60379
H	1.70877	3.81756	-2.96096
C	1.39579	1.81468	-3.53424
H	1.59178	2.17062	-4.54577
H	2.00374	0.92681	-3.35380
H	0.34127	1.52489	-3.45872
C	5.66655	-1.70034	1.08477
H	5.27077	-2.00910	2.05944
H	6.72273	-1.96458	1.03412
H	5.57541	-0.61510	1.01216

L2chNHCOCH3_

C	0.76807	-3.25211	16.29990
C	2.12108	-3.00151	16.68649
C	1.53520	-4.93305	14.74235
H	1.33928	-5.66801	13.96831
C	0.48685	-4.21810	15.28541
C	2.87120	-4.71803	15.15940
H	3.66672	-5.30229	14.71017
C	3.16612	-3.76612	16.10727
H	4.19079	-3.58120	16.41193
C	-0.94423	-4.40661	14.77812
O	-1.33480	-3.59635	13.89178
O	-1.59407	-5.36365	15.26245
N	-0.27163	-2.56580	16.84503
C	1.27720	-1.22963	18.09426
C	-0.03575	-1.56947	17.66806
C	2.33995	-1.96190	17.62554
H	3.35156	-1.73951	17.94939
H	1.42873	-0.40800	18.78414
C	-1.22843	-0.72351	18.12866
C	-1.83846	0.05187	16.95446
C	-2.10890	1.41934	17.05485
C	-2.66069	2.06040	15.94600
C	-2.91042	1.35557	14.77234
C	-2.59180	-0.00948	14.76952
N	-2.09426	-0.62838	15.84004
H	-2.88717	3.11985	15.98993
H	-1.89440	1.96418	17.96599
H	-3.32220	1.82892	13.89534
C	-2.25918	-1.55080	18.89384
C	-3.15784	-2.40380	18.25712
C	-4.05150	-3.12835	19.04505
C	-4.02053	-2.99043	20.42361
C	-3.07792	-2.10721	20.97219
N	-2.22808	-1.40252	20.22920
H	-4.76556	-3.80176	18.58493
H	-3.14888	-2.49059	17.18078
H	-4.69814	-3.54573	21.06078
H	-0.85586	0.01128	18.84232
N	-2.71958	-0.87623	13.66865
N	-3.06094	-1.95626	22.37145
H	-3.82867	-2.40311	22.85774
C	-2.18207	-1.35284	23.24754
C	-3.27891	-0.62955	12.44511
O	-2.45431	-1.37843	24.44690
O	-3.79293	0.44380	12.13449
H	-2.30822	-1.80053	13.83133
C	-3.22559	-1.79466	11.47897
H	-4.24738	-2.06079	11.19773
H	-2.70879	-1.47172	10.57224
H	-2.72333	-2.66873	11.89269
C	-0.92676	-0.69883	22.73533
H	-1.17180	0.18393	22.14292
H	-0.32376	-0.41374	23.59600
H	-0.36863	-1.36910	22.08131

L2chNHCONH2_

C	0.61089	-3.13284	6.95675
C	1.86797	-3.66691	7.38489
C	0.45293	-4.91644	5.32727
H	-0.08398	-5.42181	4.53111
C	-0.09758	-3.78694	5.90225
C	1.69978	-5.43349	5.74555
H	2.09842	-6.31867	5.26259
C	2.39927	-4.82174	6.75835
H	3.35520	-5.21100	7.09198
C	-1.43946	-3.26783	5.38747
O	-1.39574	-2.33714	4.54854
O	-2.47012	-3.85402	5.81813
N	0.06739	-2.02159	7.54036
C	1.96631	-1.88966	9.00973
C	0.71360	-1.42847	8.52271
C	2.53465	-2.99888	8.44180
H	3.49218	-3.37315	8.78891
H	2.45883	-1.36157	9.81758
C	0.08028	-0.20760	9.19586
C	-0.62906	0.70796	8.19632
C	0.12876	1.37275	7.22615
C	-0.53115	2.18731	6.31590
C	-1.91202	2.34148	6.39783
C	-2.57644	1.67897	7.43362
N	-1.94798	0.87309	8.30074
H	0.02037	2.69321	5.53191
H	1.20225	1.23833	7.17878
H	-2.44737	2.92591	5.66328
C	-0.79990	-0.61696	10.37285
C	-0.75621	0.07003	11.58086
C	-1.60521	-0.34976	12.61060
C	-2.45749	-1.42169	12.41197
C	-2.42691	-2.06023	11.15811
N	-1.61061	-1.66505	10.18265
H	-1.59793	0.16312	13.56558
H	-0.08525	0.90841	11.71872
H	-3.12640	-1.76365	13.19228
H	0.90365	0.38084	9.61124
N	-3.96652	1.73944	7.63286
N	-3.27381	-3.14397	10.92011
H	-3.89122	-3.40743	11.67432
C	-3.51753	-3.88447	9.75013
C	-4.89837	2.73750	7.39816
O	-4.41140	-4.73973	9.77661
O	-6.09054	2.52186	7.61814
N	-4.44833	3.92740	6.90168
H	-3.49136	4.21367	7.04575
H	-5.13220	4.66932	6.89849
N	-2.74052	-3.61300	8.69094
H	-2.06774	-2.85221	8.76395
H	-2.91078	-4.02657	7.77884
H	-4.33501	0.98228	8.19307

L3chH_			
C	-1.70145	-0.67358	0.39901
C	-1.95225	-1.92434	1.05755
C	-4.11113	-0.56552	-0.17230
C	-2.80499	0.03574	-0.23652
C	-4.29880	-1.82046	0.50364
H	-5.30101	-2.23679	0.52863
C	-3.27078	-2.47565	1.09465
H	-3.42626	-3.42269	1.60186
N	-0.43350	-0.17077	0.37681
C	0.38721	-2.05352	1.62560
C	0.56014	-0.82922	0.95134
C	-0.87811	-2.59351	1.66924
H	-1.06340	-3.53474	2.17758
H	1.22869	-2.55072	2.09416
C	1.97813	-0.25029	0.88800
C	2.01189	1.27181	0.76994
C	1.74979	2.04744	1.90710
C	1.78825	3.43202	1.80928
C	2.09303	4.00941	0.57720
C	2.34689	3.16239	-0.49544
N	2.31212	1.82473	-0.40993
H	1.59064	4.05028	2.67766
H	1.52132	1.56620	2.85115
H	2.13886	5.08421	0.45119
H	2.59422	3.57195	-1.47081
C	2.84801	-0.94460	-0.15924
C	4.22305	-1.07679	0.07206
C	5.01755	-1.69994	-0.88284
C	4.41657	-2.18070	-2.04441
C	3.04247	-2.01445	-2.18546
N	2.26916	-1.41515	-1.27037
H	6.08365	-1.81348	-0.72189
H	4.65831	-0.69588	0.98888
H	4.99162	-2.67670	-2.81674
H	2.53475	-2.38234	-3.07278
H	2.43613	-0.48226	1.85538
C	-5.10196	1.25158	-1.42283
C	-3.86383	1.86810	-1.50852
C	-5.24089	0.03831	-0.75898
C	-2.66189	1.32639	-0.94038
H	-3.75898	2.81634	-2.02749
H	-5.96939	1.72247	-1.87820
H	-6.20401	-0.45414	-0.68483
O	-1.56887	1.96539	-1.06692

L3chNH2_			
C	-1.91582	-0.13090	0.27436
C	-2.59964	-1.16377	1.00112
C	-4.11749	0.73896	-0.45008
C	-2.68297	0.85111	-0.48678
C	-4.74549	-0.31908	0.29619
H	-5.83001	-0.36596	0.28877
C	-4.02751	-1.23468	0.98991
H	-4.51732	-2.02718	1.54710
N	-0.55924	-0.07797	0.31297
C	-0.45953	-2.00239	1.74151
C	0.14175	-0.96119	1.00800
C	-1.83536	-2.09302	1.72732
H	-2.34426	-2.87667	2.28024
H	0.14443	-2.70769	2.30035
C	1.67610	-0.86231	1.01649
C	2.15128	0.57405	1.21329
C	2.65847	0.99999	2.44283
C	3.00190	2.34847	2.57799
C	2.77831	3.22688	1.52835
C	2.23069	2.70696	0.33937
N	2.00244	1.40005	0.17757
H	3.41721	2.71472	3.51078
H	2.77987	0.30591	3.26529
H	2.99160	4.28536	1.62381
C	2.34197	-1.52115	-0.19100
C	1.75438	-1.56875	-1.45158
C	2.46129	-2.18688	-2.48695
C	3.71246	-2.72648	-2.24540
C	4.23048	-2.63260	-0.93924
N	3.55401	-2.04877	0.05860
H	2.03129	-2.24399	-3.48110
H	0.78004	-1.13206	-1.61661
H	4.28230	-3.20940	-3.03038
H	2.02221	-1.43204	1.88106
C	-4.39377	2.67932	-1.86481
C	-3.01701	2.82172	-1.93665
C	-4.95695	1.64266	-1.13057
C	-2.08570	1.94415	-1.28672
H	-2.58114	3.62914	-2.51780
H	-5.03486	3.38281	-2.38973
H	-6.03210	1.51589	-1.07071
O	-0.83574	2.14761	-1.43401
N	1.89091	3.50423	-0.74672
H	1.81760	4.49115	-0.53919
H	1.06062	3.14327	-1.21819
N	5.49747	-3.10313	-0.63680
H	5.67013	-3.25406	0.34723
H	5.86815	-3.82958	-1.23186

L3chNHCH3_

C	1.21194	-3.38037	6.51792
C	2.42339	-2.96516	5.86984
C	1.01316	-5.19828	4.84629
C	0.47721	-4.52985	6.00292
C	2.23026	-4.73235	4.23842
H	2.59714	-5.26679	3.36764
C	2.91081	-3.66588	4.72324
H	3.82948	-3.32641	4.25496
N	0.76791	-2.69305	7.60744
C	2.64301	-1.19747	7.49608
C	1.44102	-1.65367	8.07248
C	3.12246	-1.86128	6.38957
H	4.04427	-1.54753	5.90925
H	3.16920	-0.34755	7.91521
C	0.90306	-0.89388	9.29012
C	0.05033	-1.75183	10.22580
C	0.68693	-2.66572	11.07233
C	-0.10216	-3.43519	11.92346
C	-1.48130	-3.27820	11.92456
C	-2.03590	-2.32280	11.05009
N	-1.27253	-1.58307	10.22018
H	0.35726	-4.15734	12.58994
H	1.76483	-2.77057	11.05929
H	-2.10728	-3.86680	12.58127
C	0.22657	0.42204	8.90597
C	0.33180	1.51965	9.76548
C	-0.31296	2.70192	9.40563
C	-1.02401	2.77095	8.21686
C	-1.05836	1.62156	7.40038
N	-0.44476	0.47503	7.75362
H	-0.25849	3.57212	10.05101
H	0.89592	1.44629	10.68706
H	-1.52686	3.68210	7.92269
H	1.78433	-0.61228	9.87590
C	-0.79415	-6.80436	4.83148
C	-1.34646	-6.19313	5.94614
C	0.38144	-6.31873	4.27126
C	-0.77493	-5.04674	6.59434
H	-2.26485	-6.57654	6.38133
H	-1.28581	-7.66964	4.39431
H	0.82396	-6.78790	3.39966
O	-1.35823	-4.55197	7.61229
N	-1.69416	1.60546	6.18418
H	-1.81087	0.68351	5.79101
N	-3.38314	-2.06063	11.00666
H	-3.67096	-1.51486	10.20819
C	-2.61155	2.64258	5.74513
H	-3.01712	2.35570	4.77568
H	-3.44707	2.78958	6.44150
H	-2.09482	3.59863	5.62220
C	-4.38295	-2.90814	11.63262
H	-4.27163	-2.90815	12.72061
H	-5.36894	-2.50852	11.39836
H	-4.33638	-3.94701	11.28160

