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Supplementary data

Complexation of Some Alkali and Alkaline Earth Metal Cations by Macrocyclic Compounds Containing Four Pyridine Subunits – a DFT Study

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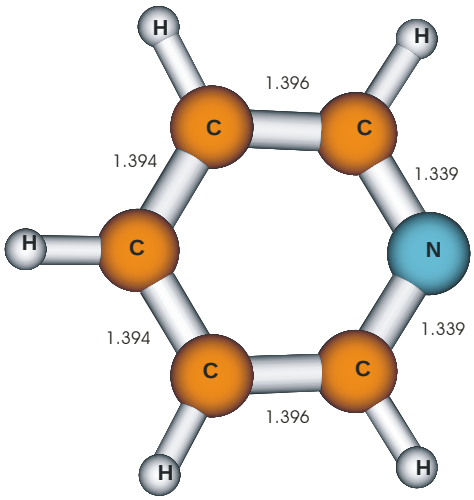
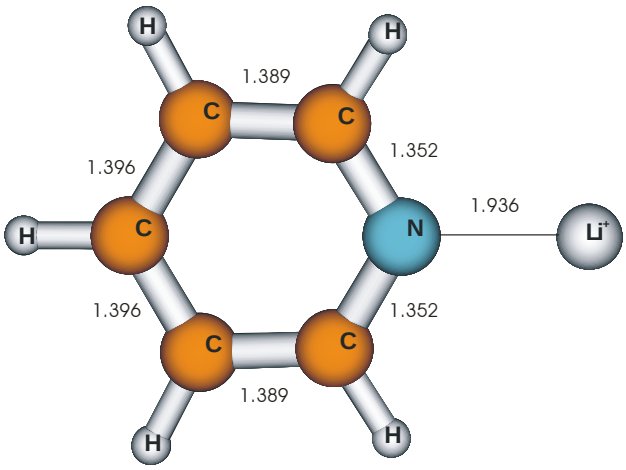


Py

Figure S1 *The structure and Cartesian coordinates of uncomplexed pyridine*

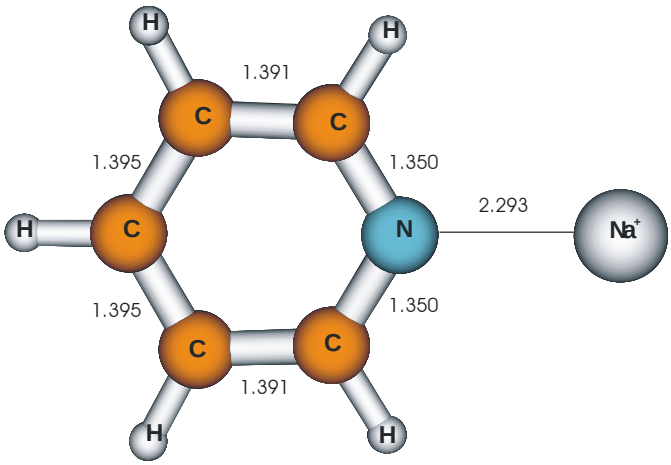
	X	Y	Z
C	-1.1821021467	0.	-0.7012122526
C	-1.1998865949	0.	0.6927548486
C	0.0162165509	0.	1.3743366152
C	1.1964671856	0.	0.6281268352
N	1.2306408063	0.	-0.7105108008
C	0.0542597967	0.	-1.3502343951
H	2.1631332783	0.	1.1300633047
H	0.0540850523	0.	2.4598997865
H	-2.1410426543	0.	1.2361315528
H	-2.1032931797	0.	-1.2767889225
H	0.1029031094	0.	-2.4383600232



Py_{Li+}

Figure S2 *The structure and Cartesian coordinates of the Li^+ complex with pyridine*

	X	Y	Z
N	0.030366551	0.	0.0175321364
C	0.0562675328	0.	1.3694619522
C	1.2367005229	0.	2.1020453387
C	2.4516641275	0.	1.415468944
C	2.4387749247	0.	0.0199914003
C	1.2141226065	0.	-0.6360018632
H	-0.905639732	0.	1.8765657688
H	1.1995342132	0.	3.1860380699
H	3.3919169473	0.	1.9583241626
H	3.3589570126	0.	-0.5541919336
H	1.1723337617	0.	-1.722589899
Li	-1.6463906362	0.	-0.950544077



Py_{Na+}

Figure S3 *The structure and Cartesian coordinates of Na^+ complex with pyridine*

	X	Y	Z
N	0.0839326593	0.	0.0484585435
C	0.1142953972	0.	1.3978106215
C	1.2944887405	0.	2.1335980915
C	2.5099612294	0.	1.4491267915
C	2.4949945189	0.	0.0542610885
C	1.2676872065	0.	-0.5999225933
H	-0.8465291035	0.	1.9076238651
H	1.2560502205	0.	3.2177177703
H	3.4502371416	0.	1.9919953425
H	3.4146504415	0.	-0.5210874857
H	1.2287861763	0.	-1.6869276412
Na	-1.9020591898	0.	-1.0981543852

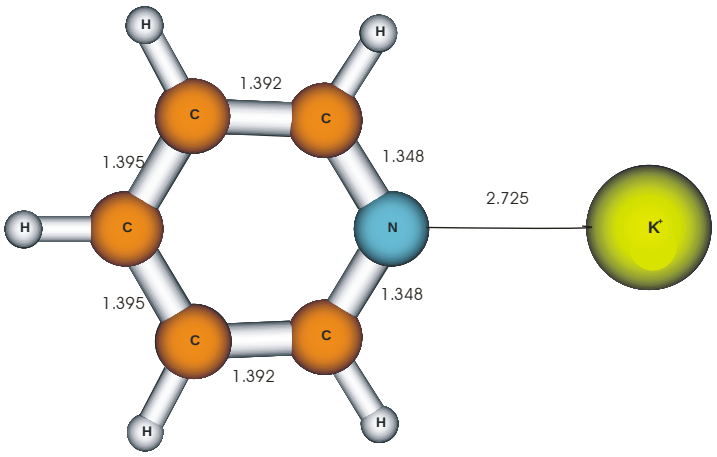
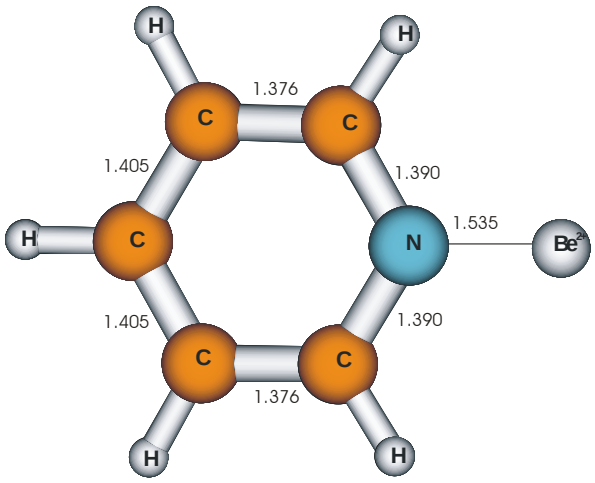


Figure S4 *The structure and Cartesian coordinates of K^+ complex with pyridine*

Py_{K+}

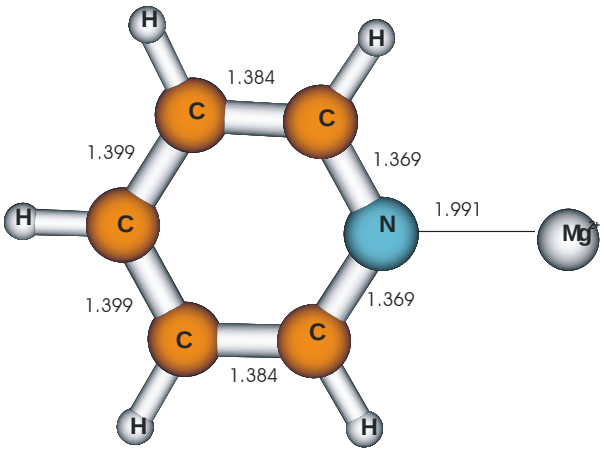
	X	Y	Z
N	0.0621850354	0.	0.0359025469
C	0.0967462306	0.	1.3829682379
C	1.2762324643	0.	2.121980568
C	2.4921599142	0.	1.4388491973
C	2.4758053103	0.	0.0442594512
C	1.246058742	0.	-0.6076994255
H	-0.8644087433	0.	1.8938391683
H	1.237346556	0.	3.2063529848
H	3.4324540492	0.	1.9817282693
H	3.3954564163	0.	-0.5316029416
H	1.2079084588	0.	-1.695519515
K	-2.2976667901	0.	-1.3265585398



Py_{Be2+}

Figure S5 *The structure and Cartesian coordinates of* Be^{2+} *complex with pyridine*

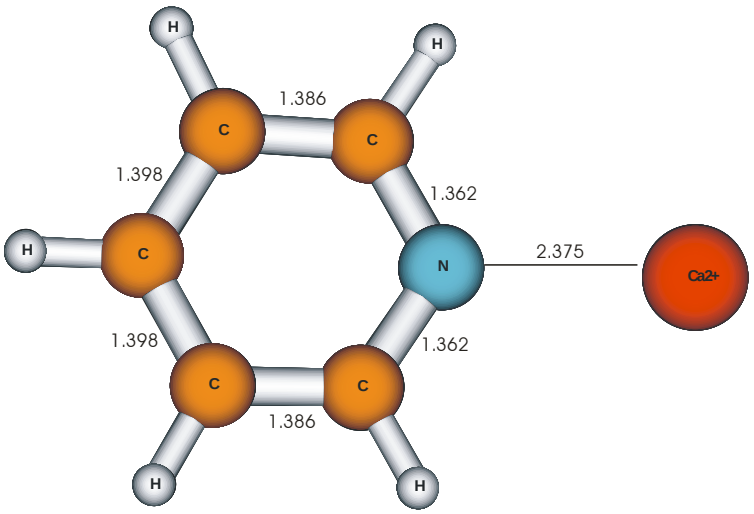
	X	Y	Z
N	0.0367786662	0.	0.0212341728
C	0.0410903044	0.	1.4113190445
C	1.2256554668	0.	2.1122754296
C	2.4433700398	0.	1.4106803502
C	2.4421119152	0.	0.0053110557
C	1.2427832976	0.	-0.6700742748
H	-0.9221527322	0.	1.9148557482
H	1.1983958269	0.	3.197935031
H	3.3849880563	0.	1.9543237655
H	3.36869089	0.	-0.5611262856
H	1.1972373564	0.	-1.7560355664
Be	-1.2924536643	0.	-0.746198471



Py_{Mg2+}

Figure S6 *The structure and Cartesian coordinates of* Mg^{2+} *complex with pyridine*

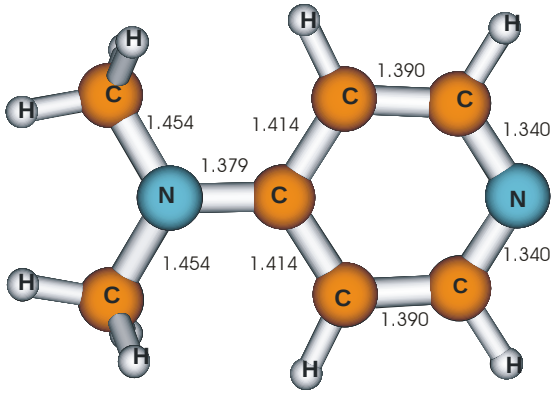
	X	Y	Z	
N	0.0707739174	0.	0.0408613403	1
C	0.0793537029	0.	1.4098681387	1
C	1.2645806884	0.	2.1247344822	1
C	2.4806712949	0.	1.4322162399	1
C	2.4723643821	0.	0.0327917602	1
C	1.2606584756	0.	-0.6362117468	1
H	-0.878792989	0.	1.9224221819	1
H	1.2289072169	0.	3.2096995267	1
H	3.4215226671	0.	1.9754170329	1
H	3.3941349371	0.	-0.5405848946	1
H	1.2254699518	0.	-1.7222681441	1
Mg	-1.6531488149	0.	-0.9544459133	2



Py_{Ca2+}

Figure S7 *The structure and Cartesian coordinates of* Ca^{2+} *complex with pyridine*

	X	Y	Z
N	0.0501651283	0.	0.0289628503
C	0.0796636809	0.	1.3907343593
C	1.260261078	0.	2.1176875582
C	2.4769312052	0.	1.4300568981
C	2.4641017616	0.	0.0325743299
C	1.2442431255	0.	-0.6263764082
H	-0.8767901979	0.	1.9103962712
H	1.2233753105	0.	3.2020686561
H	3.4173223208	0.	1.9729919618
H	3.3847604561	0.	-0.5415602308
H	1.2160566032	0.	-1.7145207208
Ca	-2.0066077495	0.	-1.1585155243



DMAP

Figure S8 *The structure and Cartesian coordinates of uncomplexed 4-dimethylaminopyridine*

	X	Y	Z
N	-0.0994868621	-0.1537241837	0.0021814337
C	0.024667712	0.2281286214	1.2808472575
C	1.2310076956	0.4206464281	1.9438305562
C	2.4449418606	0.2002315955	1.2534837162
C	2.3209240926	-0.1920851045	-0.0991075201
C	1.0547063567	-0.3509411914	-0.649857059
H	-0.9074294773	0.3972735194	1.8194771062
H	1.2183250272	0.7386087113	2.9793672773
N	3.6723770243	0.3531105936	1.8624739475
H	3.1913462083	-0.3705891589	-0.718864537
H	0.9661040605	-0.6559935724	-1.692272547
C	4.8870738917	0.26050674	1.0691247831