L3chNHCOCH3_

C	1.02715	-3.83710	6.35503
C	-0.12829	-3.93713	5.50955
C	2.34397	-4.98939	4.60429
C	2.30686	-4.35821	5.89608
C	1.15159	-5.06736	3.80322
H	1.22585	-5.54699	2.83218
C	-0.03250	-4.56207	4.22664
H	-0.92231	-4.62557	3.60814
N	0.90617	-3.26617	7.58413
C	-1.42972	-2.83519	7.22077
C	-0.26018	-2.78746	7.99716
C	-1.34875	-3.41889	5.97405
H	-2.22575	-3.48630	5.33762
H	-2.35903	-2.42524	7.59262
C	-0.24308	-2.17164	9.39910
C	-1.50641	-2.48358	10.19787
C	-1.56230	-3.62985	10.99475
C	-2.72840	-3.88295	11.70919
C	-3.80519	-3.00948	11.61076
C	-3.67036	-1.90676	10.76140
N	-2.54368	-1.64641	10.08802
H	-2.79631	-4.74696	12.35997
H	-0.70911	-4.29272	11.06488
H	-4.69449	-3.17089	12.19969
C	0.07801	-0.67760	9.40125
C	0.64987	-0.10060	10.53966
C	0.95292	1.25499	10.51446
C	0.67807	2.00573	9.37591
C	0.07665	1.34957	8.29928
N	-0.20022	0.03950	8.31096
H	1.42330	1.72831	11.36856
H	0.86686	-0.70457	11.41206
H	0.95536	3.04717	9.32756
H	0.58360	-2.66447	9.91482
C	4.70130	-5.47792	4.82365
C	4.71359	-4.86826	6.06861
C	3.52865	-5.54212	4.07954
C	3.55794	-4.27146	6.67537
H	5.63421	-4.81499	6.64230
H	5.61848	-5.90491	4.42628
H	3.50869	-6.00927	3.10126
O	3.66661	-3.71162	7.81444
N	-0.24274	1.96398	7.07131
H	-0.35636	1.29737	6.31569
N	-4.66190	-0.92420	10.57107
H	-4.29113	-0.05718	10.19816
C	-0.59920	3.24520	6.71952
O	-0.85112	3.48476	5.54043
C	-6.03761	-0.94675	10.61657
O	-6.65153	0.08967	10.37391
C	-0.69254	4.31761	7.77650
H	0.29868	4.73064	7.98240
H	-1.31801	5.11759	7.38437
H	-1.11032	3.94690	8.71292
C	-6.75933	-2.23132	10.93961
H	-6.28331	-3.10287	10.48948
H	-6.79640	-2.38084	12.02206
H	-7.78096	-2.13949	10.57529

L3chNHCONH2_

C	0.95141	-3.35091	6.69711
C	1.94783	-2.91077	5.76542
C	0.42662	-5.22526	5.16744
C	0.19288	-4.56693	6.42440
C	1.42784	-4.72653	4.26362
H	1.58070	-5.26394	3.33295
C	2.17138	-3.63005	4.55033
H	2.93144	-3.27274	3.86265
N	0.70912	-2.61284	7.81455
C	2.43248	-1.04931	7.22452
C	1.40173	-1.51510	8.06404
C	2.68811	-1.75289	6.06918
H	3.45899	-1.42404	5.37910
H	2.99438	-0.15750	7.47735
C	1.07863	-0.71641	9.33626
C	0.29905	-1.56214	10.33430
C	0.98346	-2.37174	11.24280
C	0.25046	-3.23743	12.04993
C	-1.13166	-3.27579	11.92444
C	-1.72625	-2.41669	10.99661
N	-1.03534	-1.56265	10.24342
H	0.75073	-3.87322	12.77153
H	2.06444	-2.33475	11.30296
H	-1.73968	-3.93267	12.53192
C	0.39954	0.62009	9.04552
C	0.54891	1.67937	9.94589
C	-0.06327	2.89176	9.65016
C	-0.81103	3.02389	8.48512
C	-0.93253	1.89849	7.66215
N	-0.32913	0.73455	7.93204
H	0.05800	3.74336	10.30963
H	1.14494	1.55878	10.84211
H	-1.24029	3.97646	8.20986
H	2.03888	-0.47681	9.80435
C	-1.26065	-6.89179	5.63547
C	-1.49286	-6.30865	6.87328
C	-0.29755	-6.37143	4.78154
C	-0.78133	-5.16485	7.35529
H	-2.22786	-6.73629	7.54860
H	-1.82963	-7.76957	5.34083
H	-0.09003	-6.83172	3.82204
O	-1.00324	-4.74037	8.54167
N	-1.63344	1.89353	6.44391
H	-1.38088	1.13081	5.82951
N	-3.13443	-2.38413	10.84750
H	-3.54629	-1.47024	10.71835
C	-2.72558	2.61335	5.98783
O	-3.10487	2.47310	4.82488
N	-3.32751	3.47925	6.85607
H	-4.20628	3.85548	6.53261
H	-3.25602	3.33364	7.85224
C	-3.96723	-3.42793	10.46682
N	-3.36630	-4.60147	10.12353
H	-2.45610	-4.61788	9.63175
H	-4.02282	-5.29984	9.80534
O	-5.19328	-3.26742	10.47858

L4chH_

C	-2.84057	1.86870	3.42346
C	-1.56258	2.37199	3.03261
N	-1.09866	1.79472	1.92687
C	-2.07695	0.88351	1.53414
C	-3.17611	0.93327	2.46223
C	-1.99779	0.03229	0.40560
C	-0.84334	-0.29095	-0.34326
N	0.46771	-0.06907	0.06779
C	1.24633	-0.49737	-0.91994
C	0.48742	-1.00834	-2.02321
C	-0.83633	-0.89081	-1.65250
C	-3.27895	-0.59340	-0.04683
C	2.76164	-0.43084	-0.87152
C	3.33143	0.89463	-1.37063
N	4.52104	0.81855	-1.98863
C	5.07595	1.94976	-2.44381
C	4.48429	3.20253	-2.31415
C	3.24785	3.27844	-1.67620
C	2.66296	2.11045	-1.19943
C	-3.41345	-1.98582	-0.13669
C	-4.60913	-2.56621	-0.55457
C	-5.70870	-1.77994	-0.91816
C	-5.56933	-0.38866	-0.84118
C	-4.38296	0.19443	-0.40244
C	-7.00921	-2.41018	-1.35371
C	3.30899	-0.82017	0.50225
N	3.71157	0.14361	1.33801
C	4.16634	-0.21237	2.54886
C	4.24917	-1.52961	2.98418
C	3.84032	-2.53508	2.10788
C	3.36653	-2.17617	0.85324
H	-3.41745	2.16495	4.28912
H	-0.99590	3.15114	3.53233
H	-4.06762	0.32501	2.42605
H	0.88448	-1.40661	-2.94756
H	-1.70377	-1.16397	-2.23476
H	6.03725	1.84566	-2.93937
H	4.97675	4.08488	-2.70442
H	2.74769	4.23251	-1.55205
H	1.70378	2.12607	-0.69903
H	-2.57665	-2.61891	0.13497
H	-4.68647	-3.64796	-0.60222
H	-6.39942	0.24853	-1.12999
H	-4.30239	1.27421	-0.35259
H	-6.84520	-3.39341	-1.80017
H	-7.68223	-2.54637	-0.49999
H	-7.53063	-1.78434	-2.08165
H	4.48193	0.60010	3.19754
H	4.62709	-1.75875	3.97307
H	3.89457	-3.57845	2.39763
H	3.04144	-2.93134	0.14679
H	3.13327	-1.18326	-1.57330

L4chNH2_			
C	-3.93765	-3.95670	0.68650
C	-2.70355	-3.96069	1.37078
N	-2.06819	-2.77194	1.28477
C	-2.88992	-1.95021	0.53659
C	-4.06474	-2.66252	0.16093
C	-2.61189	-0.56512	0.19658
C	-1.35990	0.04252	0.08847
N	-0.12617	-0.59622	0.08965
C	0.83314	0.35270	-0.00878
C	0.20212	1.67944	-0.06035
C	-1.14169	1.48242	-0.01826
C	-3.81318	0.27501	-0.09598
C	2.24528	0.13873	-0.12459
C	3.12136	1.33530	-0.07936
N	3.00404	2.17783	0.97499
C	3.74165	3.29544	1.02281
C	4.66817	3.64253	0.02899
C	4.80325	2.77354	-1.05059
C	4.03392	1.61933	-1.11336
C	-3.95686	0.95669	-1.31346
C	-5.08143	1.73962	-1.58262
C	-6.11039	1.87656	-0.64707
C	-5.97298	1.19472	0.57159
C	-4.85827	0.40568	0.83578
C	-7.33750	2.70697	-0.93870
C	2.86697	-1.15118	-0.30856
N	4.23445	-1.22390	-0.19270
C	4.86478	-2.38123	-0.37190
C	4.21088	-3.59058	-0.66334
C	2.81892	-3.53868	-0.75590
C	2.13716	-2.34552	-0.58100
N	3.50500	4.13940	2.10914
N	6.26572	-2.33744	-0.30003
H	-4.63607	-4.77891	0.59286
H	-2.26785	-4.78159	1.93196
H	-4.88417	-2.27915	-0.43143
H	0.71615	2.62616	-0.12625
H	-1.90816	2.24357	-0.02791
H	5.24959	4.55410	0.10335
H	5.50263	3.00732	-1.84711
H	4.12212	0.94078	-1.95099
H	-3.18002	0.86420	-2.06413
H	-5.15860	2.24704	-2.53971
H	-6.75002	1.28729	1.32500
H	-4.78211	-0.10986	1.78663
H	-7.59080	3.35360	-0.09374
H	-7.19008	3.33837	-1.81741
H	-8.20945	2.07183	-1.12961
H	4.76536	-4.51157	-0.79926
H	2.26219	-4.44673	-0.97016
H	1.06075	-2.29296	-0.62804
H	4.27549	4.73591	2.37718
H	3.08109	3.67156	2.89916
H	6.70508	-3.20075	-0.00982
H	6.60899	-1.54239	0.22306

L4chNHCH3_			
C	-3.63793	3.32928	1.98576
C	-2.41023	3.65837	1.33660
N	-1.96234	2.67680	0.55645
C	-2.90064	1.65302	0.65490
C	-3.95899	2.05921	1.54129
C	-2.81780	0.40048	-0.00307
C	-1.68208	-0.17645	-0.61324
N	-0.36682	0.24869	-0.43652
C	0.38841	-0.55244	-1.17878
C	-0.39364	-1.52271	-1.89069
C	-1.70199	-1.29556	-1.52063
C	-4.07800	-0.40501	-0.04901
C	1.90328	-0.47946	-1.23023
C	2.41960	0.95879	-1.31142
N	2.78293	1.57107	-0.17384
C	3.20655	2.84353	-0.22733
C	3.30239	3.55623	-1.44479
C	2.93913	2.90757	-2.60893
C	2.48810	1.58452	-2.55468
C	-4.13126	-1.69870	0.48765
C	-5.30878	-2.44297	0.45354
C	-6.47223	-1.93239	-0.13361
C	-6.41447	-0.64546	-0.68296
C	-5.24517	0.10936	-0.63151
C	-7.75358	-2.72992	-0.15148
C	2.60295	-1.29133	-0.13989
N	3.82582	-1.73466	-0.46442
C	4.52643	-2.45597	0.43081
C	4.00472	-2.77923	1.70054
C	2.73633	-2.31729	2.01728
C	2.01271	-1.56156	1.09441
H	-4.19370	3.94936	2.67614
H	-1.86793	4.59502	1.41755
H	-4.81477	1.46593	1.82703
H	-0.01887	-2.27359	-2.57382
H	-2.57978	-1.81906	-1.86925
H	3.65515	4.58112	-1.45493
H	3.00906	3.42283	-3.56097
H	2.19947	1.05492	-3.45422
H	-3.24404	-2.11963	0.94637
H	-5.32151	-3.43753	0.88841
H	-7.29652	-0.22743	-1.15815
H	-5.22905	1.10346	-1.06317
H	-7.55529	-3.80347	-0.11887
H	-8.37772	-2.48586	0.71533
H	-8.34307	-2.51599	-1.04611
H	4.57356	-3.37067	2.40511
H	2.30789	-2.54969	2.98659
H	1.02344	-1.18751	1.31747
H	2.19888	-0.95701	-2.16905
N	3.52957	3.45897	0.95878
H	4.04449	4.32185	0.88057
N	5.78597	-2.83907	0.03589
H	5.95711	-2.72682	-0.95235
C	6.57057	-3.84240	0.73526
H	6.04655	-4.80279	0.82470
H	7.49499	-4.00368	0.18182
H	6.83755	-3.50226	1.73966
C	3.67337	2.72997	2.20907
H	4.45335	1.96095	2.15958
H	3.93266	3.44380	2.99113