C 3.7466435346 0.9016374911 3.2067459509

H 4.7881938273 0.907682898 3.5331335863

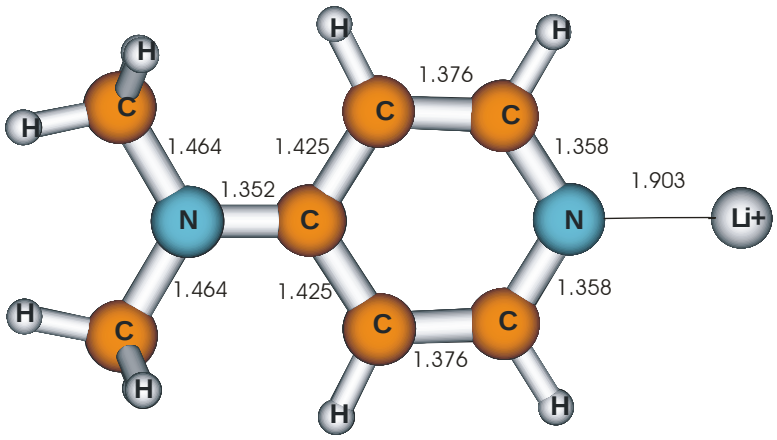
H 3.3615259514 1.931252954 3.2651826967

H 3.1794224416 0.2861593165 3.9154301586

H 5.7520516179 0.3658142266 1.726480279

H 4.9615697528 -0.7157345671 0.574969465

H 4.9465171207 1.0401997654 0.2942809075



$DMAP_{Li+}$

Figure S9 *The structure and Cartesian coordinates of Li^+ complex with 4-dimethylaminopyridine*

	X	Y	Z
N	-0.0462540717	-0.0963001361	0.0046408846
C	0.0724728895	0.2868806966	1.3025923222
C	1.2703092812	0.4816885476	1.9508334685
C	2.4967313968	0.2801061954	1.2547936721
C	2.3708051831	-0.1216409358	-0.1060720761
C	1.1226659652	-0.2888828971	-0.6602921652
H	-0.8560650186	0.4446907728	1.8471579667
H	1.2548233552	0.7876977778	2.9885200294
N	3.6991396452	0.4580796545	1.8459094576
H	3.2409100308	-0.3011421735	-0.7236251719
H	1.0422285266	-0.5960391968	-1.7008800606
C	4.9340296646	0.2388719149	1.0900078366
C	3.7792917394	0.8719376222	3.2482982525

H 4.8269660942 0.9591292214 3.533257983

H 3.3013937819 1.8463617071 3.4033050884

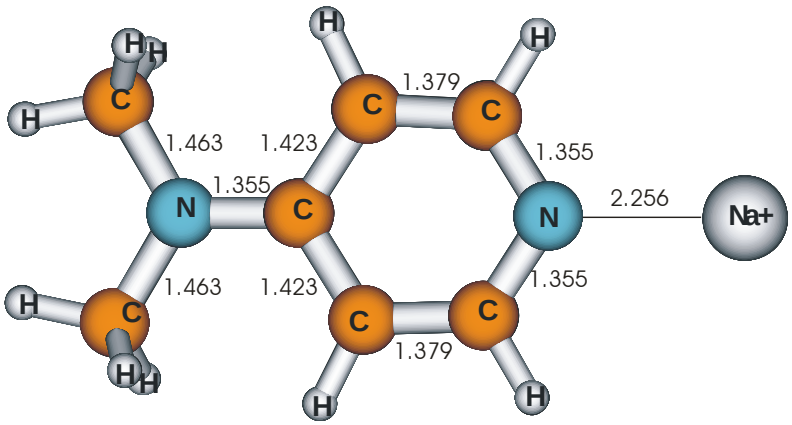
H 3.3065343821 0.1349637405 3.9080599346

H 5.7867685893 0.4329373483 1.7393160915

H 5.0043987168 -0.7958614638 0.734633206

H 4.9992399646 0.9155430438 0.2299030157

Li -1.7388618865 -0.3468363571 -0.8274522771

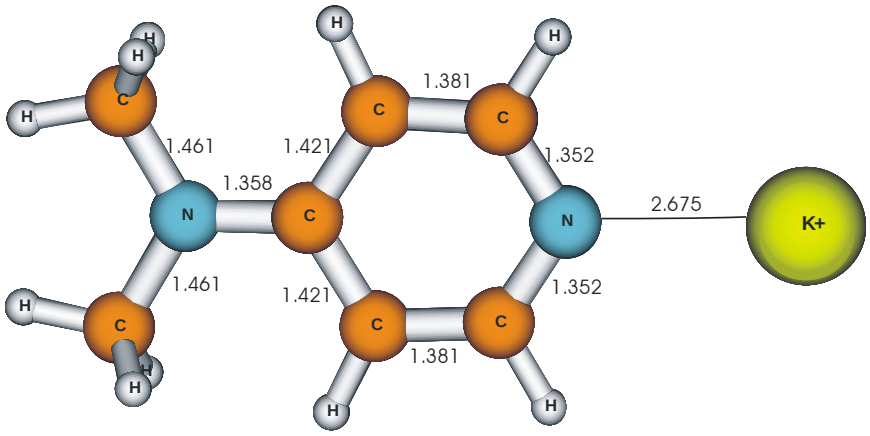


$DMAP_{Na+}$

Figure S10 *The structure and Cartesian coordinates of Na^+ complex with 4-dimethylaminopyridine*

	X	Y	Z
N	-0.0337092493	-0.1423020713	0.0262037821
C	0.0884862118	0.2599827816	1.3143336961
C	1.2874932613	0.4794274953	1.9584481541
C	2.5122787208	0.2827737044	1.2623201432
C	2.3854163047	-0.139556169	-0.0900515623
C	1.1336908165	-0.3292800652	-0.6358061205
H	-0.8385833378	0.4155485598	1.8628443959
H	1.2714819906	0.8003188121	2.9918242076
N	3.7176873169	0.4840348565	1.8475635928
H	3.2549952581	-0.3179452322	-0.7090050246
H	1.0560399583	-0.6525947549	-1.672127061
C	4.9500452227	0.2683143178	1.0897142178

C	3.7964947014	0.9186252788	3.2420143705
H	4.8438555128	1.0228481968	3.5232163952
H	3.3070215944	1.8893969567	3.3860302061
H	3.3343998485	0.1865012969	3.915204995
H	5.8040582335	0.4816022762	1.7316421496
H	5.0320100815	-0.7705191544	0.7479105244
H	5.0045843715	0.9323380518	0.2186121415
Na	-2.0402185887	-0.477330055	-0.9479857448



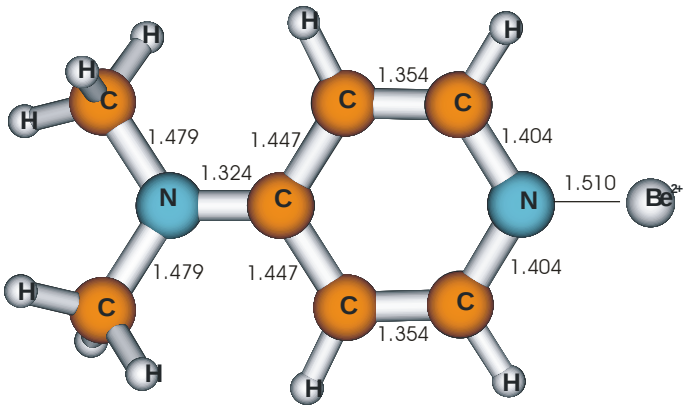
$DMAP_{K+}$

Figure S11 *The structure and Cartesian coordinates of K^+ complex with 4-dimethylaminopyridine*

$DMAP_{K+}$

	X	Y	Z
N	-0.06046035	-0.0673364751	-0.0150780865
C	0.0645234538	0.3119968363	1.2766874959
C	1.2634709085	0.497241169	1.9362712986
C	2.4876660116	0.2850606695	1.2466325312
C	2.3619089308	-0.1139088399	-0.1113673961
C	1.1070355776	-0.267958395	-0.6668024989
H	-0.8631926502	0.4795989617	1.8225231399
H	1.2466598146	0.8028248962	2.9744994463
N	3.6954976016	0.4522560794	1.8446952235
H	3.2321684917	-0.3016298977	-0.7269903028
H	1.0315164094	-0.574360157	-1.7094478823

K	-2.4395183562	-0.397297157	-1.1926321894
C	4.9266717716	0.2210545374	1.0924450161
C	3.7719232929	0.8629959331	3.2449263744
H	5.7812759181	0.406343702	1.7425778635
H	4.9895284296	-0.814127798	0.7347670243
H	5.002480696	0.895662842	0.23068191
H	4.8189526999	0.9411496438	3.5363981414
H	3.301280971	1.8414404328	3.4018249383
H	3.2890414065	0.1311780993	3.9042954113

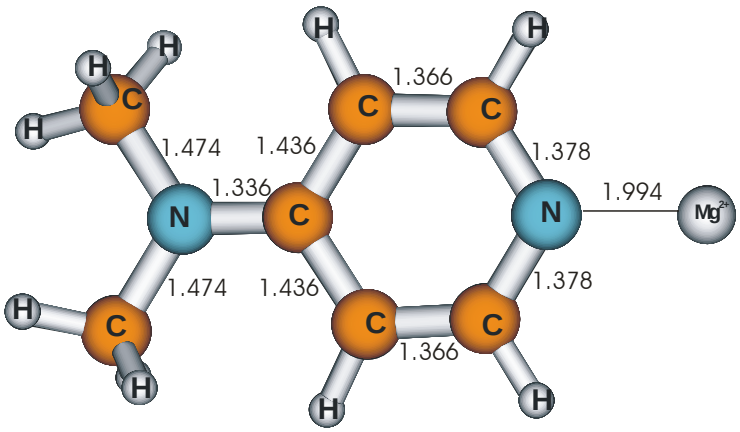


$DMAP_{Be2+}$

Figure S12 *The structure and Cartesian coordinates of* Be^{2+} *complex with 4-dimethylaminopyridine*

	X	Y	Z
N	-0.0802978111	-0.1199472214	-0.0022007139
C	0.0292488899	0.2901128578	1.3362742207
C	1.2219177495	0.4723447239	1.9502782103
C	2.4678635518	0.2718179369	1.2429705699
C	2.3362952521	-0.1552827627	-0.1334492214
C	1.1198467816	-0.3360958475	-0.6988699193
H	-0.9000880352	0.4620221119	1.8705488543
H	1.2064039542	0.7938762753	2.9835467032
N	3.6466517321	0.4563979657	1.817146531
H	3.2055035282	-0.3828725205	-0.7367591906
H	1.0318168474	-0.6709548377	-1.728054086
C	4.9192528432	0.3800409353	1.0672004252

C	3.7947926264	0.7540213466	3.2583896191
H	4.7688137551	0.3844874604	3.5809009184
H	3.752153502	1.8361562915	3.4247430766
H	3.0284231542	0.2487539972	3.8454837479
H	5.6447796681	1.0226259261	1.5675052773
H	5.2954118431	-0.6491780035	1.0703351174
H	4.7964973081	0.7380499601	0.0456524181
Be	-1.4177589113	-0.2041915123	-0.6987350997



$DMAP_{Mg2+}$

Figure S13 *The structure and Cartesian coordinates of Mg^{2+} complex with 4-dimethylaminopyridine*

	X	Y	Z
C	0.0332312511	-0.0507389811	0.0042572782
N	0.0297915326	-0.0918523117	1.3824038559
C	1.2575616716	-0.0459028248	2.0072571495
C	2.4444098667	-0.0158819787	1.3307267349
C	2.4648565797	0.0084435796	-0.1052022205
C	1.1768102029	-0.0147008107	-0.7421335568
N	3.6022238224	0.0334807251	-0.8059781663
C	4.9202204587	-0.0583671888	-0.151481294
C	3.5922536258	0.1634669927	-2.2755575469
Mg	-1.6285326842	0.3764527785	2.3855806205
H	1.2595190991	-0.0750287811	3.0934230823
H	3.3585736069	-0.0227266092	1.9100192717

H 1.0824390045 -0.0580695556 -1.8194961958

H -0.9322447444 -0.0979479823 -0.4924920769

H 5.6530794364 -0.3786649343 -0.8910527687

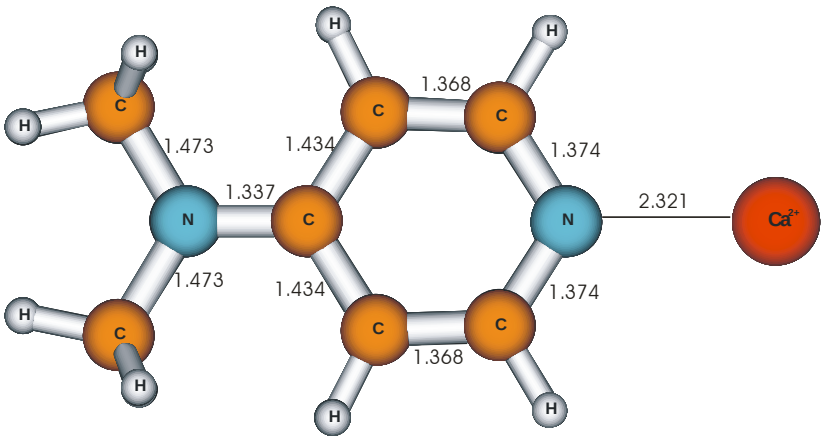
H 5.2222013183 0.917584221 0.246083613

H 4.9031498346 -0.7978141573 0.6516304493

H 4.59570115 0.4236883838 -2.608891911

H 3.30186145 -0.7849484062 -2.7430538975

H 2.9113249786 0.9577732683 -2.5890718461



$DMAP_{Ca2+}$

Figure S14 *The structure and Cartesian coordinates of* Ca^{2+} *complex with 4-dimethylaminopyridine*

	X	Y	Z
N	-0.0702609623	-0.0732518114	-0.0172652547
C	0.0561013567	0.3113755588	1.2958717894
C	1.2488682664	0.4937861345	1.939858437
C	2.4857963761	0.2836136558	1.246474616
C	2.3543496757	-0.1173438647	-0.1235410002
C	1.1156200154	-0.2743439198	-0.6817251396
H	-0.8668739699	0.4789018923	1.8493649303
H	1.2318293632	0.7985863662	2.9779441592
N	3.6747877996	0.4493962872	1.8343955436
H	3.2239066936	-0.3027636072	-0.7402262643
H	1.0481345604	-0.5797497073	-1.7250255824
Ca	-2.1350418826	-0.3663291139	-1.0367123256

C 4.9207363135 0.2222115397 1.0827247814

C 3.7621266186 0.8626191854 3.2452712294

H 5.7680702188 0.4096381489 1.7394067685

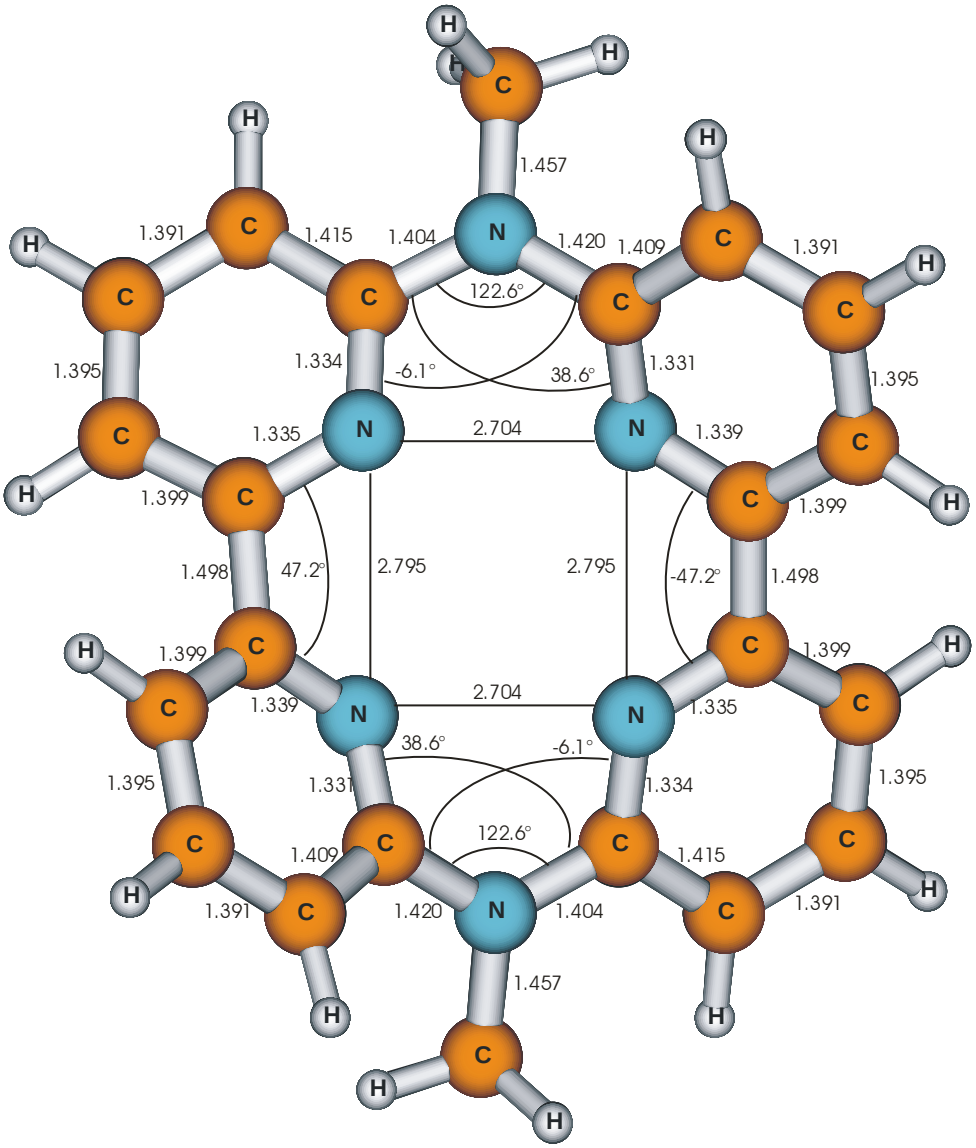
H 4.9814585323 -0.8132056715 0.7317802037

H 4.9912290828 0.9040918037 0.2289096195

H 4.8107284504 0.9386632813 3.526332716

H 3.295230599 1.8416979604 3.3947724041

H 3.2848390021 0.1245909645 3.8982958273



1a

Figure S15 *The structure and Cartesian coordinates of molecule* ***1a***

	X	Y	Z
N	-1.2225976625	1.5111600256	-0.1785326361
C	-0.4241335011	2.487912533	0.2698248015

C -0.8827871908 3.5174392503 1.0992006772

C -2.2102092263 3.4673011199 1.5258049212

C -3.0209520982 2.4094994241 1.128077497

C -2.4803527574 1.4484630223 0.2506745171

C 1.0105264832 2.3783659906 -0.146018485

N 1.5437872956 1.1658377464 0.0181510409

C 2.7893490744 0.9239875368 -0.3924719041

C 3.5946415032 1.9479151505 -0.9446282648

C 3.0427993544 3.2183130635 -1.0717132926

C 1.7258756054 3.4567273775 -0.6786196431

N 3.2860201527 -0.3776197226 -0.2189162612

C 4.6832270991 -0.6361866535 -0.54266096

N -3.2864288642 0.3772834969 -0.2176037671

C -4.6833068461 0.6359397175 -0.5427553129

C 2.4801692038 -1.4485606306 0.2502250023

N 1.2222010067 -1.5113279288 -0.178341259

C 0.4239313415 -2.4879793122 0.270555178

C 0.8829066481 -3.5173091287 1.0999810403

C 2.2105290684 -3.4670856467 1.525959633

C 3.0211628058 -2.4094368123 1.1275704355

C -1.0107559381 -2.3784780112 -0.1452289553

N -1.5441835033 -1.1660963705 0.0194717767

C -2.7894527574 -0.9240600333 -0.3919703522

C -3.594214684 -1.9475766913 -0.9456331257

C -3.0423412296 -3.2179465803 -1.0728823411

C -1.7257464009 -3.4565860235 -0.6788199063

H 2.6015684416 -4.2254548451 2.1994195167

H 0.2121212186 -4.3026099434 1.4339388558

H -1.2623539986 -4.4296604809 -0.8058721857

H -3.6413861246 -4.0195757403 -1.4977230325

H -4.6146246646 -1.7722566237 -1.2620475708

H 4.033641395 -2.3190784067 1.5071523896

H -4.0332182173 2.3191004055 1.5082188077

H -2.6009500078 4.2258087923 2.1992806886

H -0.2118497481 4.3027925719 1.4327219845

H 1.2626095055 4.4298855186 -0.8054933327

H 3.6422168814 4.0202064537 -1.4955269803

H 4.6154772131 1.7729821039 -1.2598748746

H 4.9015131779 -0.3439971785 -1.577400416

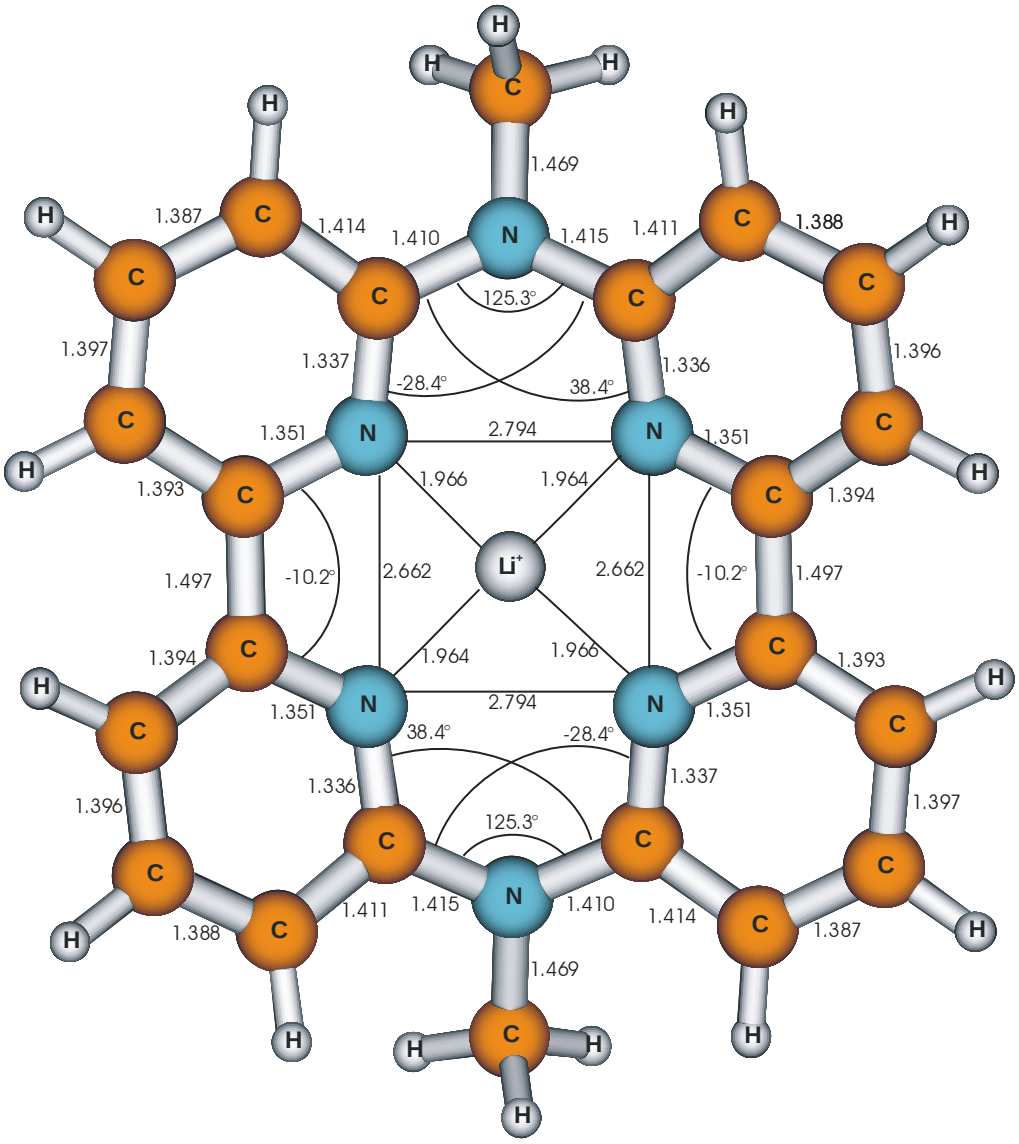
H 5.3728581533 -0.096121662 0.1206205514

H 4.8796777209 -1.7042301071 -0.4580347494

H -4.880760838 1.7035138767 -0.4548235516

H -4.8999533646 0.3469309873 -1.5787823716

H -5.3733690632 0.0931515747 0.1177970509



$1a_{Li+}$

Figure S16 *The structure and Cartesian coordinates of molecule* ***$1a_{Li+}$***