H 2.73577 2.24231 2.47998

L4chNHCOCH3_

C	-3.80380	2.96791	-2.52463
C	-2.43465	2.60203	-2.70446
N	-2.09678	1.51773	-2.01180
C	-3.25420	1.11401	-1.34844
C	-4.33052	2.01275	-1.67593
C	-3.34921	0.00055	-0.48163
C	-2.27945	-0.70259	0.12114
N	-0.97596	-0.23190	0.24071
C	-0.28378	-1.20005	0.83399
C	-1.09427	-2.34523	1.12136
C	-2.36403	-2.02389	0.68483
C	-4.72630	-0.48921	-0.16961
C	1.19079	-1.08286	1.17075
C	2.13197	-1.32937	-0.00666
N	3.37370	-1.70751	0.33109
C	4.26457	-1.96648	-0.63060
C	3.95062	-1.89857	-1.99155
C	2.66734	-1.49032	-2.33395
C	1.74139	-1.19318	-1.33829
C	-5.17132	-0.59757	1.15640
C	-6.45743	-1.04433	1.44782
C	-7.34267	-1.42010	0.42962
C	-6.89285	-1.32735	-0.89261
C	-5.61435	-0.85945	-1.18914
C	-8.74275	-1.88472	0.74867
C	1.50100	0.22245	1.90386
N	1.98677	1.25332	1.19866
C	2.22783	2.40211	1.82762
C	2.00769	2.58608	3.20085
C	1.52088	1.51006	3.92721
C	1.26133	0.30649	3.27669
H	-4.31266	3.81387	-2.96655
H	-1.71148	3.10371	-3.33943
H	-5.33962	1.96407	-1.29453
H	-0.76638	-3.26383	1.58971
H	-3.24468	-2.64788	0.72003
H	4.65943	-2.18093	-2.75459
H	2.38779	-1.42222	-3.37916
H	0.73681	-0.87378	-1.57669
H	-4.50541	-0.31566	1.96373
H	-6.77742	-1.10455	2.48345
H	-7.55060	-1.62589	-1.70285
H	-5.29193	-0.79853	-2.22211
H	-8.76897	-2.46511	1.67408
H	-9.41597	-1.03072	0.88204
H	-9.15075	-2.50070	-0.05546
H	2.21636	3.53728	3.67524
H	1.34663	1.60878	4.99252
H	0.88312	-0.55072	3.81980
H	1.41072	-1.88516	1.88113
N	2.75556	3.48840	1.10403
H	3.06825	4.26660	1.67162
N	5.51809	-2.37990	-0.13084
H	5.47477	-2.71163	0.82630
C	6.80389	-2.25117	-0.60089
C	2.90892	3.74341	-0.24331
O	7.72936	-2.69119	0.07871
O	3.43939	4.80363	-0.57299
C	2.41893	2.75108	-1.26185
H	2.97895	1.81841	-1.19231
H	1.37300	2.49540	-1.08807

H	2.54306	3.19400	-2.24880
C	7.05638	-1.56211	-1.91955
H	8.09172	-1.22576	-1.92613
H	6.92340	-2.26725	-2.74449
H	6.39060	-0.71453	-2.08350

	L4chNHCONH2_		
C	4.44965	-0.08498	3.85430
C	3.12657	-0.61637	3.93401
N	2.57417	-0.80221	2.73763
C	3.53400	-0.40600	1.80917
C	4.71587	0.03506	2.50305
C	3.36856	-0.42286	0.40354
C	2.15756	-0.54135	-0.31561
N	0.88376	-0.37809	0.22270
C	0.02952	-0.58035	-0.77391
C	0.69569	-0.89431	-2.00286
C	2.04481	-0.85744	-1.71600
C	4.61791	-0.30503	-0.41087
C	-1.47534	-0.49536	-0.60658
C	-2.11793	-1.79755	-0.13034
N	-3.41645	-1.94130	-0.46263
C	-4.06933	-3.04180	-0.08858
C	-3.45523	-4.07182	0.64702
C	-2.12342	-3.91810	0.98409
C	-1.43327	-2.76646	0.59254
C	4.78330	0.72852	-1.34371
C	5.95306	0.83941	-2.09179
C	6.99336	-0.08767	-1.95348
C	6.82129	-1.12804	-1.03280
C	5.66195	-1.22920	-0.26694
C	8.26767	0.04649	-2.75120
C	-1.89246	0.70069	0.24744
N	-2.05773	1.84995	-0.42119
C	-2.39607	2.95742	0.25118
C	-2.59141	2.97658	1.63785
C	-2.42250	1.77713	2.31843
C	-2.07234	0.61988	1.62842
H	5.09938	0.16524	4.68203
H	2.58962	-0.87655	4.84062
H	5.61639	0.41901	2.04731
H	0.22504	-1.10891	-2.95311
H	2.86121	-1.05334	-2.39509
H	-4.01318	-4.95531	0.93254
H	-1.61712	-4.69186	1.54989
H	-0.39145	-2.62148	0.84183
H	3.99239	1.45822	-1.47353
H	6.05722	1.65835	-2.79682
H	7.60398	-1.87064	-0.91305
H	5.55535	-2.04458	0.43918
H	8.07644	0.47151	-3.73927
H	8.97788	0.70881	-2.24393
H	8.75874	-0.92027	-2.88174
H	-2.86598	3.88992	2.14011
H	-2.56495	1.74836	3.39299
H	-1.93684	-0.31894	2.14827
H	-1.89646	-0.30523	-1.59696
N	-5.41471	-3.18782	-0.43988
H	-5.86562	-4.03784	-0.13342
N	-2.52606	4.07763	-0.58265
H	-2.33568	3.86337	-1.55261
N	-2.99864	6.20691	-1.33597
H	-3.10978	7.18394	-1.11256
H	-2.50320	6.00407	-2.19118
N	-5.78444	-1.19988	-1.61856
H	-4.81574	-0.96053	-1.42430
H	-6.40243	-0.58663	-2.12437
C	-6.28520	-2.36299	-1.15529

C	-2.93476	5.35803	-0.26056
O	-3.25281	5.71065	0.87265
O	-7.45014	-2.73366	-1.32790

L5chH_			
C	0.12545	-1.16162	-1.11150
C	-0.16516	-0.43401	0.03444
N	1.01720	-0.02122	0.59691
C	1.97495	-0.50723	-0.23475
N	1.48587	-1.20992	-1.28393
C	3.42328	-0.35068	0.06166
C	3.87888	-0.73699	1.32828
C	5.21499	-0.63233	1.72992
C	6.13872	-0.11924	0.81315
C	5.72486	0.28417	-0.45058
C	4.36048	0.21250	-0.89418
O	4.02274	0.65159	-2.05880
C	-1.49238	-0.06989	0.65988
C	-1.94989	1.36868	0.41322
N	-2.82120	1.86464	1.30810
C	-3.26704	3.11609	1.13978
C	-2.87582	3.93680	0.08576
C	-1.96888	3.42337	-0.83892
C	-1.49810	2.12541	-0.67115
C	-2.58072	-1.06680	0.27267
N	-3.23250	-0.87367	-0.88301
C	-4.16109	-1.76881	-1.24850
C	-4.49405	-2.88710	-0.49195
C	-3.82439	-3.08290	0.71540
C	-2.85749	-2.16255	1.10116
H	-0.55385	-1.64489	-1.80162
H	3.14931	-1.14383	2.02328
H	5.52307	-0.95086	2.72002
H	7.18723	-0.02993	1.08752
H	6.44681	0.69822	-1.15048
H	-3.96771	3.47974	1.88666
H	-3.26681	4.94335	-0.00064
H	-1.63255	4.02572	-1.67569
H	-0.78824	1.69030	-1.36277
H	-4.66460	-1.57671	-2.19212
H	-5.25649	-3.57552	-0.83567
H	-4.05423	-3.93554	1.34457
H	-2.31705	-2.28479	2.03263
H	-1.37192	-0.14816	1.74544

L5chNH2_

C	-0.08256	0.03630	1.11949
C	-0.68227	0.12999	2.36693
C	-2.21619	0.18687	0.86466
C	-3.56757	0.19358	0.23758
C	-4.41214	-0.89667	0.47029
C	-5.70352	-0.99331	-0.06145
C	-6.16204	0.05497	-0.86629
C	-5.35494	1.15886	-1.11433
C	-4.03185	1.30112	-0.57490
C	1.39552	-0.08799	0.82325
C	2.06869	1.18400	0.30489
N	3.40373	1.23087	0.47915
C	4.08044	2.30873	0.06512
C	3.44834	3.40205	-0.55875
C	2.07699	3.34292	-0.73513
C	1.36356	2.22309	-0.29659
C	1.69778	-1.29847	-0.06302
N	1.83108	-2.46874	0.58534
C	2.05648	-3.58641	-0.11801
C	2.16048	-3.58729	-1.52148
C	2.02743	-2.37638	-2.18019
C	1.79769	-1.20806	-1.45094
H	-4.03595	-1.70594	1.09140
H	-6.32399	-1.85980	0.14042
H	-7.15810	0.01210	-1.30064
H	-5.72583	1.97395	-1.73115
H	4.02528	4.26032	-0.88242
H	1.55820	4.16718	-1.21300
H	0.29194	2.14620	-0.41552
H	2.34401	-4.50916	-2.06059
H	2.10139	-2.33854	-3.26180
H	1.69147	-0.25370	-1.94901
H	-0.21419	0.13374	3.34470
H	1.88468	-0.30595	1.77703
N	2.24389	-4.74967	0.61351
H	1.86561	-4.72225	1.55021
H	2.06725	-5.61936	0.13186
N	5.44108	2.32772	0.33148
H	5.84878	1.41948	0.50498
H	6.00959	2.92157	-0.25483
O	-3.33429	2.36337	-0.79914
N	-1.06425	0.06914	0.16112
N	-2.04379	0.22580	2.20865

L5chNHCH3_

C	-0.25013	-1.02427	1.44506
C	0.40536	-0.66263	0.27351
N	-0.27669	-1.18044	-0.79612
C	-1.32035	-1.83102	-0.24236
N	-1.34980	-1.76805	1.11645
C	-2.35236	-2.55978	-0.98722
C	-2.33407	-2.64759	-2.38900
C	-3.31647	-3.33674	-3.09506
C	-4.35519	-3.96273	-2.40069
C	-4.40007	-3.89409	-1.01002
C	-3.41419	-3.20336	-0.29824
O	-3.50223	-3.16636	1.05748
C	1.65308	0.16477	0.06321
C	1.40059	1.63933	-0.26347
N	2.44079	2.27320	-0.84122
C	2.31889	3.56798	-1.16213
C	1.13425	4.29844	-0.90447
C	0.07810	3.63536	-0.31391
C	0.19887	2.27793	0.01316
C	2.63480	0.01049	1.22372
N	2.41889	0.74668	2.31908
C	3.24037	0.61036	3.37839
C	4.33768	-0.27533	3.36570
C	4.55226	-1.02645	2.21949
C	3.69702	-0.89303	1.12645
H	0.00402	-0.79797	2.47002
H	-1.52494	-2.15910	-2.91922
H	-3.27319	-3.38550	-4.17740
H	-5.12760	-4.50258	-2.93762
H	-5.19802	-4.37385	-0.45347
H	-2.70791	-2.63178	1.38564
H	1.06654	5.34613	-1.17416
H	-0.84442	4.16658	-0.10445
H	-0.61499	1.73455	0.47313
H	4.99571	-0.36375	4.21944
H	5.39139	-1.71261	2.17581
H	3.84794	-1.46895	0.22205
H	2.15193	-0.24430	-0.82055
N	3.38026	4.17661	-1.79086
H	3.35210	5.18371	-1.82129
N	2.92708	1.37365	4.47584
H	2.25027	2.09943	4.29286
C	4.69739	3.56481	-1.87114
H	5.35864	4.24888	-2.40324
H	5.12450	3.35617	-0.88286
H	4.65235	2.62469	-2.42329
C	3.82409	1.56427	5.60241
H	4.79681	1.97557	5.30331
H	3.35678	2.25717	6.30122
H	3.99740	0.62248	6.13060

L5chNHCOCH3_

C	0.09134	0.28393	1.09339
C	-0.51378	0.90823	2.17657
N	-1.87512	0.88872	2.00477
C	-2.04277	0.24721	0.82020
N	-0.88616	-0.14296	0.23406
C	-3.39086	-0.06577	0.27597
C	-4.26879	-0.80876	1.07305
C	-5.56191	-1.16033	0.66932
C	-5.98894	-0.74839	-0.59749
C	-5.15022	0.00023	-1.41455
C	-3.82603	0.40013	-1.02788
O	-3.10738	1.14312	-1.79965
C	2.30351	1.14587	0.07183
N	1.64101	1.83271	-0.86148
C	2.28548	2.77304	-1.56319
C	3.63443	3.08720	-1.37425
C	4.31716	2.37180	-0.39483
C	3.65607	1.39481	0.33911
C	1.87013	-1.33399	0.35439
N	2.10022	-1.49587	-0.95094
C	2.32689	-2.72802	-1.42721
C	2.34996	-3.86971	-0.62312
C	2.12104	-3.68905	0.73923
C	1.87807	-2.41775	1.24150
H	-3.91506	-1.12939	2.04950
H	-6.20691	-1.74326	1.31798
H	-6.98436	-1.01013	-0.94868
H	-5.49813	0.32913	-2.39103
H	4.10855	3.85573	-1.96300
H	5.36339	2.58519	-0.20585
H	4.17243	0.83284	1.10833
H	2.54271	-4.83974	-1.05174
H	2.13730	-4.54617	1.40315
H	1.69462	-2.25790	2.29701
H	-0.04915	1.36202	3.04462
N	2.53802	-2.73835	-2.81982
H	2.46880	-1.81691	-3.23043
N	1.45219	3.40771	-2.50540
H	0.50626	3.05047	-2.48735
C	2.97654	-3.41288	-5.11612
H	3.99034	-3.67185	-5.43020
H	2.28294	-4.01216	-5.70930
H	2.80064	-2.35677	-5.32037
C	0.57053	4.84403	-4.25976
H	0.35713	5.89306	-4.04116
H	0.86287	4.77732	-5.30948
H	-0.33520	4.25842	-4.10231
C	1.73876	4.40147	-3.40357
C	2.81222	-3.78721	-3.65786
O	2.84950	4.91168	-3.51859
O	2.92390	-4.94839	-3.27583
C	1.57414	0.07063	0.88072
H	2.02636	0.10973	1.87779