	X	Y	Z
C	-0.0084736168	0.8821625501	0.1562726162
C	-0.0754753034	0.2259992206	1.3830713746

N 1.0395651576 -0.1707197242 2.0335328221

C 2.2562565644 0.0910071114 1.5449015685

C 2.4012132567 0.7793403448 0.318605286

C 1.2567868579 1.1562882199 -0.3680961437

C -1.3649553987 -0.0900555635 2.0753971569

N -1.2644757639 -0.9118848892 3.1428770074

C -2.3357421535 -1.2122468086 3.8829615337

C -3.6075244282 -0.7000691667 3.5488781497

C -3.720996344 0.1158224208 2.432414831

C -2.5921028975 0.4363820614 1.6758034891

N -2.1932145023 -2.0696060368 4.9993090457

C -3.3822571469 -2.8348912482 5.3983392345

N 3.3952554275 -0.3292009282 2.2616522621

C 4.670328483 -0.3597553893 1.5322943004

C -1.0991037415 -2.0745499181 5.8884209155

N 0.1043287625 -1.6901678153 5.4506997375

C 1.174219057 -1.6691986979 6.2745309673

C 1.0817067796 -2.089355036 7.5992890475

C -0.1688919327 -2.4991167798 8.0673598735

C -1.2739449184 -2.4864131857 7.2294721197

C 2.4434831798 -1.1661442604 5.659820132

N 2.4141518157 -1.0024800606 4.3191611505

C 3.4630229512 -0.4949651662 3.6650562266

C 4.6414900419 -0.1439443825 4.3574190397

C 4.6883546364 -0.3436742877 5.7296281371

C 3.5805573645 -0.8593749964 6.4052447538

H -4.6892829359 0.5278067368 2.1645598418

H -2.6757853188 1.0980523515 0.8223802769

H -0.9006321748 1.1698479895 -0.3860960102

H 1.3497377959 1.682272349 -1.3135318794

H 3.3738361107 1.0385578047 -0.0769427196

H -4.476107082 -0.9031583558 4.1620039838

H 5.4835386233 0.3045817136 3.8461626692

H 5.5825942903 -0.0706968975 6.2817831068

H 3.6064416363 -0.9864092126 7.4805744833

H 1.9448322253 -2.1084475615 8.253141974

H -0.2843958437 -2.816456494 9.0993977702

H -2.2447235416 -2.7626899791 7.6179394504

H -3.0668206293 -3.7772570973 5.8498192188

H -4.023635778 -2.2970681785 6.1086982474

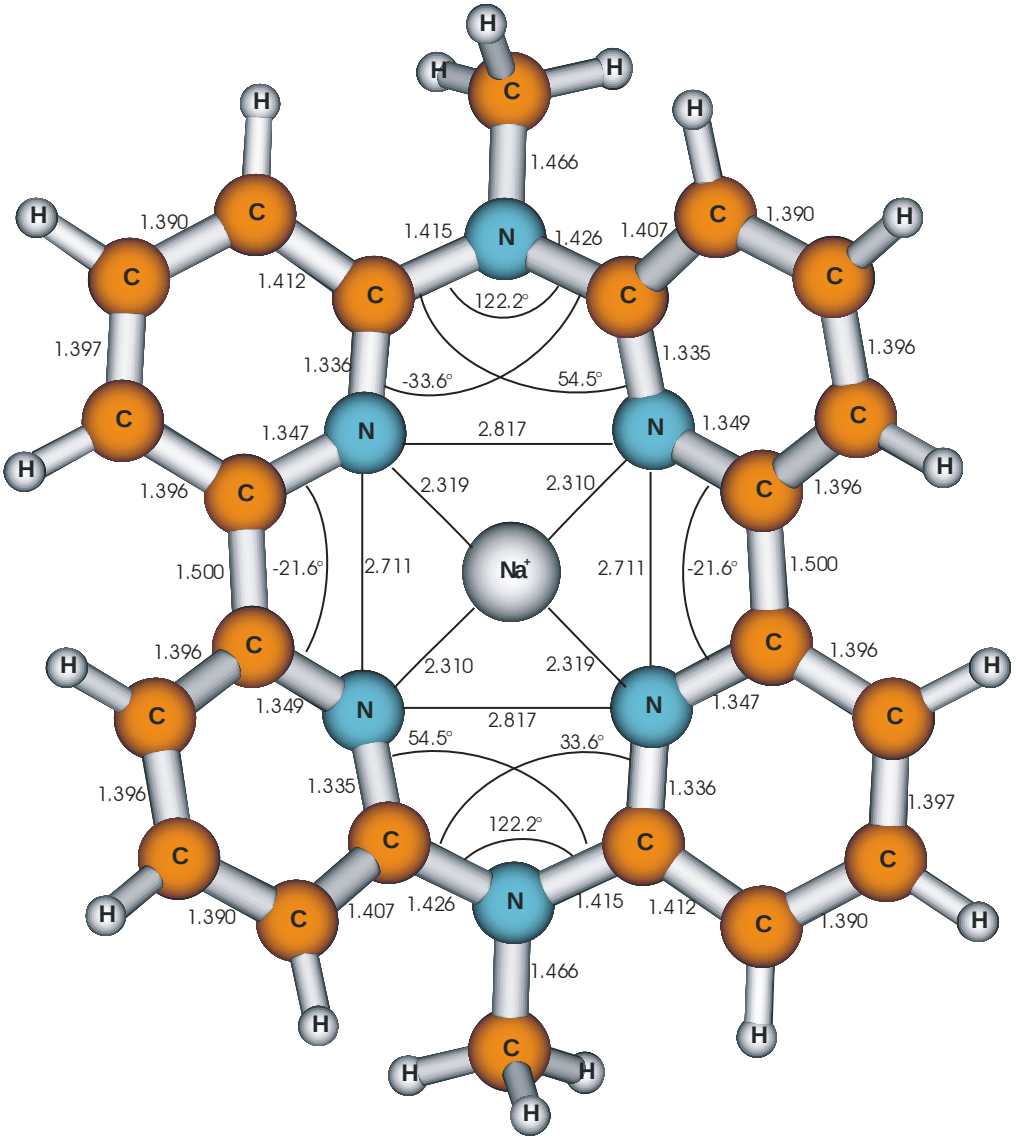
H -3.963895459 -3.0751293952 4.5078642834

H 5.3518487207 -1.0434768249 2.0392641768

H 4.49898216 -0.7503176466 0.5275606774

H 5.1469933477 0.6261192484 1.4543700749

Li 0.6101951097 -1.2843062823 3.5952422167



1a$_{Na+}$

Figure S17 *The structure and Cartesian coordinates of molecule* ***1a$_{Na+}$***

	X	Y	Z
C	0.1727747752	-0.2657578679	0.0268937066
C	-0.0335723931	-0.0191084237	1.3856956448

N 0.9806405941 0.3500311742 2.1952235771

C 2.2351656872 0.3749940057 1.739429444

C 2.5250113675 0.1314709348 0.3840299963

C 1.4721039937 -0.1660261911 -0.4728393803

C -1.3664926094 -0.2278423204 2.0409488516

N -1.3229464695 -0.4704401185 3.3649037524

C -2.4265370378 -0.7848809375 4.0481763382

C -3.6865781426 -0.8082778805 3.410541447

C -3.7407147003 -0.5019969762 2.0561739596

C -2.574330628 -0.2155037712 1.3421255013

N -2.2907382576 -1.086574343 5.4238420421

C -3.5216415454 -1.1934531022 6.2135226258

N 3.2866849864 0.6685064183 2.6570817557

C 4.4524337213 1.3746041033 2.1161602296

C -1.1363529149 -1.7390975529 5.9487512747

N 0.0629551486 -1.2063186143 5.7037759276

C 1.1864268015 -1.8419927242 6.0961496619

C 1.1330954796 -3.0025806823 6.8707139001

C -0.1205016713 -3.5228795817 7.1958567731

C -1.2723490213 -2.9104621503 6.7167571823

C 2.4811067111 -1.2815698726 5.5869035958

N 2.3820454734 -0.5283878348 4.4749186533

C 3.4692529951 -0.0632826279 3.8541925587

C 4.7570439082 -0.2951077779 4.3858684848

C 4.8571081446 -1.0237807536 5.5648820801

C 3.7158381002 -1.5412503148 6.1830434092

H -4.7000491133 -0.5057266953 1.5470126509

H -2.6178970102 0.0233687456 0.2858662575

H -0.6434419428 -0.5656192883 -0.6201214983

H 1.6692904106 -0.3657293729 -1.521874868

H 3.5440929573 0.1406721213 0.0164555048

H -4.5924159222 -1.0755986509 3.9384574234

H 5.6536388781 0.0572123715 3.893236881

H 5.8367898414 -1.2071875663 5.9963532461

H 3.7951924281 -2.1092840255 7.102653465

H 2.03741291 -3.5129508505 7.1813382216

H -0.1970959906 -4.4322333644 7.7844557022

H -2.2447464434 -3.3490001961 6.9061000015

H -4.1015249133 -2.1013748974 5.9973284941

H -3.2613359249 -1.186514586 7.2727765343

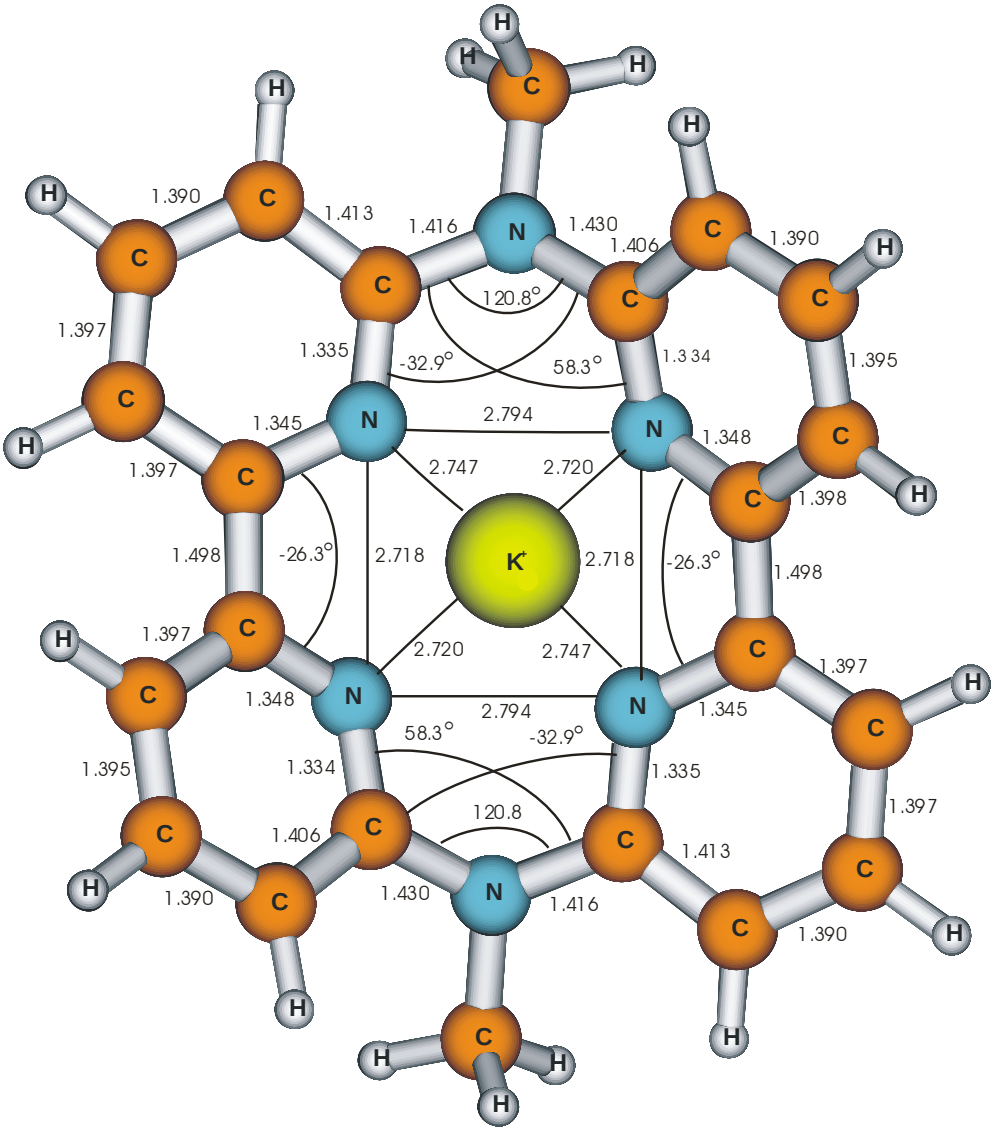
H -4.1517409767 -0.3224682982 6.017820123

H 4.9249426787 1.953141539 2.9136362048

H 5.2039386677 0.7039960454 1.6770105283

H 4.1152921925 2.0743055941 1.3502751859

Na 0.4017586836 0.6757938528 4.4078095608



$1a_{K+}$

Figure S18 *The structure and Cartesian coordinates of molecule* ***$1a_{K+}$***

	X	Y	Z
C	-0.000663675	-0.4908941357	0.1630742232
C	0.0204296914	-0.050997303	1.4892138959
N	1.1757256156	0.2191669339	2.12825694