L5chNHCONH2_

C	-0.21341	-0.47524	0.17580
C	-1.09719	-0.31309	1.23330
N	-2.27638	0.21557	0.76243
C	-2.05441	0.34858	-0.56971
N	-0.84225	-0.07912	-0.97786
C	-3.02000	1.01819	-1.49070
C	-4.09427	0.29165	-2.01279
C	-5.04112	0.84480	-2.88193
C	-4.89952	2.18829	-3.23966
C	-3.84679	2.94463	-2.73704
C	-2.86456	2.41499	-1.84306
O	-1.91388	3.18211	-1.38878
C	2.02998	0.66225	0.11425
N	1.27176	1.71067	-0.17233
C	1.79591	2.92152	-0.37146
C	3.16762	3.16719	-0.23093
C	3.96663	2.07369	0.10713
C	3.41520	0.80287	0.27466
C	1.80693	-1.74120	-0.70088
N	1.94990	-2.97710	-0.20054
C	2.36655	-3.96763	-1.00065
C	2.67030	-3.77893	-2.35352
C	2.52582	-2.49198	-2.86124
C	2.09422	-1.45662	-2.03923
H	-4.18759	-0.75348	-1.72729
H	-5.85858	0.24484	-3.26674
H	-5.61551	2.65084	-3.91428
H	-3.74907	3.99063	-3.01616
H	3.57722	4.15430	-0.38448
H	5.03460	2.21796	0.23228
H	4.04150	-0.04722	0.51883
H	3.00448	-4.60366	-2.96187
H	2.75321	-2.30154	-3.90441
H	1.97831	-0.45152	-2.42099
H	-0.93921	-0.51536	2.28674
N	2.46915	-5.19567	-0.32822
H	2.18522	-5.13120	0.64040
N	0.80038	3.83141	-0.73344
H	-0.12152	3.38573	-0.85076
C	0.90864	5.13287	-1.16791
C	2.87458	-6.42305	-0.81414
O	1.96128	5.77904	-1.18382
O	3.20735	-6.62305	-1.98025
N	2.83296	-7.43067	0.11665
H	2.82190	-7.22705	1.10482
H	3.29393	-8.28691	-0.15036
N	-0.30160	5.64520	-1.55153
H	-0.28937	6.52220	-2.04672
H	-1.08689	5.00381	-1.68606
C	1.28546	-0.68308	0.26444
H	1.50486	-1.06581	1.26664

Table S3. B3LYP/6-311++G(d,p) optimized geometry coordinates (Å) for the Be²⁺ complexes of **L1-L5** with their corresponding buttress groups.

L1chH_Be

C	-1.699750	-0.001090	-1.301120
C	-0.892060	-0.002570	-3.582520
C	0.430050	-0.001940	-3.123420
H	-1.092740	-0.003380	-4.647250
C	0.623660	-0.001000	-1.756720
H	1.268690	-0.002220	-3.806400
C	1.991530	-0.000260	-1.074700
H	2.777940	-0.000460	-1.824960
C	3.102170	2.204320	-0.353800
C	3.119570	3.290750	0.519210
H	3.837590	2.107130	-1.141590
C	1.200260	2.381970	1.619390
C	2.156510	3.383200	1.520260
H	3.878580	4.056700	0.416200
H	0.424460	2.400070	2.374620
H	2.141520	4.213530	2.213440
C	2.117540	-1.240160	-0.192120
C	3.121210	-3.289050	0.522600
C	1.201410	-2.380100	1.621830
C	2.158160	-3.380970	1.523720
H	3.880580	-4.054730	0.420380
H	0.425600	-2.397830	2.377040
H	2.143550	-4.210610	2.217720
C	2.116900	1.240640	-0.193430
C	3.103300	-2.203510	-0.351490
H	3.838680	-2.106750	-1.139380
N	-0.410130	-0.000650	-0.893890
N	1.187660	1.336100	0.779610
N	1.188320	-1.335080	0.780990
C	-1.948140	-0.002160	-2.687940
H	-2.958770	-0.002710	-3.066360
C	-2.752350	-0.000420	-0.269940
C	-4.111380	-0.000280	-0.652120
C	-2.446170	0.000140	1.128630
C	-5.141510	0.000260	0.271840
H	-4.371110	-0.000520	-1.702480
C	-3.513030	0.000600	2.051810
C	-4.833020	0.000650	1.638340
H	-6.171600	0.000370	-0.062820
H	-3.257960	0.000950	3.105370
H	-5.627430	0.001040	2.376700
O	-1.211990	0.000210	1.621370
Be	0.042050	0.000210	0.745510

L1chNH2_Be

C	-1.719050	-0.000350	1.512580
C	-0.924200	-0.000790	3.796580
C	0.399210	-0.000610	3.344730
H	-1.130740	-0.001030	4.860230
C	0.602300	-0.000320	1.978010
H	1.233960	-0.000700	4.032560
C	1.969910	-0.000110	1.299450
H	2.752650	-0.000180	2.053620
C	3.084300	-2.196760	0.609260
C	3.100250	-3.296530	-0.267780
H	3.811910	-2.097520	1.402780
C	1.190840	-2.388080	-1.414370
C	2.167120	-3.401920	-1.273480
H	3.853200	-4.067150	-0.151210
H	2.166010	-4.240030	-1.958310
C	2.105880	1.246420	0.425540
C	3.099800	3.296960	-0.266740
C	1.190560	2.388580	-1.413660
C	2.166680	3.402520	-1.272430
H	3.852630	4.067660	-0.149920
H	2.165470	4.240830	-1.957020
C	2.106060	-1.246350	0.425150
C	3.083980	2.196920	0.609960
H	3.811600	2.097550	1.403470
N	-0.428640	-0.000210	1.112610
N	1.177670	-1.340380	-0.561200
N	1.177500	1.340620	-0.560800
C	-1.976850	-0.000660	2.896000
H	-2.989520	-0.000820	3.269100
C	-2.765750	-0.000150	0.471790
C	-4.126560	-0.000140	0.844320
C	-2.455440	0.000030	-0.922470
C	-5.150940	0.000010	-0.087130
H	-4.393110	-0.000230	1.892850
C	-3.510680	0.000170	-1.854080
C	-4.835020	0.000150	-1.450360
H	-6.183000	0.000020	0.241410
H	-3.248250	0.000290	-2.905780
H	-5.623970	0.000260	-2.194280
O	-1.209260	0.000090	-1.412280
N	0.268170	2.407890	-2.404750
H	-0.490420	1.736410	-2.383830
N	0.268410	-2.407250	-2.405420
H	-0.490240	-1.735850	-2.384310
H	0.154600	3.239360	-2.961270
H	0.154990	-3.238520	-2.962240
Be	0.052510	0.000050	-0.514460

L1chNHCH3_Be

C	-1.738160	-0.000710	1.482010
C	-1.060220	-0.001230	3.803180
C	0.284350	-0.001060	3.419630
H	-1.320770	-0.001500	4.854930
C	0.556730	-0.000750	2.064680
H	1.083200	-0.001180	4.148930
C	1.955960	-0.000540	1.455890
H	2.699610	-0.000650	2.248450
C	3.118290	-2.186620	0.820030
C	3.187500	-3.281660	-0.057010
H	3.804940	-2.079660	1.648250
C	1.316940	-2.399340	-1.293130
C	2.302560	-3.399860	-1.106050
H	3.943600	-4.043760	0.092100
H	2.352870	-4.242420	-1.780280
C	2.138030	1.245130	0.588300
C	3.187110	3.281280	-0.055790
C	1.316670	2.399180	-1.292250
C	2.302170	3.399760	-1.104800
H	3.943120	4.043420	0.093610
H	2.352380	4.242580	-1.778720
C	2.138180	-1.245880	0.587840
C	3.118030	2.185910	0.820850
H	3.804680	2.078730	1.649040
N	-0.429080	-0.000590	1.148760
N	1.260140	-1.345120	-0.438520
N	1.260000	1.344640	-0.438040
C	-2.066120	-0.001070	2.850320
H	-3.096300	-0.001220	3.172640
C	-2.729070	-0.000470	0.387610
C	-4.107220	-0.000430	0.689050
C	-2.347240	-0.000260	-0.988690
C	-5.082300	-0.000230	-0.293960
H	-4.427310	-0.000540	1.722340
C	-3.352900	-0.000070	-1.973550
C	-4.696490	-0.000060	-1.638890
H	-6.129940	-0.000200	-0.019150
H	-3.036550	0.000070	-3.010330
H	-5.445860	0.000090	-2.422680
O	-1.077030	-0.000210	-1.413150
N	0.416940	2.434240	-2.297360
H	-0.278740	1.696810	-2.312840
N	0.417200	-2.434130	-2.298240
H	-0.278590	-1.696800	-2.313420
Be	0.137700	-0.000290	-0.450240
C	0.321690	-3.509640	-3.272850
H	-0.486070	-3.270490	-3.961840
H	1.245390	-3.610130	-3.849810
H	0.097180	-4.469900	-2.797910
C	0.321330	3.510080	-3.271590
H	0.096720	4.470160	-2.796320
H	1.245020	3.610860	-3.848520
H	-0.486400	3.271100	-3.960680

L1chNHCOCH3_Be

C	0.071170	-0.025650	2.241920
C	2.288590	-0.011650	3.208380
C	2.855740	-0.005560	1.929880
H	2.928950	-0.008540	4.082230
C	1.988910	-0.008870	0.855490
H	3.927090	0.001880	1.782980
C	2.414090	-0.002370	-0.610040
H	3.498810	0.002920	-0.678240
C	2.683140	-2.208550	-1.875980
C	2.068080	-3.322850	-2.450860
H	3.758790	-2.100620	-1.860080
C	-0.081660	-2.405760	-1.905690
C	0.688440	-3.436720	-2.460890
H	2.670740	-4.114070	-2.879840
H	0.221830	-4.319270	-2.865610
C	1.858710	1.245200	-1.295160
C	2.040540	3.317550	-2.444320
C	-0.103040	2.396120	-1.879660
C	0.660780	3.426960	-2.445130
H	2.636770	4.109550	-2.880790
H	0.191350	4.305220	-2.854330
C	1.870210	-1.250870	-1.302050
C	2.664380	2.207110	-1.871550
H	3.740560	2.104110	-1.861660
N	0.653650	-0.018210	1.021640
N	0.521710	-1.350170	-1.316800
N	0.509550	1.339410	-1.300760
C	0.913000	-0.021550	3.369150
H	0.499080	-0.025520	4.365640
C	-1.402460	-0.037810	2.308020
C	-2.051800	-0.051570	3.560640
C	-2.216830	-0.037310	1.138270
C	-3.431250	-0.063510	3.678290
H	-1.463850	-0.053850	4.468530
C	-3.615010	-0.049200	1.274520
C	-4.217800	-0.062060	2.521510
H	-3.891130	-0.074120	4.658760
H	-4.207410	-0.048300	0.367130
H	-5.299450	-0.071220	2.595690
O	-1.724560	-0.026650	-0.113720
N	-1.489550	2.362840	-1.813210
H	-1.865530	1.654990	-1.178810
N	-1.469550	-2.380000	-1.859540
H	-1.860530	-1.702660	-1.201640
Be	-0.215070	-0.014460	-0.429650
C	-2.492800	3.000500	-2.534730
C	-2.447130	-2.963050	-2.657850
C	-2.064080	-3.784250	-3.861580
H	-1.816200	-4.805560	-3.560060
H	-2.930550	-3.828130	-4.518730
H	-1.214010	-3.366220	-4.401280
C	-2.154030	3.920850	-3.677510
H	-3.053270	4.045630	-4.277480
H	-1.859320	4.903120	-3.298160
H	-1.348100	3.532910	-4.301160
O	-3.650960	2.766110	-2.219060
O	-3.616390	-2.760960	-2.361690

L1chNHCONH_Be

C	-0.049830	0.036470	2.049280
C	2.141660	0.079160	3.070010
C	2.743080	0.061830	1.806580
H	2.759930	0.102390	3.959380
C	1.905200	0.035440	0.709370
H	3.818130	0.069880	1.689230
C	2.367790	0.016840	-0.746760
H	3.453890	0.024560	-0.787320
C	2.670230	-2.161280	-2.052330
C	2.066300	-3.239300	-2.705920
H	3.744070	-2.037270	-2.036200
C	-0.090960	-2.429120	-2.030030
C	0.690410	-3.379940	-2.707450
H	2.675820	-3.967270	-3.227450
H	0.223320	-4.188630	-3.247560
C	1.824880	1.241160	-1.481940
C	2.014840	3.209830	-2.799540
C	-0.129050	2.387170	-2.096500
C	0.636960	3.329490	-2.802810
H	2.612640	3.931570	-3.342830
H	0.156820	4.115100	-3.365140
C	1.844470	-1.236970	-1.445320
C	2.635840	2.160490	-2.115840
H	3.711500	2.054040	-2.096950
N	0.566990	0.024080	0.847890
N	0.497530	-1.364590	-1.440730
N	0.476120	1.347970	-1.479280
C	0.762150	0.067420	3.198000
H	0.324150	0.083250	4.184230
C	-1.526140	0.016390	2.067480
C	-2.210910	0.014410	3.300890
C	-2.308060	-0.002790	0.872960
C	-3.593080	-0.002330	3.380890
H	-1.647600	0.024450	4.224310
C	-3.709570	-0.018420	0.972730
C	-4.346740	-0.018020	2.202590
H	-4.079970	-0.003600	4.348300
H	-4.277170	-0.031560	0.049640
H	-5.430020	-0.030710	2.246550
O	-1.782560	-0.007230	-0.364450
N	-1.508830	2.397740	-2.008940
H	-1.929710	1.557320	-1.614440
N	-1.470750	-2.456290	-1.945430
H	-1.904140	-1.610640	-1.576780
Be	-0.261880	-0.001950	-0.613560
C	-2.456030	3.403230	-2.241100
C	-2.405100	-3.477520	-2.160150
O	-3.637160	3.090650	-2.335190
O	-3.588950	-3.180430	-2.269030
N	-2.010110	4.683820	-2.358920
H	-2.736780	5.383450	-2.402660
H	-1.154340	4.973740	-1.909010
N	-1.944500	-4.755560	-2.245550
H	-1.089780	-5.026370	-1.781940
H	-2.663610	-5.463580	-2.278400

L2chH_Be

C	-2.002970	0.000030	-0.407690
C	-2.730210	0.000130	-1.633590
C	-4.061000	-0.000060	0.829510
H	-4.583820	-0.000130	1.777360
C	-2.678790	-0.000060	0.847050
C	-4.794320	0.000030	-0.376570
H	-5.876690	0.000020	-0.337950
C	-4.146630	0.000120	-1.589040
H	-4.704360	0.000190	-2.518230
C	-1.966750	-0.000140	2.189240
O	-2.629980	-0.000220	3.218970
O	-0.657660	-0.000130	2.201270
N	-0.644100	0.000030	-0.445490
C	-0.612540	0.000200	-2.828120
C	0.034910	0.000100	-1.582570
C	-1.990580	0.000210	-2.841550
H	-2.524470	0.000290	-3.785130
H	-0.038220	0.000270	-3.744640
C	1.548810	0.000070	-1.377880
C	1.942800	1.241660	-0.576910
C	2.820540	2.207720	-1.045280
C	3.112350	3.296670	-0.225060
C	2.521430	3.387190	1.031930
C	1.652470	2.382430	1.434410
N	1.374070	1.335270	0.643180
H	3.794250	4.065520	-0.567300
H	3.264080	2.109990	-2.027290
H	2.725680	4.218720	1.692850
H	1.161840	2.399130	2.399390
C	1.942790	-1.241610	-0.577050
C	2.820500	-2.207630	-1.045530
C	3.112300	-3.296670	-0.225430
C	2.521390	-3.387330	1.031550
C	1.652440	-2.382600	1.434140
N	1.374060	-1.335350	0.643030
H	3.794190	-4.065500	-0.567770
H	3.264040	-2.109800	-2.027540
H	2.725630	-4.218930	1.692370
H	1.161820	-2.399400	2.399130
H	2.062770	0.000130	-2.335300
Be	0.288150	-0.000060	0.977410

L2chNH2_Be

C	-2.132020	-0.000020	-0.483670
C	-2.944990	-0.000060	-1.653720
C	-4.098730	0.000030	0.897860
H	-4.552430	0.000070	1.880670
C	-2.718430	0.000030	0.815440
C	-4.915410	-0.000010	-0.252670
H	-5.992290	-0.000010	-0.137740
C	-4.354400	-0.000060	-1.508100
H	-4.976680	-0.000090	-2.395390
C	-1.916770	0.000080	2.100540
O	-2.494150	0.000130	3.177960
O	-0.601640	0.000070	2.017990
N	-0.779730	-0.000030	-0.617780
C	-0.917980	-0.000110	-2.995850
C	-0.181470	-0.000070	-1.799410
C	-2.292900	-0.000110	-2.911830
H	-2.893070	-0.000140	-3.814730
H	-0.410310	-0.000140	-3.950970
C	1.340420	-0.000060	-1.699640
C	1.798150	1.245910	-0.937890
C	2.635590	2.190670	-1.482950
C	2.994320	3.288540	-0.679000
C	2.519320	3.395820	0.606850
C	1.663970	2.388110	1.112380
N	1.318450	1.341010	0.330460
H	3.649640	4.055060	-1.075460
H	3.002020	2.088150	-2.494840
H	2.786840	4.231590	1.240260
C	1.798150	-1.245970	-0.937800
C	2.635570	-2.190780	-1.482800
C	2.994300	-3.288600	-0.678790
C	2.519310	-3.395780	0.607080
C	1.663990	-2.388020	1.112560
N	1.318460	-1.340980	0.330560
H	3.649590	-4.055170	-1.075210
H	3.001990	-2.088340	-2.494710
H	2.786820	-4.231510	1.240540
H	1.781850	-0.000090	-2.692610
Be	0.266770	0.000030	0.715110
N	1.191560	-2.420780	2.379580
H	0.493560	-1.751040	2.675150
H	1.328280	-3.244110	2.942700
N	1.191470	2.421000	2.379370
H	0.493610	1.751180	2.675080
H	1.328420	3.244240	2.942560

L2chNHCH3_Be

C	-2.292800	0.059980	-0.283110
C	-3.283970	0.512920	-1.202310
C	-4.009410	-0.901970	1.099940
H	-4.295370	-1.441200	1.993970
C	-2.665600	-0.653320	0.890060
C	-4.998160	-0.471640	0.190960
H	-6.039020	-0.691620	0.394220
C	-4.646640	0.226610	-0.940140
H	-5.399960	0.567680	-1.640790
C	-1.662030	-1.131910	1.915060
O	-2.057010	-1.685710	2.936170
O	-0.394280	-0.941010	1.672010
N	-0.979930	0.327420	-0.530610
C	-1.517930	1.501610	-2.540260
C	-0.599690	1.020070	-1.592240
C	-2.853770	1.238350	-2.340310
H	-3.593040	1.590130	-3.051060
H	-1.172580	2.062410	-3.398210
C	0.899130	1.243600	-1.636110
C	1.310890	1.965290	-0.354910
C	1.646190	3.296920	-0.353500
C	1.937600	3.899380	0.884170
C	1.951540	3.138360	2.024820
C	1.672380	1.748290	1.948800
N	1.268460	1.199240	0.774330
H	2.178870	4.954550	0.932930
H	1.666200	3.860840	-1.275710
H	2.223310	3.566770	2.981340
C	1.652660	-0.078770	-1.743580
C	2.634070	-0.231540	-2.692830
C	3.377970	-1.423570	-2.693620
C	3.072670	-2.406740	-1.790800
C	2.008360	-2.221420	-0.868030
N	1.344900	-1.036140	-0.812620
H	4.172560	-1.572500	-3.414910
H	2.834940	0.558170	-3.403340
H	3.603710	-3.350350	-1.790330
H	1.157740	1.864820	-2.489710
Be	0.297770	-0.268780	0.451930
N	1.828110	0.980190	3.056080
H	2.098410	1.501490	3.876130
N	1.693660	-3.258000	-0.048290
H	2.300790	-4.054230	-0.167470
C	0.375210	-3.585680	0.495410
H	-0.413310	-3.174030	-0.137110
H	0.278880	-4.671410	0.498160
H	0.246620	-3.214300	1.509740
C	2.233350	-0.428280	3.062000
H	2.900350	-0.582150	3.910030
H	1.378710	-1.095640	3.145540
H	2.781260	-0.666420	2.147260

L2chNHCOCH3_Be

C	0.548730	-2.836090	7.072200
C	1.875460	-3.345030	6.968840
C	-0.185850	-4.371760	5.375420
H	-0.976410	-4.772590	4.754150
C	-0.500100	-3.356700	6.260610
C	1.122750	-4.887040	5.265320
H	1.320610	-5.682690	4.557880
C	2.138930	-4.386110	6.044260
H	3.146820	-4.775800	5.962390
C	-1.926810	-2.859650	6.310400
O	-2.770550	-3.336930	5.571200
O	-2.226890	-1.900820	7.175590
N	0.292030	-1.838010	7.958690
C	2.560980	-1.762870	8.683100
C	1.232360	-1.313940	8.730350
C	2.869960	-2.776620	7.802310
H	3.885420	-3.150760	7.738930
H	3.311630	-1.319970	9.323310
C	0.703360	-0.209960	9.639030
C	0.105140	0.910990	8.785920
C	0.568940	2.210210	8.829040
C	-0.066000	3.155980	8.019600
C	-1.126380	2.792270	7.207980
C	-1.547080	1.453840	7.212380
N	-0.927650	0.541730	7.992790
H	0.271130	4.185460	8.025530
H	1.395420	2.478540	9.472550
H	-1.633750	3.504150	6.578990
C	-0.387030	-0.785800	10.544230
C	-0.289120	-0.794130	11.921110
C	-1.339390	-1.363770	12.644570
C	-2.445150	-1.876330	11.989500
C	-2.504270	-1.797320	10.591440
N	-1.468340	-1.278210	9.895870
H	-1.285530	-1.421160	13.724770
H	0.582200	-0.386740	12.414590
H	-3.232710	-2.353430	12.548430
H	1.505920	0.192510	10.250840
Be	-1.248950	-1.176840	8.151750
N	-2.594810	0.956270	6.448660
N	-3.557130	-2.262970	9.814850
H	-3.340960	-2.389970	8.826880
C	-4.913360	-2.437300	10.075570
C	-3.439880	1.645440	5.592030
O	-5.608960	-2.883900	9.175280
O	-3.373200	2.850770	5.412070
H	-2.748170	-0.046210	6.527100
C	-5.491580	-2.053270	11.412340
H	-5.053470	-1.138840	11.813260
H	-6.563510	-1.919120	11.279900
H	-5.338920	-2.858780	12.135790
C	-4.439380	0.769900	4.873010
H	-5.377140	1.315990	4.774620
H	-4.059640	0.566240	3.867480
H	-4.617860	-0.181980	5.373360

L2chNHCONH2_Be

C	0.673060	-3.003030	7.157290
C	2.029880	-3.433040	7.102440
C	0.042840	-4.745580	5.628210
H	-0.718180	-5.259870	5.055460
C	-0.339830	-3.670240	6.409260
C	1.383350	-5.180860	5.562620
H	1.634370	-6.027660	4.936030
C	2.363180	-4.541100	6.284430
H	3.394250	-4.871530	6.238330
C	-1.798740	-3.271920	6.421970
O	-2.611470	-3.891390	5.758100
O	-2.161640	-2.237930	7.170920
N	0.351040	-1.939220	7.938540
C	2.603810	-1.650530	8.655170
C	1.249720	-1.282750	8.657100
C	2.981040	-2.723230	7.875900
H	4.018460	-3.036320	7.848350
H	3.321760	-1.103100	9.250540
C	0.644150	-0.129210	9.452330
C	-0.016000	0.861180	8.490720
C	0.359040	2.187410	8.404000
C	-0.327070	3.002630	7.500470
C	-1.349210	2.487450	6.721520
C	-1.676040	1.131600	6.860150
N	-1.012930	0.346450	7.734510
H	-0.059950	4.048070	7.405480
H	1.158360	2.575170	9.020170
H	-1.892920	3.096390	6.018250
C	-0.419530	-0.676050	10.406530
C	-0.351440	-0.518520	11.776780
C	-1.388470	-1.049250	12.547830
C	-2.446760	-1.709460	11.946870
C	-2.451080	-1.832890	10.550780
N	-1.448170	-1.319900	9.807850
H	-1.368100	-0.945720	13.625860
H	0.481140	0.001030	12.230510
H	-3.258130	-2.126590	12.520180
H	1.414470	0.381100	10.023800
Be	-1.225400	-1.367140	8.064190
N	-2.676380	0.494330	6.133920
N	-3.453010	-2.473540	9.829680
H	-3.311590	-2.522990	8.822180
C	-4.605470	-3.057260	10.299230
C	-3.534250	1.033550	5.204830
O	-4.962290	-3.114150	11.460030
O	-3.572560	2.195670	4.849860
H	-2.782080	-0.504040	6.306410
H	-5.192880	-3.483720	9.473830
H	-4.210210	0.265760	4.802530