C 2.3407886188 -0.0495415774 1.536695107

C 2.4086247658 -0.5057340339 0.2082947013

C 1.2180397553 -0.6981033509 -0.4836777763

C 1.2309530398 0.0614507562 2.305580336

N -1.0652178495 -0.1322409755 3.6257489101

C -2.1153388467 -0.1648227825 4.449457206

C -3.4241368218 0.0649195027 3.9704261053

C -3.5875557577 0.3162506817 2.6126877002

C -2.4887081722 0.3087800271 1.7502515913

N -1.8610572478 -0.4316283799 5.8170897362

C -2.9870954447 -0.3172363743 6.7471911423

N 3.5370814538 0.1461992498 2.2947664314

C 4.7266660888 0.5654005425 1.5495856255

C -0.7909525397 -1.2954562268 6.2079589568

N 0.4444470774 -0.9735549374 5.8210629032

C 1.4676167406 -1.8128371539 6.0756253283

C 1.2993083622 -2.9633380203 6.8506223573

C 0.020508088 -3.2607623719 7.3225026888

C -1.0495527647 -2.4411016554 6.9812537706

C 2.7707261121 -1.490940145 5.4097822002

C 4.0085507512 -1.9056228714 5.9071143538

C 5.1442511563 -1.6036499165 5.1519227543

C 5.0309521637 -0.9314816568 3.94003164

C 3.7415019098 -0.5392839706 3.5172989667

N 2.6645371037 -0.7972574476 4.262891854

K 1.0193139189 1.3795980149 4.5835205942

H -0.1495043958 -4.1554303874 7.9141473769

H 2.1298253813 -3.6320475907 7.0473661353

H 4.0936193994 -2.4293281705 6.8526146083

H 6.1257959626 -1.9104828176 5.5015989321

H 5.9145667452 -0.745288951 3.3436734664

H -2.0577731989 -2.7019169067 7.2811233766

H 3.3586862176 -0.7332903197 -0.2608070488

H 1.2389860949 -1.0551322453 -1.5090899711

H -0.9365154132 -0.706658718 -0.340181546

H -2.6128130816 0.5047056016 0.6911548234

H -4.5835388802 0.501850343 2.2209984645

H -4.2899558741 0.0281456603 4.6185700419

H -3.4701228077 0.6543623229 6.6140717564

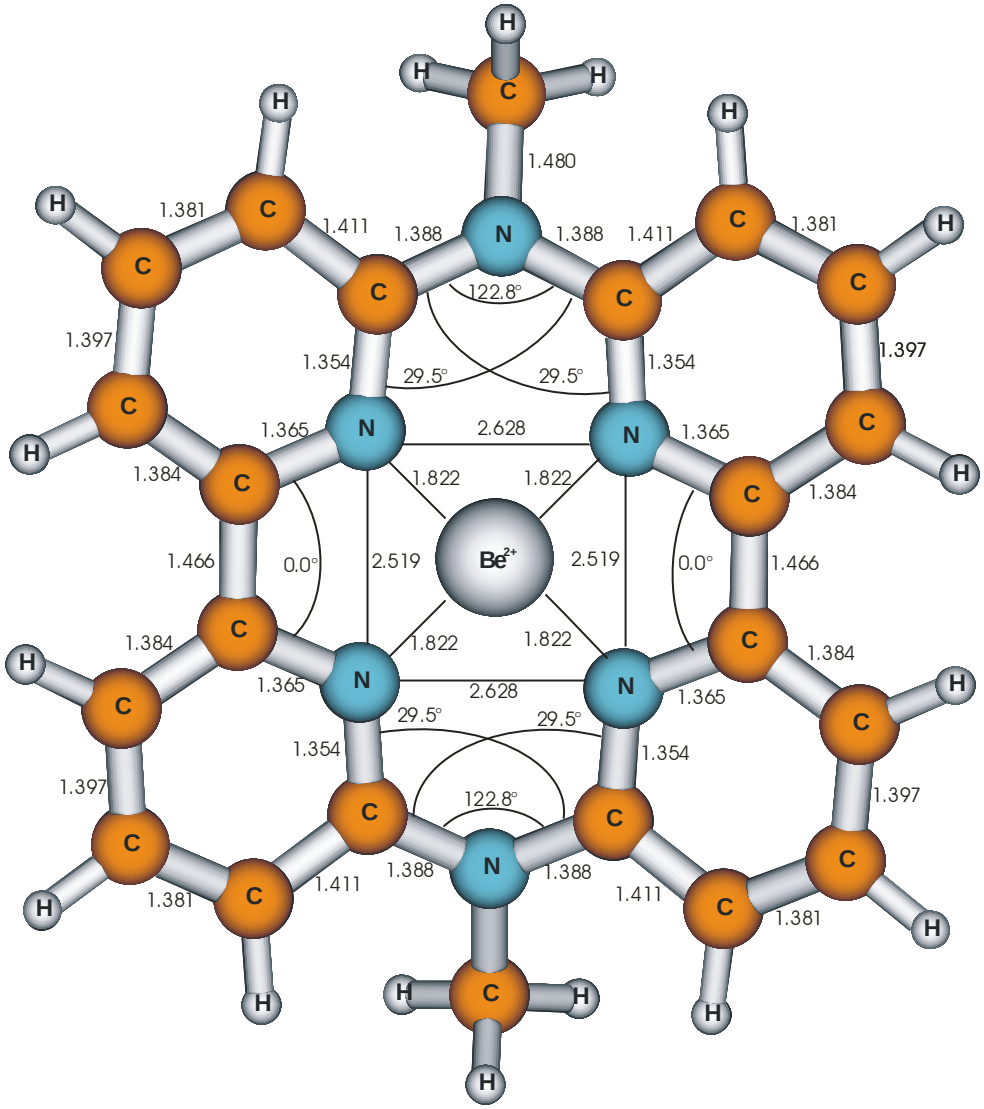
H -3.7444157262 -1.1029749932 6.616039306

H -2.6055582645 -0.3650999218 7.7681174497

H 4.4189135458 1.2328302672 0.7433735095

H 5.3919479248 1.1241797272 2.213066187

H 5.2905110624 -0.273463511 1.1177221177



1a$_{Be2+}$

Figure S19 *The structure and Cartesian coordinates of molecule* ***1a$_{Be2+}$***

	X	Y	Z
C	0.0253749209	0.0845330879	0.0047691355
C	-0.0004209185	-0.1579357505	1.3669906029
N	1.1241613321	-0.2336279531	2.1372458382

C 2.3197020333 -0.0129057368 1.5402327679

C 2.4134871088 0.2434134118 0.1556433993

C 1.2648211514 0.2775497711 -0.6103501906

C -1.2325135869 -0.2830060397 2.1515324339

N -0.9928749452 -0.4485184917 3.4852820326

C -2.0549163254 -0.4569737698 4.3257922208

C -3.3758447395 -0.344271901 3.842027783

C -3.5957514785 -0.2158622508 2.4846414007

C -2.5032791139 -0.1721643346 1.6149012162

N -1.8443547819 -0.5835205936 5.6917973425

C -2.9128447814 -0.1332075181 6.6109630891

N 3.4797095633 -0.0430703836 2.3016730508

C 4.6828740494 0.6378416736 1.7743473338

C -0.7623760517 -1.2691189683 6.2262070858

N 0.400361263 -1.3239432194 5.5337504242

C 1.4567176748 -1.9727295339 6.1054979123

C 1.3834122245 -2.6142730958 7.329488264

C 0.1707339376 -2.5824403204 8.0224908174

C -0.9006899862 -1.8994757548 7.4812375754

C 2.6888105881 -1.8476579619 5.3209564844

C 3.9120648116 -2.3575965849 5.7193482442

C 5.0313050213 -2.0890492151 4.9274913443

C 4.8886407504 -1.3118007053 3.7948495619

C 3.6122423853 -0.8250457073 3.4406498364

N 2.517399851 -1.1090305313 4.1857221505

Be 0.7709949964 -0.7054252301 3.8609091214

H 0.0671849232 -3.0915441165 8.9753780701

H 2.2406511379 -3.1239289644 7.7493474429

H 4.0090648626 -2.944435875 6.6232841216

H 6.0041849305 -2.4888894178 5.1949528666

H 5.7440314854 -1.1159951618 3.1636719412

H -1.8495183843 -1.8868143125 7.9989079896

H 3.3789030061 0.3700872662 -0.313764551

H 1.3281948321 0.4491823647 -1.6801301856

H -0.8869029804 0.131864509 -0.5752292998

H -2.6553204529 -0.0476743255 0.5508170418

H -4.6088078056 -0.1535057606 2.1002825376

H -4.2146491984 -0.4007502974 4.5214652109

H -3.3906917486 0.7491965369 6.1861153362

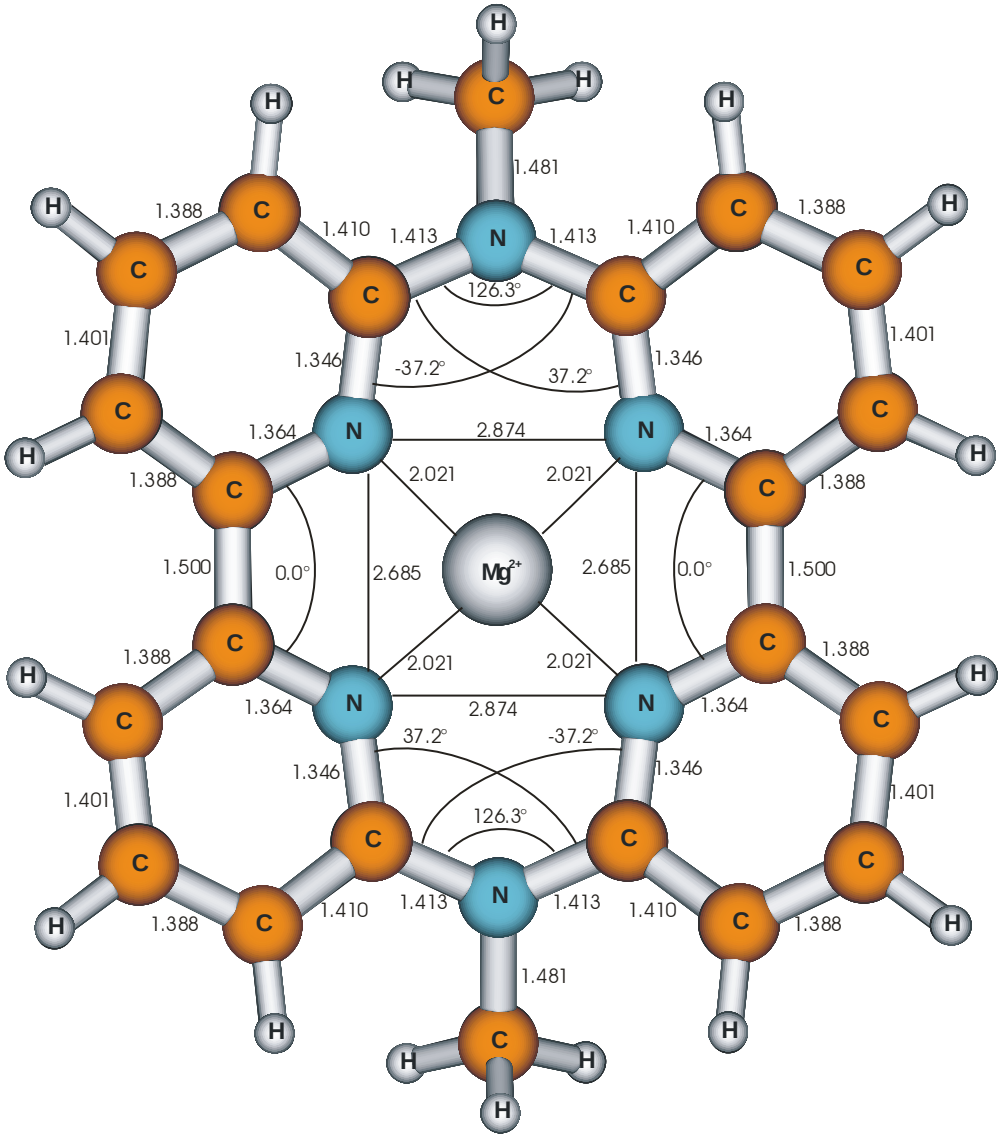
H -3.665136431 -0.9082363549 6.7914184864

H -2.4589203629 0.1637403484 7.5560799184

H 4.3713659943 1.5371369825 1.2435917293

H 5.3031334103 0.9516642387 2.6135519478

H 5.266777733 -0.0015442411 1.1039603467



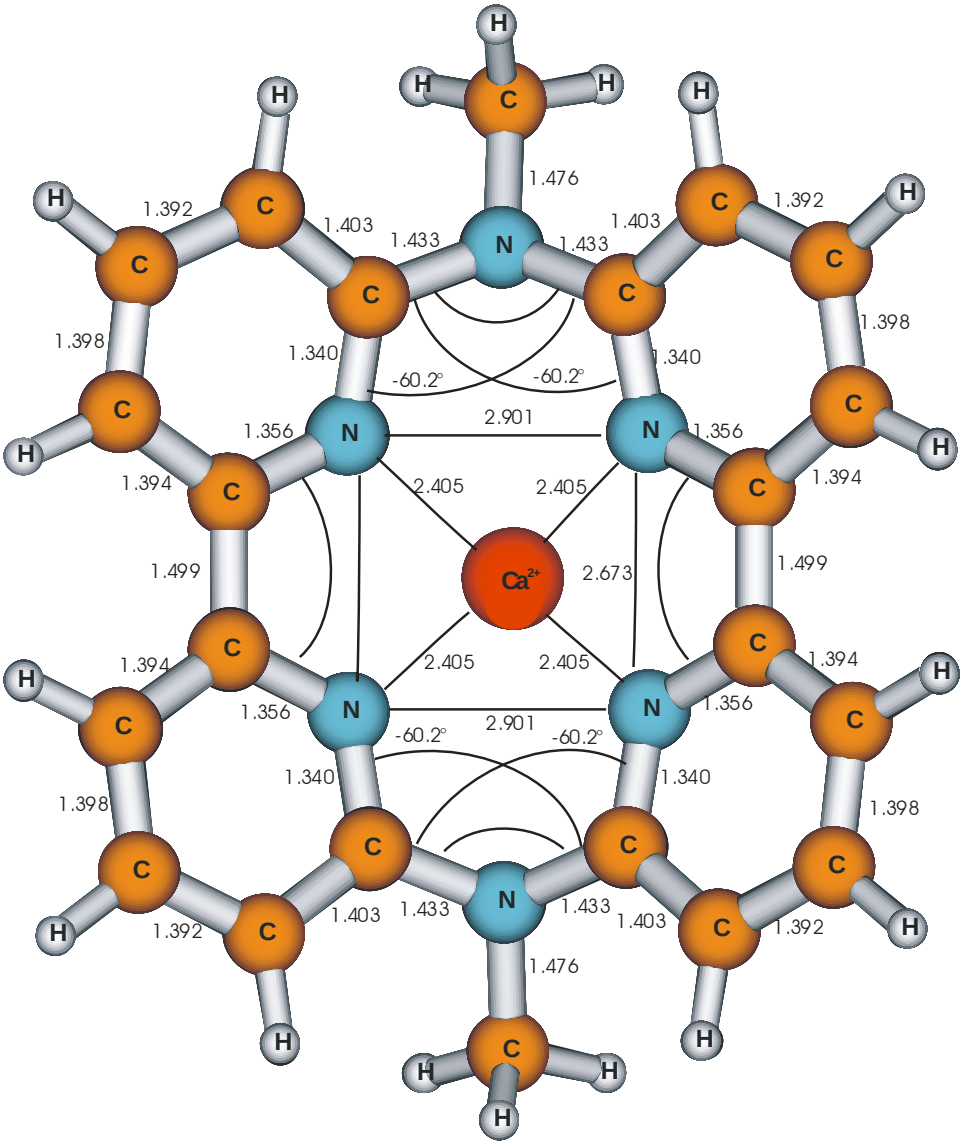
1a$_{Mg2+}$

Figure S20 *The structure and Cartesian coordinates of molecule* ***1a$_{Mg2+}$***

	X	Y	Z
N	0.1152418008	0.2657747735	0.0223002449
C	0.0405373717	0.2418779745	1.3837009287

C	1.1927709779	0.1184875536	2.1474233989
C	2.4162776582	-0.0198166222	1.4799279522
C	2.4734119291	-0.0452757053	0.0938211828
C	1.2768410179	0.099398031	-0.6370990172
C	-1.341395241	0.3225975381	1.9623064828
N	-2.3582525145	0.4101760766	1.0579291933
C	-3.6525500543	0.3872553229	1.4268037847
C	-3.9813443837	0.3317432979	2.7963934401
C	-2.9542875877	0.2939492075	3.7285558123
C	-1.6138839047	0.2825033841	3.3225561148
N	-4.6649668558	0.445640008	0.4429719084
C	-5.9843098207	0.9480802281	0.890782003
N	1.2891011898	0.0979988873	-2.0499608482
C	2.5762947866	0.4482302293	-2.6934775115
C	-4.6296363852	-0.1674764431	-0.829490736
N	-3.4722353304	-0.2222698448	-1.5144862684
C	-3.3736760928	-0.8311899231	-2.7306572468
C	-4.5014445002	-1.3568629633	-3.3454276976
C	-5.7227226265	-1.2778023281	-2.6643414064
C	-5.8006384792	-0.7011512547	-1.4047368747
C	-1.9917406105	-0.9118905208	-3.309260927
C	-1.6947713916	-1.520806614	-4.5205283463
C	-0.3521338203	-1.5914557254	-4.9129332415
C	0.6541371203	-1.0780775218	-4.107287543
C	0.2997603138	-0.4553028872	-2.8933980044

N	-0.998746396	-0.3666696563	-2.5501411206
Mg	-1.6955882218	0.4750381394	-0.8501497263
H	-3.1959754138	0.2447558004	4.7857752803
H	-0.8243307061	0.2291425408	4.0614196645
H	1.1622519063	0.1129514626	3.2296427927
H	3.3308682105	-0.1366063034	2.0530164126
H	3.4204807606	-0.2068129251	-0.4031039964
H	-5.0102593082	0.2856195843	3.1268090775
H	1.6890041627	-1.1897522588	-4.4014764054
H	-0.0902123481	-2.0787564026	-5.8470002849
H	-2.4662369078	-1.9469890335	-5.1493132313
H	-4.4528493261	-1.8308849832	-4.3175915475
H	-6.6170902094	-1.6975544092	-3.1142979445
H	-6.7417635261	-0.6974451023	-0.8715972797
H	-6.5108959227	1.3675664461	0.0332359375
H	-6.6008767404	0.1674049702	1.3497263236
H	-5.829075599	1.7546685683	1.6076952062
H	2.3755483567	0.8487106028	-3.6874413217
H	3.0573701737	1.2357742159	-2.1129704646
H	3.2545844538	-0.4080618624	-2.7767014292



1a$_{Ca2+}$

Figure S21 *The structure and Cartesian coordinates of molecule* ***1a$_{Ca2+}$***

	X	Y	Z
C	0.1013393496	-0.1120945302	0.0469889222
C	0.0406329704	0.0503720458	1.4298262546

N 1.1717633576 0.2693447139 2.1458344937

C 2.382294262 0.2062473583 1.5741474529

C 2.5152559511 0.0420326417 0.1871146445

C 1.3554242562 -0.0916317905 -0.5706707668

C -1.2199495162 -0.0771098973 2.2311153476

N -1.0760961511 0.0420116096 3.574687178

C -2.0823009064 -0.2452647259 4.4120739731

C -3.3606967265 -0.5521903986 3.9221723185

C -3.5424174708 -0.5869334887 2.5426481029

C -2.4648973671 -0.3716118714 1.6782189141

N -1.7867168233 -0.1986390368 5.8137114646

C -2.9318457802 0.070352602 6.7060114208

N 3.5131581164 0.3373677122 2.4448276231

C 4.751013086 0.8473788532 1.8223493987

C -0.7749456281 -1.0679540771 6.3378749294

N 0.460154041 -0.9246808786 5.8376812865

C 1.4649965346 -1.7666391598 6.1862040615

C 1.2711498416 -2.7226071383 7.1816287128

C 0.0077815793 -2.8210267958 7.7722760614

C -1.0399129618 -2.0126482047 7.3407940834

C 2.725588635 -1.6391190922 5.3849357623

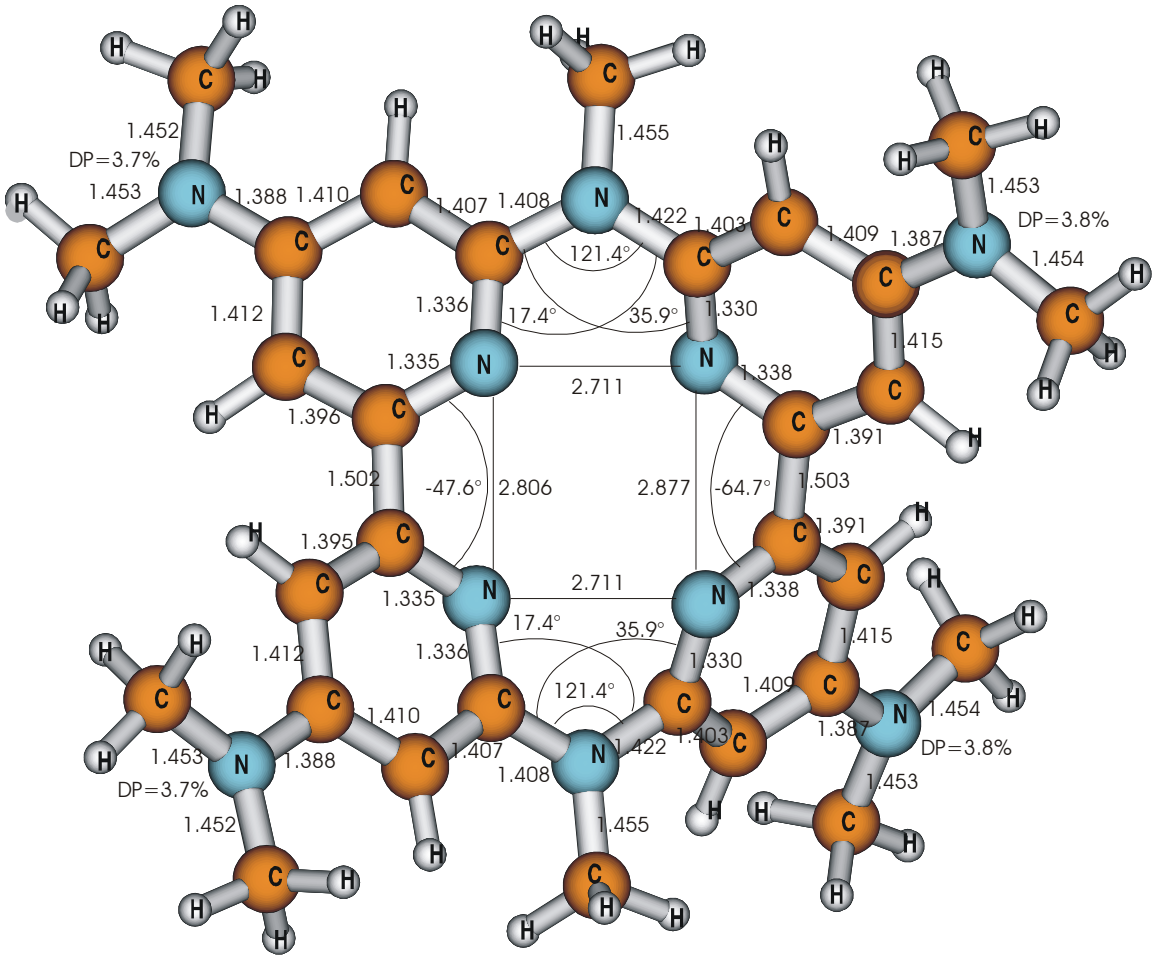
C 3.8374350389 -2.4629554892 5.5504961864

C 4.9056914956 -2.3255139248 4.6590984283

C 4.8360912401 -1.4182488399 3.6058461605

C 3.6896617316 -0.616377461 3.4999767517

N	2.7080060337	-0.6973357843	4.4088173239
Ca	0.9697074384	0.9640608388	4.4391727864
H	-0.1689468997	-3.5608596431	8.5469454429
H	2.0661997682	-3.3889711292	7.4931081811
H	3.8834882179	-3.2050399417	6.3381220977
H	5.7810910973	-2.9588741282	4.7650637674
H	5.6386733158	-1.3594123749	2.8815606814
H	-2.0317898231	-2.1353287939	7.7571105469
H	3.4868651938	-0.0055262811	-0.2881778214
H	1.4287607653	-0.2203460494	-1.6461951342
H	-0.791076452	-0.2636661451	-0.547809286
H	-2.6082981931	-0.4474360108	0.6073072923
H	-4.521178461	-0.822035177	2.1358897803
H	-4.1835295723	-0.7812116624	4.5875178958
H	-3.4883217453	0.9238556548	6.3141582768
H	-3.6172940552	-0.7797861614	6.8081524694
H	-2.5512202005	0.3341409874	7.6945564833
H	4.5071416953	1.7324711587	1.2317398832
H	5.444251885	1.1428343994	2.6121643158
H	5.2483097415	0.116845319	1.1727150795



1b

Figure S22 *The structure and Cartesian coordinates of molecule* ***1b***

	X	Y	Z
N	1.5232159676	-1.3371968294	0.3771475407
C	1.5188074135	-1.2847822525	1.7143435844
C	2.6673019366	-1.1839659043	2.4920486143
C	3.9168168973	-1.0459647648	1.8422984901
C	3.897905538	-0.9712520242	0.4350465277

C 2.6823399909 -1.141535217 -0.2449583942

C 0.1355421739 -1.2569878262 2.3017435828

N -0.5520948401 -0.154847432 1.9803376069

C -1.8520724017 -0.134098712 2.2605083442

C -2.5046876051 -1.1693099722 2.9471186839

C -1.7563598661 -2.2733983442 3.4024124531

C -0.390170268 -2.314658747 3.0359011917

N -2.5897324936 1.0021808248 1.8270006266

C -3.5300327173 1.6285522079 2.7435259242

N 2.6558077894 -1.1036948331 -1.6666006425

C 3.6657623783 -1.837084566 -2.4140332461

C -2.2973649953 1.647048391 0.6104362823

N -1.5660078386 0.9619574681 -0.2725519183

C -1.2320348842 1.5642233237 -1.4157920178

C -1.6764944057 2.8345865592 -1.7845924245

C -2.5069161813 3.5448396209 -0.8906002486

C -2.7964511408 2.936163282 0.3474075384

C -0.2964841701 0.784222948 -2.2948337733

N 0.7651222881 0.2685417293 -1.6716767618

C 1.5741973243 -0.535957219 -2.3659966011

C 1.3993463175 -0.7896264149 -3.7390106124

C 0.3207235513 -0.1859348911 -4.4165873313

C -0.5634234503 0.6068635371 -3.6530192593

N -3.0079443376 4.7998884796 -1.2084928256

H -1.3452896588 3.2629643568 -2.7213684033

H -1.4567922855 1.0422043286 -4.0809491263

N 0.1299210772 -0.3780449117 -5.778175178

H 2.0694537929 -1.4499281639 -4.2678952692

H -3.3799603325 3.4634107663 1.0865209886

H 4.7961588924 -0.7396021985 -0.1215728018

N 5.1004734524 -0.9513712756 2.5592572335

H 2.5786498041 -1.1558025787 3.570458806

H 0.2357787411 -3.1683360396 3.2618301648

N -2.3394395509 -3.2907292256 4.1434097177

H -3.5777672747 -1.1323531464 3.0793302206

H -3.1678426518 2.6092080718 3.0865213136

H -4.5137902803 1.7714733825 2.2778937426

H -3.6483737168 0.9974487703 3.623396953

H 4.4297357964 -2.1979369778 -1.7265746329

H 3.2361730959 -2.7141876234 -2.9206462547

H 4.1451387136 -1.2050694807 -3.1728309186

C -3.7835967547 -3.323632055 4.2960507661

C -1.607915061 -4.5308304311 4.3470188999

H -4.05303392 -4.1435566525 4.9656034249

H -4.145465934 -2.3936845036 4.7492414518

H -4.3159043921 -3.4671161287 3.3416474337

H -2.1982229774 -5.190446609 4.9868753503

H -1.3923072422 -5.0618428402 3.4062440638

H -0.656212222 -4.3421892911 4.8559043484

C 6.3235205401 -0.5787536949 1.8698491121

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H 7.1582860956 -0.6274118105 2.5726807729