L3chH_Be

C	-1.582440	-0.268740	0.827440
C	-2.082300	-0.688100	2.091400
C	-3.872120	0.007710	-0.012850
C	-2.465980	0.087930	-0.251310
C	-4.346750	-0.420360	1.276270
H	-5.419230	-0.471390	1.428780
C	-3.500380	-0.754170	2.285040
H	-3.880900	-1.074420	3.248060
N	-0.242490	-0.205180	0.638460
C	0.211900	-0.940450	2.856020
C	0.631790	-0.522610	1.594590
C	-1.152410	-1.019110	3.092660
H	-1.514630	-1.340810	4.062840
H	0.932920	-1.194430	3.621310
C	2.088430	-0.381210	1.153310
C	2.346280	1.064060	0.728710
C	3.293720	1.883150	1.326000
C	3.443910	3.185190	0.851240
C	2.646790	3.628670	-0.200330
C	1.718650	2.753790	-0.747820
N	1.577390	1.500880	-0.290520
H	4.176590	3.844860	1.299990
H	3.898570	1.510710	2.142200
H	2.737470	4.632730	-0.592380
H	1.069030	3.042250	-1.564690
C	2.336630	-1.295370	-0.046080
C	3.274660	-2.317770	-0.052180
C	3.415450	-3.086650	-1.206390
C	2.618930	-2.813410	-2.314890
C	1.700690	-1.775450	-2.235740
N	1.568370	-1.036240	-1.124480
H	4.140310	-3.891060	-1.237000
H	3.879910	-2.506670	0.824630
H	2.702380	-3.390960	-3.225680
H	1.051340	-1.517820	-3.063060
H	2.755840	-0.652040	1.967570
C	-4.301090	0.756810	-2.268470
C	-2.929770	0.840350	-2.518840
C	-4.778400	0.346250	-1.033590
C	-1.987250	0.514340	-1.537420
H	-2.562660	1.161890	-3.486630
H	-4.998990	1.018520	-3.056340
H	-5.843250	0.282950	-0.843180
O	-0.694000	0.611660	-1.832010
Be	0.432680	0.281740	-0.843800

L3chNH2_Be

C	-1.687650	1.013340	-0.066800
C	-2.242740	2.318280	-0.155480
C	-3.937830	0.035280	0.001980
C	-2.523020	-0.157390	0.014370
C	-4.469320	1.369290	-0.087830
H	-5.547580	1.484610	-0.093700
C	-3.667820	2.463740	-0.163130
H	-4.089560	3.459930	-0.230060
N	-0.341820	0.869450	-0.059060
C	0.016190	3.215300	-0.221840
C	0.492190	1.906950	-0.132830
C	-1.356210	3.408490	-0.231710
H	-1.761280	4.412080	-0.298990
H	0.703890	4.048170	-0.281030
C	1.963550	1.500030	-0.108590
C	2.252610	0.578540	-1.294840
C	3.169220	0.879050	-2.276770
C	3.339010	-0.049970	-3.319330
C	2.610370	-1.216820	-3.340470
C	1.688220	-1.470640	-2.298650
N	1.527060	-0.569740	-1.304900
H	4.048270	0.154500	-4.112720
H	3.734540	1.800110	-2.243850
H	2.729410	-1.942880	-4.134150
C	2.258380	0.755610	1.194040
C	3.180500	1.191190	2.118050
C	3.357580	0.418030	3.279820
C	2.631150	-0.735120	3.468700
C	1.703880	-1.133830	2.477460
N	1.533120	-0.379090	1.369960
H	4.071190	0.732320	4.032400
H	3.744830	2.098200	1.951750
H	2.755910	-1.342390	4.355880
H	2.595300	2.382420	-0.171980
C	-4.268930	-2.352140	0.164290
C	-2.886170	-2.557420	0.178610
C	-4.798450	-1.075670	0.077510
C	-1.993080	-1.487020	0.105540
H	-2.476460	-3.558470	0.247020
H	-4.931100	-3.208950	0.222490
H	-5.870700	-0.919610	0.066900
O	-0.678580	-1.745910	0.123420
Be	0.413910	-0.643700	0.046620
N	0.966420	-2.615340	-2.236340
H	0.942220	-3.229530	-3.034170
H	0.217020	-2.685940	-1.557750
N	0.986390	-2.277840	2.579810
H	0.238160	-2.452200	1.919340
H	0.981100	-2.784980	3.449660

L3chNHCH3_Be

C	1.244010	-3.066700	6.794100
C	2.603820	-3.384460	6.520240
C	0.505140	-4.583720	5.014490
C	0.165150	-3.658380	6.047950
C	1.888530	-4.884060	4.761700
H	2.115270	-5.590090	3.970630
C	2.896350	-4.317380	5.474240
H	3.931330	-4.560980	5.263900
N	0.962010	-2.185160	7.781870
C	3.257460	-1.859990	8.301720
C	1.905950	-1.594610	8.516100
C	3.593280	-2.758730	7.298950
H	4.636040	-2.987390	7.106550
H	4.018790	-1.377590	8.901010
C	1.337600	-0.638520	9.564060
C	0.417720	-1.408940	10.514700
C	0.634610	-1.486730	11.872960
C	-0.287370	-2.220050	12.638680
C	-1.363140	-2.837300	12.040900
C	-1.532520	-2.722820	10.638870
N	-0.638000	-2.005780	9.910700
H	-0.150750	-2.303940	13.710710
H	1.484580	-0.998790	12.330000
H	-2.071270	-3.405400	12.626640
C	0.531190	0.460510	8.867440
C	0.834420	1.800020	8.976100
C	0.014190	2.711150	8.289590
C	-1.050300	2.268500	7.536910
C	-1.312420	0.878110	7.463580
N	-0.514920	0.007950	8.135250
H	0.221390	3.773400	8.349840
H	1.674430	2.134260	9.569570
H	-1.679990	2.966520	7.004450
H	2.146550	-0.186050	10.133940
C	-1.836060	-4.891320	4.512990
C	-2.184790	-3.987810	5.520950
C	-0.510160	-5.191150	4.255860
C	-1.213500	-3.360580	6.297830
H	-3.225150	-3.756610	5.718450
H	-2.619160	-5.360130	3.928140
H	-0.243680	-5.891510	3.473560
O	-1.610720	-2.498020	7.254480
Be	-0.619300	-1.743430	8.176540
N	-2.335730	0.357530	6.753660
H	-2.390960	-0.654780	6.715170
N	-2.557400	-3.293510	9.971370
H	-2.544660	-3.204000	8.960820
C	-3.256890	1.143790	5.947100
H	-3.973440	0.463930	5.489280
H	-3.812960	1.860260	6.558430
H	-2.740280	1.684730	5.147830
C	-3.579380	-4.122680	10.591660
H	-4.145400	-3.565430	11.343650
H	-4.273580	-4.443180	9.816680
H	-3.152200	-5.015990	11.058360

L3chNHCOCH3_Be

C	1.342690	-3.070800	6.780440
C	2.700800	-3.384360	6.504020
C	0.606300	-4.584780	4.994290
C	0.266190	-3.664110	6.030970
C	1.990330	-4.880640	4.737530
H	2.218780	-5.582520	3.943180
C	2.995610	-4.312250	5.453140
H	4.032050	-4.549230	5.242860
N	1.058390	-2.193480	7.772590
C	3.358670	-1.869420	8.288810
C	2.006660	-1.607990	8.504020
C	3.693790	-2.762230	7.282910
H	4.735830	-2.989410	7.087480
H	4.116100	-1.386300	8.891040
C	1.444320	-0.655820	9.555260
C	0.528440	-1.431730	10.502640
C	0.766840	-1.538660	11.858710
C	-0.126390	-2.297950	12.617930
C	-1.222090	-2.898520	12.022320
C	-1.433150	-2.714170	10.648720
N	-0.546220	-2.006670	9.915330
H	0.043210	-2.433560	13.679110
H	1.626950	-1.061690	12.307700
H	-1.883370	-3.516720	12.606090
C	0.640450	0.444080	8.860650
C	0.960770	1.784190	8.954520
C	0.164670	2.693520	8.254260
C	-0.918590	2.254720	7.512700
C	-1.216630	0.885150	7.493040
N	-0.422450	0.008790	8.145870
H	0.401370	3.750270	8.276520
H	1.810080	2.109490	9.539190
H	-1.503230	2.957260	6.942880
H	2.254540	-0.207810	10.124390
C	-1.737800	-4.896140	4.497610
C	-2.086540	-3.995600	5.509430
C	-0.411330	-5.192510	4.235620
C	-1.111510	-3.370050	6.283480
H	-3.125760	-3.765340	5.711870
H	-2.522100	-5.364710	3.913770
H	-0.144090	-5.889590	3.450320
O	-1.505040	-2.509690	7.241760
Be	-0.522960	-1.753340	8.169050
N	-2.272540	0.303680	6.802850
H	-2.200020	-0.709420	6.689590
N	-2.489950	-3.245540	9.920530
H	-2.358510	-3.228080	8.907040
C	-3.499440	0.792930	6.369210
C	-3.771700	-3.649370	10.276850
O	-4.233220	0.025020	5.762910
O	-4.493530	-4.088880	9.392820
C	-3.909960	2.210730	6.670100
H	-3.625700	2.525610	7.674680
H	-3.457230	2.896790	5.949140
H	-4.990990	2.270590	6.559440
C	-4.249460	-3.517660	11.699320
H	-3.886390	-4.356710	12.299010
H	-3.921070	-2.589130	12.167000
H	-5.336950	-3.557450	11.686580

L3chNHCONH2_Be

C	1.327560	-3.080400	6.773680
C	2.680740	-3.405130	6.486180
C	0.564080	-4.589690	4.994930
C	0.239820	-3.665720	6.033870
C	1.943550	-4.896720	4.726810
H	2.159710	-5.600900	3.931060
C	2.959330	-4.336040	5.433560
H	3.992040	-4.581370	5.214630
N	1.058610	-2.199760	7.767000
C	3.365660	-1.893860	8.263830
C	2.017540	-1.621050	8.490020
C	3.685180	-2.790380	7.256220
H	4.723670	-3.026400	7.052450
H	4.132030	-1.416380	8.859240
C	1.472540	-0.662370	9.545000
C	0.558850	-1.430620	10.500950
C	0.807470	-1.541250	11.854320
C	-0.084430	-2.298530	12.619560
C	-1.189400	-2.889390	12.033340
C	-1.409290	-2.701250	10.659250
N	-0.524450	-1.997660	9.920510
H	0.094990	-2.438990	13.678570
H	1.673490	-1.069710	12.297580
H	-1.852780	-3.511560	12.614010
C	0.672650	0.442310	8.853170
C	1.006330	1.779410	8.934780
C	0.213650	2.691690	8.231840
C	-0.880960	2.259180	7.504900
C	-1.192040	0.889920	7.498780
N	-0.400680	0.011080	8.150500
H	0.463260	3.745730	8.242010
H	1.862790	2.101200	9.510880
H	-1.467120	2.956510	6.926440
H	2.291450	-0.220240	10.106230
C	-1.786220	-4.883340	4.517600
C	-2.119490	-3.979680	5.531750
C	-0.464270	-5.190060	4.244920
C	-1.133630	-3.360880	6.297740
H	-3.155280	-3.741390	5.742620
H	-2.578910	-5.346130	3.940530
H	-0.208720	-5.889640	3.457940
O	-1.513690	-2.497460	7.258510
Be	-0.516970	-1.746830	8.176970
N	-2.256430	0.324990	6.818290
H	-2.211210	-0.685990	6.693570
N	-2.470700	-3.232020	9.947850
H	-2.363670	-3.228850	8.933680
C	-3.450310	0.871620	6.334660
C	-3.717720	-3.719330	10.354250
N	-4.122300	-3.447580	11.625140
H	-5.075320	-3.707580	11.833070
H	-3.774100	-2.637200	12.115660
N	-3.794520	2.118980	6.756870
H	-3.461030	2.476290	7.639940
H	-4.718510	2.421030	6.484610
O	-4.128110	0.215040	5.552480
O	-4.386590	-4.370640	9.560010