H 6.5361513093 -1.2794138202 1.054375533

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H 6.0631453664 -0.7476808936 4.3955784603

H 4.559390791 0.1958715826 4.2821555161

H 4.5040193122 -1.5696434362 4.4849921191

C -1.113809321 0.0597549422 -6.3893224473

C 0.914313241 -1.3823437245 -6.4748071191

H 0.6469773031 -1.3730693516 -7.533713987

H 1.9857391173 -1.1605098178 -6.4030291591

H 0.7514840062 -2.4007591007 -6.086176177

H -1.0651772246 -0.1213361564 -7.4654482751

H -1.9975703652 -0.4631003709 -5.9898412881

H -1.2618438544 1.1353557627 -6.2413927014

C -2.4990553895 5.4910958914 -2.3812242926

C -3.6548205683 5.5929024207 -0.1780254505

H -4.0039159223 6.530732477 -0.6155701755

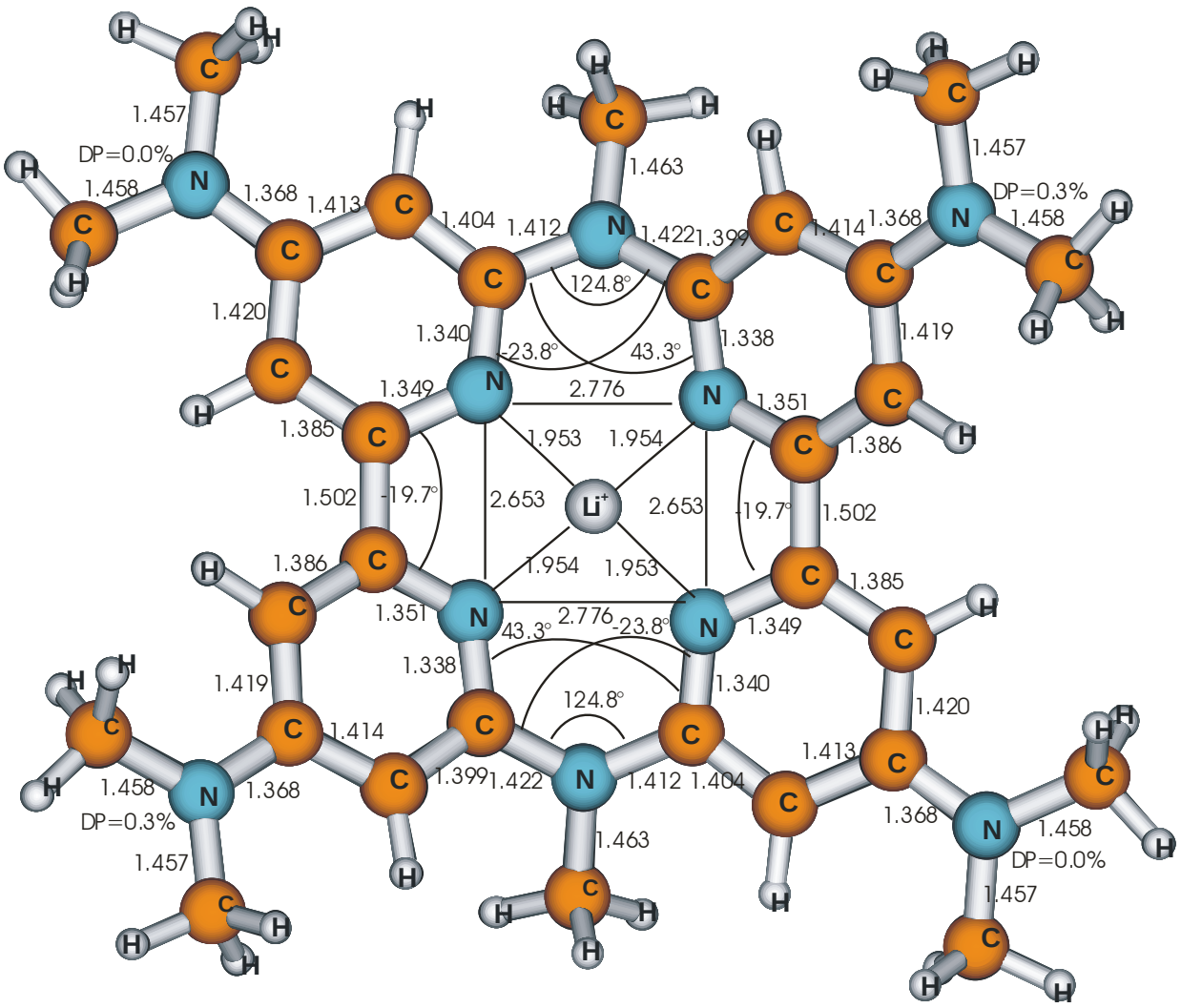
H -4.5306869983 5.0706049005 0.2249378739

H -2.9851039645 5.8325204116 0.6638652463

H -3.0416556078 6.4311258659 -2.5042465604

H -1.4230827952 5.7186352584 -2.3141032551

H -2.6625738153 4.894159242 -3.2854604465



$1b_{Li+}$

Figure S23 *The structure and Cartesian coordinates of molecule* ***$1b_{Li+}$***

	X	Y	Z
C	-0.1634102896	0.1070758252	0.1719776163
C	-0.0814608902	0.2568794602	1.5471622061
N	1.0959040503	0.3437874389	2.2039461444
C	2.2365484572	0.2042275609	1.5185450035

C 2.2507428259 0.032307319 0.1298630352

C 1.0324889587 0.0138150072 -0.5869046262

C -1.2967072242 0.2835421931 2.4295449974

N -1.0504922394 -0.0292780366 3.7187260431

C -2.0626509137 -0.0726605753 4.5952692422

C -3.382650332 0.198256735 4.2028586012

C -3.654298853 0.5645198663 2.8656688187

C -2.5593688707 0.6072270582 1.9623655283

N -1.7747047377 -0.3976673799 5.9392220509

C -2.833422308 -0.1820576222 6.9262049564

N 3.4688056061 0.2645544495 2.225168632

C 4.61809746 0.8097568173 1.5017127861

C -0.6372925838 -1.1340306308 6.369891937

N 0.5539825737 -0.8482960122 5.831802253

C 1.6359183314 -1.5629856623 6.2109329002

C 1.5843722595 -2.5345330185 7.1977095957

C 0.3435998191 -2.8182039906 7.8260321787

C -0.7882040586 -2.1105227333 7.3607927717

C 2.8905536176 -1.2587842358 5.4431531537

C 4.1556395241 -1.5621058814 5.9173858525

C 5.2799235315 -1.2728267798 5.0994888328

C 5.0354080217 -0.6786476873 3.8412434354

C 3.7200582242 -0.3686739997 3.4623610923

N 2.6785645457 -0.6584684454 4.2535533742

Li 0.8598593568 0.0410379059 4.1194632934

N 0.2418570816 -3.7610755114 8.8119273879

H 2.4718078007 -3.0990297717 7.4455859222

H 4.2795026698 -1.9877353774 6.9029491414

N 6.5512358396 -1.5675409384 5.5104988788

H 5.8579714207 -0.495397404 3.1690980899

H -1.7724236984 -2.3523742192 7.7331599839

H 3.1866682885 -0.1315078175 -0.3830170398

N 1.0054385889 -0.1251731869 -1.94752882

H -1.1291496488 0.0138268267 -0.3037251555

H -2.6978244286 0.9102809971 0.9343451387

N -4.9258216374 0.8574657509 2.4540461991

H -4.1950611951 0.1002878686 4.9045431447

H -3.3041488592 0.7871023335 6.7443315621

H -3.6115899957 -0.9586548613 6.9067463462

H -2.3883401245 -0.1563440821 7.9211826187

H 4.261889057 1.5305700531 0.7653136512

H 5.2672952104 1.3397366847 2.2028519434

H 5.2123663329 0.0416228596 0.9861145079

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C 2.2475172439 -0.2870868002 -2.6924382644

C -6.0262770238 0.8520049225 3.4090575889

C -5.1877248416 1.1994848344 1.0613495563

H 2.0242535905 -0.309488218 -3.759355459

H 2.9290968518 0.5524918096 -2.5095600963

H 2.7669640643 -1.2200060117 -2.4322990389

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H -0.821382422 -1.1429591806 -2.3492076186

H -0.9028565987 0.6330072139 -2.4677664776

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H -4.6790107857 2.1267997032 0.7657725969

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H -6.1989689353 -0.149500731 3.8257703019

H -5.8394876066 1.5454180522 4.239271574

C 7.6924864118 -1.2194024487 4.6741823379

C 6.7771237732 -2.2120871084 6.7984077108

H 8.612812752 -1.4767393855 5.1988128834

H 7.6809132525 -1.7657114359 3.7213454646

H 7.7163066374 -0.1437072865 4.4567430799

H 7.8428896469 -2.4091741706 6.9164321532

H 6.4543060792 -1.5778844846 7.6348551769

H 6.2480627177 -3.1712663413 6.8650991086

C 1.4074038822 -4.5461835065 9.2004170299

C -1.0573362378 -4.0789289895 9.3906600135

H 1.1335867926 -5.2068040551 10.023381844

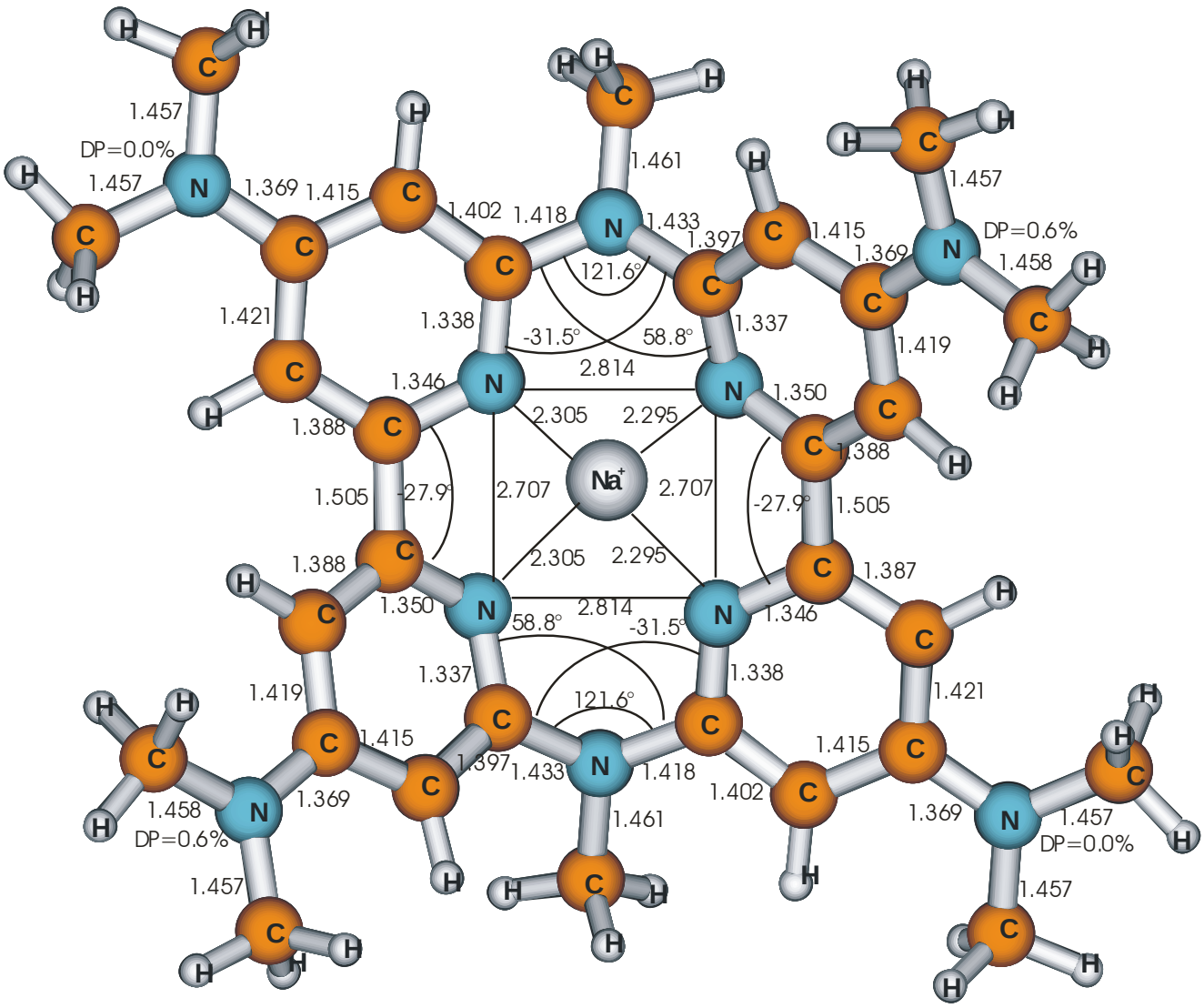
H 1.7801422615 -5.1669560445 8.3741058628