L4chH_Be

C	-1.180330	1.039480	3.608000
C	0.110440	0.950780	3.054770
N	0.066990	0.571760	1.765340
C	-1.294830	0.405340	1.432740
C	-2.062530	0.693570	2.594140
C	-1.777610	-0.020260	0.167380
C	-0.897360	-0.382940	-0.871370
N	0.451850	-0.328380	-0.626530
C	1.122650	-0.633930	-1.728250
C	0.214830	-0.924070	-2.780180
C	-1.060760	-0.761360	-2.240310
C	-3.238650	-0.082970	-0.077990
C	2.624430	-0.509250	-1.554020
C	2.941190	0.949540	-1.199340
N	2.341750	1.418750	-0.081560
C	2.559020	2.683070	0.310180
C	3.389040	3.539660	-0.400640
C	4.011620	3.062710	-1.549750
C	3.787690	1.747950	-1.955170
C	-3.832710	-1.265360	-0.540650
C	-5.203110	-1.324740	-0.782380
C	-6.022780	-0.207290	-0.592490
C	-5.422040	0.977150	-0.144040
C	-4.058450	1.040360	0.117560
C	-7.507120	-0.268430	-0.853060
C	3.064490	-1.376940	-0.368370
N	2.490550	-1.085050	0.822250
C	2.823720	-1.792700	1.912130
C	3.749470	-2.826220	1.863960
C	4.346230	-3.129600	0.644640
C	4.001560	-2.393610	-0.487740
H	-1.419710	1.314820	4.623580
H	1.056960	1.141830	3.541790
H	-3.136690	0.632950	2.664570
H	0.465910	-1.204820	-3.791520
H	-1.997960	-0.887640	-2.759610
H	2.049200	3.002120	1.210740
H	3.538330	4.554140	-0.056180
H	4.665570	3.704910	-2.127170
H	4.259420	1.348940	-2.843630
H	-3.224100	-2.149630	-0.687930
H	-5.640190	-2.256990	-1.124210
H	-6.030240	1.864440	-0.000830
H	-3.618850	1.973240	0.449620
H	-7.794180	-1.223260	-1.296590
H	-8.072550	-0.144950	0.076040
H	-7.821660	0.531340	-1.529420
H	2.329170	-1.517920	2.835400
H	3.990880	-3.374920	2.764420
H	5.072630	-3.929940	0.571890
H	4.450620	-2.605420	-1.449250
Be	1.280620	0.211980	0.685490
H	3.168590	-0.800270	-2.448820

L4chNH2_Be

C	-1.254640	2.030630	3.043630
C	0.025120	1.706670	2.574650
N	-0.031660	0.961120	1.444800
C	-1.401890	0.792950	1.149260
C	-2.152880	1.453240	2.152690
C	-1.922430	0.050730	0.049530
C	-1.078850	-0.650180	-0.822270
N	0.275070	-0.616430	-0.588160
C	0.909070	-1.279430	-1.541370
C	-0.028620	-1.806150	-2.473430
C	-1.281180	-1.405170	-2.023080
C	-3.386380	0.014750	-0.184470
C	2.412850	-1.227050	-1.399310
C	2.862070	0.234810	-1.490290
N	2.312920	1.077190	-0.570170
C	2.647920	2.386440	-0.593250
C	3.578070	2.879040	-1.536560
C	4.133790	2.012260	-2.447420
C	3.771460	0.655810	-2.434590
C	-4.061150	-1.212790	-0.268770
C	-5.432500	-1.254350	-0.498210
C	-6.175230	-0.080400	-0.675830
C	-5.496220	1.141520	-0.599420
C	-4.127920	1.193640	-0.350340
C	-7.654290	-0.134830	-0.965460
C	2.816810	-1.758060	-0.021180
N	2.272140	-1.112120	1.049330
C	2.578730	-1.531290	2.296740
C	3.476790	-2.602610	2.501100
C	4.029590	-3.232660	1.411520
C	3.694880	-2.810280	0.115290
N	2.097110	3.215650	0.335220
N	2.031990	-0.875480	3.357870
H	-1.481110	2.608450	3.926310
H	0.976990	1.980910	3.009620
H	-3.228970	1.480800	2.211220
H	0.195640	-2.390250	-3.352720
H	-2.230440	-1.613610	-2.491370
H	3.830290	3.931730	-1.531500
H	4.844060	2.377940	-3.179520
H	4.187770	-0.045020	-3.145030
H	-3.513410	-2.136590	-0.124870
H	-5.933680	-2.215940	-0.537330
H	-6.044580	2.067650	-0.736410
H	-3.627570	2.153660	-0.306700
H	-8.131010	-0.966440	-0.441740
H	-8.152410	0.790860	-0.670630
H	-7.833840	-0.278880	-2.036460
H	3.705950	-2.914190	3.511960
H	4.715370	-4.059470	1.553760
H	4.109750	-3.293830	-0.758330
H	2.200250	4.209170	0.198050
H	1.244850	2.928790	0.793270
H	2.114740	-1.307250	4.265520
H	1.188340	-0.340950	3.213780
Be	1.167870	0.209410	0.521100
H	2.914030	-1.806680	-2.170010

L4chNHCH3_Be

C	-1.282350	0.191900	3.500960
C	-0.016270	0.209720	2.887540
N	-0.114750	0.116500	1.551930
C	-1.492090	0.043370	1.248640
C	-2.210230	0.081860	2.475240
C	-2.030130	-0.076060	-0.057430
C	-1.194180	-0.186020	-1.184760
N	0.166390	-0.186310	-0.991740
C	0.783390	-0.236700	-2.163660
C	-0.172240	-0.280370	-3.212690
C	-1.420780	-0.243520	-2.594480
C	-3.501330	-0.078750	-0.249670
C	2.285270	-0.173620	-2.053410
C	2.717960	1.133320	-1.378900
N	2.154310	1.393900	-0.170800
C	2.541530	2.500810	0.505790
C	3.584170	3.309930	0.023660
C	4.168440	3.020090	-1.193560
C	3.712600	1.922280	-1.926640
C	-4.129370	-1.133750	-0.926600
C	-5.509720	-1.138570	-1.110070
C	-6.307360	-0.085990	-0.647460
C	-5.674020	0.971310	0.018650
C	-4.298320	0.975710	0.222070
C	-7.798070	-0.073870	-0.876770
C	2.821700	-1.274630	-1.132150
N	2.277660	-1.336960	0.111870
C	2.748540	-2.255560	0.987190
C	3.860730	-3.051590	0.665330
C	4.427650	-2.956900	-0.590280
C	3.884210	-2.069240	-1.521690
H	-1.476390	0.244610	4.561330
H	0.951720	0.278630	3.361580
H	-3.282130	0.021060	2.574610
H	0.033090	-0.324260	-4.271360
H	-2.381460	-0.248690	-3.085380
H	3.885120	4.178160	0.596050
H	4.956290	3.652140	-1.585750
H	4.136700	1.672880	-2.889780
H	-3.538370	-1.967820	-1.286160
H	-5.972980	-1.977490	-1.618750
H	-6.265650	1.804320	0.384370
H	-3.834550	1.812050	0.731220
H	-8.175240	-1.074080	-1.097760
H	-8.330670	0.310920	-0.003710
H	-8.054930	0.571640	-1.723540
H	4.229850	-3.761860	1.394130
H	5.270220	-3.583410	-0.857920
H	4.292090	-1.981580	-2.519490
Be	1.065910	0.014440	0.367510
H	2.766510	-0.252660	-3.024830
N	2.111050	-2.382440	2.216830
H	2.695960	-2.905100	2.857980
N	1.894930	2.809740	1.698300
H	2.440830	3.485090	2.220150
C	0.489840	3.263140	1.621880
H	0.065400	3.264800	2.625520
H	0.418520	4.271760	1.198630
H	-0.090720	2.581030	1.008010
C	0.742550	-2.941720	2.224310
H	0.746600	-4.010620	1.981550
H	0.310620	-2.800540	3.214510
H	0.120050	-2.419100	1.503660

L4chNHCOCH3_Be

H	2.451160	-5.326670	1.793900
H	0.817760	-5.064800	2.402020

C	-1.171510	-0.200390	3.296610
C	0.039300	-0.089500	2.594530
N	-0.151880	-0.048040	1.262150
C	-1.549300	-0.129240	1.063430
C	-2.171150	-0.231310	2.336320
C	-2.196300	-0.153810	-0.196100
C	-1.461030	-0.153040	-1.394200
N	-0.087320	-0.136260	-1.325590
C	0.409220	-0.072740	-2.554790
C	-0.636590	-0.054590	-3.509070
C	-1.820260	-0.100000	-2.774650
C	-3.677700	-0.178390	-0.262670
C	1.916050	0.026950	-2.575330
C	2.316400	1.319220	-1.861050
N	1.937220	1.432860	-0.562960
C	2.258770	2.554480	0.113230
C	2.957620	3.601170	-0.491990
C	3.315640	3.488620	-1.824720
C	2.997690	2.326150	-2.523470
C	-4.341280	-1.189530	-0.973420
C	-5.730570	-1.209500	-1.048200
C	-6.505230	-0.216360	-0.436820
C	-5.837470	0.800050	0.257560
C	-4.449610	0.817470	0.354000
C	-8.011480	-0.253150	-0.503310
C	2.498090	-1.167560	-1.821540
N	2.174910	-1.269430	-0.507940
C	2.685200	-2.289550	0.210200
C	3.493290	-3.266500	-0.371280
C	3.784240	-3.180000	-1.723220
C	3.293410	-2.105250	-2.460070
H	-1.281200	-0.258800	4.368310
H	1.028880	-0.049290	3.025670
H	-3.230850	-0.332390	2.506650
H	-0.530400	-0.006870	-4.581800
H	-2.823590	-0.087640	-3.170760
H	3.243450	4.465400	0.088830
H	3.861810	4.288310	-2.309600
H	3.276700	2.200600	-3.560820
H	-3.767430	-1.975560	-1.449790
H	-6.219930	-2.010480	-1.592480
H	-6.410400	1.592800	0.727190
H	-3.959170	1.623460	0.886610
H	-8.357690	-0.748880	-1.412630
H	-8.423030	-0.806070	0.348180
H	-8.435510	0.752790	-0.474360
H	3.913800	-4.051260	0.240580
H	4.414880	-3.924860	-2.192600
H	3.525890	-1.993140	-3.510340
Be	0.924460	-0.008580	-0.032010
H	2.306170	0.040020	-3.589520
N	1.901950	2.599380	1.466870
H	2.059260	1.759540	2.008720
N	2.414710	-2.287140	1.587820
H	2.612160	-1.427730	2.085090
C	1.352090	3.631490	2.208680
C	2.016640	-3.325330	2.409750
O	1.219440	3.480200	3.415340
O	1.980840	-3.141520	3.618930
C	0.900930	4.887630	1.504540
H	0.631190	4.726580	0.461540
H	0.043750	5.279910	2.050430
H	1.694180	5.638720	1.547790
C	1.604610	-4.634960	1.783270
H	1.252680	-4.533380	0.757480

L4chNHCONH2_Be

C	-1.249470	0.040180	3.286810
C	0.004770	0.091740	2.650300
N	-0.116870	0.054710	1.313490
C	-1.500940	-0.014310	1.034750
C	-2.195050	-0.032590	2.276460
C	-2.063680	-0.086740	-0.259730
C	-1.248230	-0.150610	-1.408610
N	0.116980	-0.159660	-1.246310
C	0.702300	-0.162480	-2.439000
C	-0.275110	-0.162420	-3.462460
C	-1.509130	-0.150440	-2.810540
C	-3.537690	-0.090980	-0.424830
C	2.207950	-0.101400	-2.364420
C	2.630320	1.189620	-1.656710
N	2.137420	1.368070	-0.407710
C	2.512460	2.456770	0.292320
C	3.405270	3.390650	-0.226480
C	3.916880	3.200580	-1.503030
C	3.520420	2.084150	-2.232610
C	-4.170880	-1.117760	-1.141490
C	-5.552580	-1.121990	-1.304730
C	-6.349490	-0.097850	-0.778450
C	-5.711460	0.933820	-0.079260
C	-4.332040	0.936750	0.104420
C	-7.848900	-0.118740	-0.939350
C	2.746240	-1.249050	-1.505520
N	2.261280	-1.333900	-0.241040
C	2.733480	-2.297060	0.573830
C	3.737300	-3.175080	0.170000
C	4.246820	-3.071770	-1.115930
C	3.736020	-2.100240	-1.972320
H	-1.421770	0.046420	4.352040
H	0.979810	0.148160	3.111070
H	-3.264390	-0.105800	2.392990
H	-0.095880	-0.163060	-4.526610
H	-2.481730	-0.133910	-3.276880
H	3.675840	4.251480	0.369920
H	4.611210	3.915610	-1.926770
H	3.900200	1.902400	-3.229030
H	-3.580440	-1.927800	-1.552960
H	-6.018550	-1.935220	-1.851480
H	-6.300560	1.750460	0.324850
H	-3.864290	1.755710	0.637560
H	-8.142280	-0.606990	-1.871140
H	-8.318410	-0.672020	-0.118640
H	-8.263970	0.891200	-0.932080
H	4.087200	-3.932280	0.858620
H	5.023170	-3.747370	-1.453250
H	4.105390	-1.995750	-2.983630
Be	1.037370	-0.004300	0.107200
H	2.664770	-0.140460	-3.349870
N	1.978430	2.612580	1.595760
H	2.656170	2.660290	2.345850
N	2.181230	-2.383580	1.873300
H	2.855370	-2.431190	2.626920
C	0.811730	3.313920	1.901240
C	1.011100	-3.080930	2.195400
O	0.579150	3.649810	3.059190
O	0.773630	-3.369790	3.364140
N	-0.013870	3.607310	0.861450
H	-0.925610	3.966070	1.098270
H	0.084720	3.178660	-0.045140
N	0.197810	-3.423190	1.162980
H	-0.712280	-3.782540	1.405120
H	0.307410	-3.045800	0.235230

L5chH_Be

C	-0.501750	0.000510	1.813440
C	0.201840	0.002330	3.010170
N	1.559260	0.002140	2.741620
C	1.641760	0.000290	1.397120
N	0.427010	-0.000840	0.832270
C	2.788260	-0.000340	0.486570
C	4.104950	-0.000180	0.969700
C	5.203850	-0.000760	0.117000
C	4.990130	-0.001530	-1.264120
C	3.695260	-0.001690	-1.772730
C	2.564000	-0.001100	-0.935130
O	1.353590	-0.001240	-1.524400
C	-1.905070	0.000710	1.233150
C	-2.067320	-1.235750	0.337600
N	-1.210040	-1.329860	-0.707710
C	-1.288240	-2.379040	-1.538620
C	-2.228390	-3.387330	-1.370830
C	-3.114200	-3.297870	-0.301560
C	-3.034520	-2.207720	0.562640
C	-2.066300	1.236620	0.336690
N	-1.208720	1.329420	-0.708520
C	-1.286080	2.378000	-1.540250
C	-2.225550	3.387090	-1.373420
C	-3.111580	3.299030	-0.304210
C	-3.032830	2.209460	0.560830
Be	0.015320	-0.000830	-0.732030
H	4.251270	0.000400	2.044570
H	6.209940	-0.000630	0.520510
H	5.832840	-0.001990	-1.947580
H	3.524960	-0.002250	-2.844240
H	-0.573760	-2.399560	-2.352780
H	-2.259320	-4.217790	-2.063570
H	-3.860740	-4.066320	-0.140330
H	-3.712030	-2.111500	1.401360
H	-0.570940	2.397670	-2.353870
H	-2.255910	4.217010	-2.066830
H	-3.857640	4.068110	-0.143690
H	-3.710590	2.114300	1.399460
H	-0.172940	0.003960	4.023320
H	-2.677040	0.001280	1.999210

L5chNH2_Be

C	0.475190	-0.000010	2.051220
C	-0.240960	-0.000020	3.242310
N	-1.597080	-0.000010	2.962090
C	-1.666820	0.	1.616610
N	-0.448090	0.000010	1.066410
C	-2.799420	0.000010	0.686480
C	-4.123450	0.000010	1.149230
C	-5.209970	0.000010	0.280650
C	-4.978130	0.000020	-1.096690
C	-3.675180	0.000020	-1.585950
C	-2.559450	0.000010	-0.731950
O	-1.334950	0.000010	-1.313390
C	1.881880	-0.000010	1.472080
C	2.051050	1.240850	0.579600
N	1.184790	1.331620	-0.466890
C	1.235450	2.382570	-1.308150
C	2.194520	3.402310	-1.122840
C	3.074290	3.300690	-0.067260
C	3.013300	2.203080	0.807510
C	2.051030	-1.240870	0.579590
N	1.184780	-1.331620	-0.466900
C	1.235420	-2.382560	-1.308170
C	2.194480	-3.402320	-1.122870
C	3.074250	-3.300710	-0.067280
C	3.013280	-2.203110	0.807500
H	-4.285710	0.	2.221730
H	-6.221450	0.000010	0.670470
H	-5.810700	0.000020	-1.792200
H	-3.488920	0.000020	-2.654680
H	2.222950	4.241750	-1.805620
H	3.816360	4.075000	0.089820
H	3.696200	2.111510	1.641270
H	2.222900	-4.241750	-1.805650
H	3.816310	-4.075040	0.089800
H	3.696180	-2.111560	1.641250
H	0.123380	-0.000030	4.259310
Be	-0.003350	0.000010	-0.480730
H	2.651930	-0.000020	2.240060
N	0.355080	-2.392010	-2.348700
H	-0.443280	-1.768120	-2.298500
H	0.226630	-3.251110	-2.859860
N	0.355110	2.392030	-2.348690
H	-0.443260	1.768160	-2.298490
H	0.226670	3.251140	-2.859830

L5chNHCH3_Be

C	-0.947320	-1.135040	-1.204980
C	0.225010	-1.460490	-0.539970
N	-0.061270	-2.361770	0.469710
C	-1.391160	-2.549890	0.393150
N	-1.935820	-1.832590	-0.604800
C	-2.298690	-3.350400	1.210530
C	-1.833300	-4.160580	2.256370
C	-2.699450	-4.908650	3.046950
C	-4.072750	-4.851050	2.792560
C	-4.561770	-4.055850	1.760770
C	-3.707580	-3.288760	0.946180
O	-4.267020	-2.545120	-0.023020
C	-1.506030	-0.228060	-2.273100
C	-2.520080	0.711920	-1.610020
N	-3.683060	0.134930	-1.175130
C	-4.634000	0.927890	-0.625010
C	-4.375940	2.298160	-0.371280
C	-3.185670	2.849760	-0.776880
C	-2.242790	2.050870	-1.442690
C	-2.237660	-1.025570	-3.356350
N	-3.221560	-1.893430	-2.956000
C	-3.896400	-2.577110	-3.912270
C	-3.648940	-2.346860	-5.288920
C	-2.672310	-1.461410	-5.669080
C	-1.935520	-0.793180	-4.682110
H	-0.764770	-4.190680	2.440370
H	-2.312260	-5.526710	3.848980
H	-4.764950	-5.426780	3.398090
H	-5.626890	-4.006210	1.561320
H	-5.141980	2.899000	0.102990
H	-2.988980	3.902180	-0.608260
H	-1.312270	2.464530	-1.807230
H	-4.218840	-2.901570	-6.024060
H	-2.464290	-1.294040	-6.719440
H	-1.151860	-0.095190	-4.943860
H	1.231370	-1.109540	-0.716370
H	-0.733270	0.372840	-2.747330
N	-4.860640	-3.494840	-3.586040
H	-5.254860	-3.928840	-4.407590
N	-5.859440	0.419710	-0.304820
H	-6.490950	1.116610	0.059780
C	-4.798260	-4.405530	-2.438460
H	-5.562550	-5.167580	-2.587760
H	-3.821920	-4.899270	-2.371090
H	-4.994930	-3.888030	-1.504250
C	-6.520170	-0.667390	-1.032530
H	-6.149980	-1.638800	-0.712390
H	-7.585640	-0.610680	-0.813130
H	-6.382070	-0.560750	-2.113480
Be	-3.478800	-1.695870	-1.080590

L5chNHCOCH3_Be

C	0.701220	0.136360	1.986300
C	-0.194820	0.291810	3.023040
N	-1.482960	0.359290	2.516430
C	-1.356880	0.241780	1.197300
N	-0.054720	0.110370	0.856770
C	-2.301870	0.213900	0.093410
C	-3.689540	0.313380	0.257980
C	-4.543020	0.270290	-0.837510
C	-4.014730	0.124060	-2.122090
C	-2.638580	0.022930	-2.310230
C	-1.781060	0.067900	-1.215300
O	-0.421010	-0.024970	-1.491960
C	2.515460	1.040570	0.605850
N	1.734670	1.082640	-0.522870
C	1.936400	2.052210	-1.460290
C	2.966370	2.990790	-1.276770
C	3.757290	2.923660	-0.149460
C	3.534390	1.936250	0.815820
C	2.202280	-1.391980	0.850880
N	1.478550	-1.418180	-0.312100
C	1.440340	-2.552860	-1.049760
C	2.055850	-3.717320	-0.586010
C	2.761460	-3.696770	0.602890
C	2.860290	-2.505360	1.323180
H	-4.084550	0.424110	1.260810
H	-5.613830	0.348520	-0.693390
H	-4.673080	0.088210	-2.982070
H	-2.218070	-0.089470	-3.301870
H	3.112290	3.746710	-2.029410
H	4.552940	3.645610	-0.012550
H	4.135760	1.872010	1.711730
H	2.002720	-4.611700	-1.191640
H	3.254450	-4.593250	0.957380
H	3.424220	-2.446750	2.243730
H	0.000140	0.357460	4.081680
N	0.784070	-2.564510	-2.281200
H	0.349030	-3.444580	-2.526920
N	1.094090	2.054300	-2.548270
H	0.425090	1.290840	-2.576600
C	0.505660	-2.118710	-4.658800
H	0.635580	-1.307030	-5.371080
H	1.008740	-3.011290	-5.042570
H	-0.555010	-2.352320	-4.548710
C	0.003320	2.598160	-4.642510
H	-0.987690	2.616640	-4.182060
H	0.041340	3.325490	-5.450110
H	0.166140	1.595860	-5.046730
C	1.066970	2.937490	-3.626330
C	1.120310	-1.725250	-3.340560
O	1.821420	3.887100	-3.736300
O	1.865300	-0.774610	-3.187690
C	2.150100	-0.061440	1.598410
H	2.838730	-0.064780	2.437370
B	0.566280	-0.052520	-0.481960

L5chNHCONH2_Be

C	0.555820	-0.005390	1.857410
C	-0.331810	-0.009200	2.926520
N	-1.629780	-0.007380	2.444420
C	-1.496830	-0.002430	1.104750
N	-0.208890	-0.001340	0.745100
C	-2.475310	0.002190	0.013460
C	-3.854110	0.001410	0.270690
C	-4.795400	0.005780	-0.753090
C	-4.359140	0.011030	-2.079430
C	-2.996800	0.012030	-2.365740
C	-2.028370	0.007820	-1.351280
O	-0.722210	0.009440	-1.742180
C	2.329690	1.241980	0.637660
N	1.632490	1.343530	-0.522360
C	1.802360	2.402610	-1.337340
C	2.723650	3.413340	-1.020280
C	3.443420	3.296060	0.156350
C	3.253330	2.202330	1.006490
C	2.331950	-1.238670	0.625730
N	1.634370	-1.331300	-0.534940
C	1.805480	-2.383170	-1.358950
C	2.729500	-3.394420	-1.051620
C	3.450150	-3.285780	0.125250
C	3.258100	-2.200130	0.985260
H	-4.176910	-0.002750	1.306090
H	-5.854180	0.005020	-0.520950
H	-5.076970	0.014400	-2.892530
H	-2.649430	0.016210	-3.393330
H	2.849880	4.249710	-1.687450
H	4.157980	4.066900	0.420330
H	3.807940	2.103240	1.929860
H	2.856930	-4.224750	-1.726080
H	4.166770	-4.057210	0.381770
H	3.813080	-2.108070	1.909150
H	-0.125320	-0.012960	3.986650
N	0.984310	-2.366620	-2.477830
H	0.279260	-1.629470	-2.478820
N	0.982970	2.393310	-2.457650
H	0.279940	1.654300	-2.465870
C	1.030110	3.253870	-3.551710
C	1.030650	-3.219260	-3.578110
O	1.863950	4.142890	-3.683430
O	1.866930	-4.104580	-3.718920
N	0.074150	-2.947250	-4.511150
H	-0.722790	-2.363850	-4.307490
H	-0.025630	-3.611690	-5.262470
N	0.077570	2.985500	-4.489840
H	-0.022060	3.655090	-5.236590
H	-0.717730	2.397370	-4.293540
C	2.032340	-0.002690	1.490210
H	2.683430	-0.006300	2.361210
Be	0.459050	0.005680	-0.710910