H 2.2237995602 -3.9006371265 9.5464349325

H -0.9219361203 -4.7945867785 10.2019315625

H -1.5323250483 -3.1831714467 9.8088602669

H -1.7407386131 -4.5232084637 8.6534947547



1b$_{Na+}$

Figure S24 *The structure and Cartesian coordinates of molecule* ***1b$_{Na+}$***

	X	Y	Z
C	-0.1465472372	0.0779553332	0.0191513667
C	-0.0961946271	0.160164958	1.4031696046
N	1.0608040324	0.2046514612	2.0895760819

C 2.2223560237 0.2423457136 1.426263831

C 2.2768219108 0.1910275104 0.026086218

C 1.0729324662 0.0811983689 -0.7096326961

C -1.3263613625 0.2480992426 2.2648444236

N -1.1951641054 -0.2166534256 3.5255398827

C -2.1582831062 0.0588251463 4.4104577585

C -3.3556959898 0.681180463 4.0506836767

C -3.5702223652 1.052727609 2.7026661541

C -2.4852785655 0.8611185093 1.8087499036

N -1.9403853134 -0.3183547487 5.7752431868

C -3.1100231898 -0.7662743878 6.5280963422

N 3.4046033501 0.3283593843 2.2041892893

C 4.6828429042 0.1950562409 1.5086272592

C -0.8338240271 0.1727210594 6.5132416734

N 0.2869607021 0.4285968475 5.8284232944

C 1.3583324617 0.93134791 6.4696586091

C 1.3859253381 1.1353644977 7.8416703458

C 0.2211005176 0.8396142469 8.5992867818

C -0.9156640632 0.370541951 7.8989784768

C 2.5051983997 1.2892292835 5.564039706

C 3.3512686783 2.3505279606 5.8550966203

C 4.3266674721 2.7451899244 4.903391577

C 4.306929997 2.0742510423 3.6581319572

C 3.4248806118 1.0088201436 3.4647230434

N 2.5934838179 0.5793378354 4.4191289447

Na 0.9092646992 -0.9431132368 4.083172178

N 0.1939800601 1.0179703862 9.9565628345

H 2.2887397618 1.489753142 8.3195885211

H 3.2200298873 2.9008428216 6.7765714508

N 5.2079272559 3.7611583897 5.158779193

H 4.9338025134 2.4078985697 2.8435711667

H -1.839564098 0.1984177726 8.4283536087

H 3.2192074468 0.2642197744 -0.4935369703

N 1.0822943422 -0.0021251556 -2.0762761565

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H -2.5271861978 1.2374618661 0.7959343142

N -4.7470183583 1.618433001 2.2913729041

H -4.0887470272 0.9157871717 4.8092316136

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H -3.7818194135 -1.2956375682 5.850871914

H -2.7935018625 -1.4648969756 7.3076081472

H 4.6648879671 -0.7042112645 0.8866196218

H 4.9263026153 1.0547823162 0.8659881216

H 5.4752259354 0.079054102 2.2494653691

C 6.127574507 4.2100403637 4.121786745

C 5.1127734632 4.5179887589 6.4006805176

C 1.3591929303 1.5516658788 10.650353766

C -0.9953877938 0.6661173564 10.7205721286

H 6.8028331676 4.9562535344 4.5417354374

H 6.7371114035 3.3772790859 3.7515957195

H 5.6034406554 4.6633046086 3.2681655489

H 5.9335258025 5.2345441715 6.4449053999

H 4.1678375617 5.0743010037 6.4764770821

H 5.1974696223 3.8574436365 7.2717289576

H 1.1247346927 1.6614976573 11.7094504207

H 2.2276227222 0.8852189125 10.562081192

H 1.6402013113 2.5395886853 10.2632184819

H -0.7921627692 0.8031515939 11.7829448953

H -1.8545078677 1.2973118957 10.4550170103

H -1.2752282737 -0.3833536594 10.5625885307

C -0.1714911045 -0.0617978287 -2.8167887225

C 2.3449704646 -0.0426192629 -2.8016146917

H 2.143766325 -0.1904825454 -3.8629195687

H 2.9115016864 0.8920944765 -2.6904122897

H 2.9759669504 -0.8724964693 -2.4583856886

H 0.0453480232 -0.0773472969 -3.8851792943

H -0.7465742763 -0.9653088563 -2.5737638391

H -0.8007803696 0.8142456103 -2.6133831345

C -5.8023412606 1.8956684367 3.2567917232

C -4.8851779772 2.1102669252 0.9263906198

H -6.6846020495 2.2573061417 2.7276420962

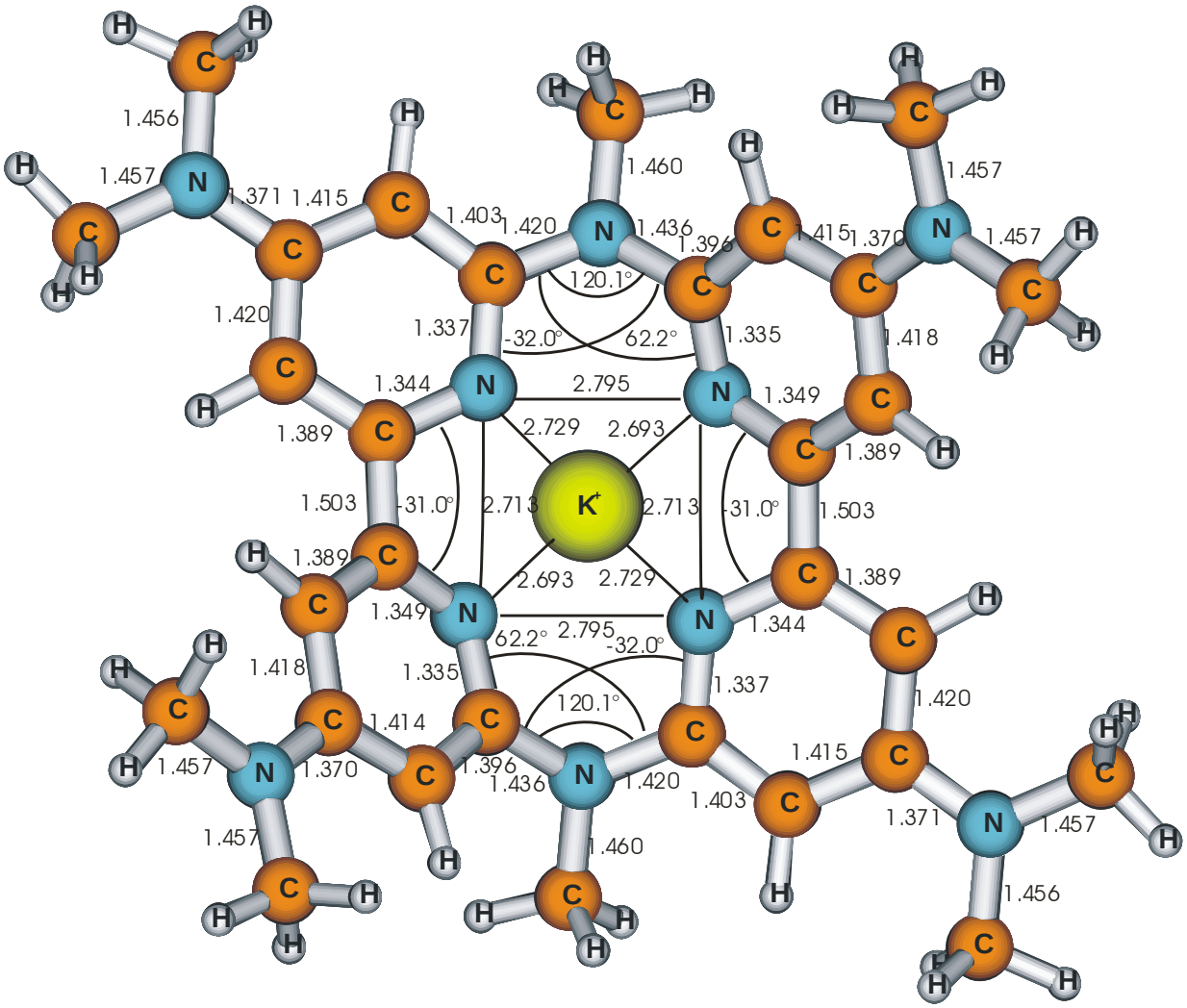
H -6.0862806262 0.9858708562 3.7987463151

H -5.505491265 2.6587978859 3.9905133563

H -5.905846392 2.4636385951 0.7767031031

H -4.19974392 2.9427776294 0.7136975049

H -4.6971979552 1.311480702 0.1991886012



$1b_{K+}$

Figure S25 *The structure and Cartesian coordinates of molecule* ***$1b_{K+}$***

	X	Y	Z
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C	0.0230865626	0.2718462981	1.2501388996
C	1.1794827357	0.2157668997	2.0182147854
C	2.4363689052	0.2110731021	1.3581883384

C 2.4328913447 0.2471420921 -0.0565029753

C 1.2077552106 0.3241793548 -0.7353020088

C -1.3562473831 0.1988216671 1.8424614748

N -2.3211945049 0.8470760055 1.1589026736

C -3.5924707726 0.6040143767 1.4857618884

C -3.9615509207 -0.1734193137 2.5853761862

C -2.9562711304 -0.7459995897 3.3991544399

C -1.6169327328 -0.5774546029 2.9648701769

N -4.6082949236 1.1833385962 0.6526647689

C -5.8294786031 1.6286572434 1.3182834588

N -3.2632333039 -1.4720854516 4.5202215441

C -4.6546402958 -1.7285181273 4.8659384838

N 3.6104530897 0.1584979571 2.0635472877

C 3.5894699615 0.0572791047 3.5166620873

N 1.1522563688 0.3798004304 -2.1528635984

C 2.4171833455 0.4576224471 -2.8785015768

C -4.6988084299 0.8201759849 -0.71685088

N -3.5496457745 0.5169448694 -1.3301806884

C -3.5762966846 0.1291395443 -2.617005919

C -4.7404779796 0.0920940266 -3.3744007196

C -5.968492047 0.4420843904 -2.7539909777

C -5.9325447012 0.7943504126 -1.383851897

C -2.2389799836 -0.3003390821 -3.1516763225

C -2.1302291278 -1.3411366351 -4.0656110662

C -0.8450448282 -1.8202578204 -4.4255871188

C 0.2556215048 -1.2520519512 -3.7426910055

C 0.0397221371 -0.1975004386 -2.8532623797

N -1.1681375762 0.3178719425 -2.6134196371

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N -7.1483656833 0.4254100899 -3.451407414

C -7.1715903129 -0.0020838311 -4.8438649154

C -2.2114432883 -2.1664765923 5.2513480745

C 4.8879648177 0.1828495958 1.365302011

C -1.8473510701 -3.4791209503 -5.9244872234

C -8.3912424501 0.8152742905 -2.8006855186

K -1.5944228591 2.3792752019 -0.9334092414

H -0.803407052 -1.0918919428 3.4579948804

H 1.1127199536 0.196262161 3.0973876831

H 3.3637130578 0.1824082672 -0.5979998247

H -5.0066452068 -0.3676338189 2.7813423527

H 1.250868609 -1.6539891701 -3.8702600324

H -3.0262082855 -1.8128059821 -4.445599939

H -4.6981218723 -0.1803110324 -4.4200840072

H -6.8510357031 1.0065617651 -0.8592768028

H -6.2845774547 2.43909631 0.7412708851

H -6.5799561 0.8329170507 1.4428574957

H -5.5696879452 2.0180061865 2.3039696413

H 2.2062410896 0.6524744742 -3.9312110021

H 3.0097522313 1.2912164345 -2.4901035455

H 3.0245844732 -0.4577222902 -2.8067693332

H 0.5793831755 -4.0880759984 -6.4221187498

H 1.3440981123 -2.5845667876 -5.8976724964

H 1.0521439046 -3.8914581438 -4.7234108937

H -1.5158592126 -4.1931395957 -6.6792872583

H -2.4335403976 -4.0239173026 -5.1705901254

H -2.5056423186 -2.7537767451 -6.4169476332

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H -6.5799492607 0.6646344117 -5.4855563316

H -6.7862339862 -1.0236066074 -4.9590769078

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H -8.6620575548 0.1280709943 -1.9871282018

H -8.3245074625 1.829826422 -2.3867991679

H 5.6961111589 0.205257511 2.0969523168

H 5.0271106765 -0.7045811747 0.7323962639

H 4.9806780285 1.0751638078 0.7326480631

H 4.6132735121 -0.0183616184 3.8842208172

H 3.1273072022 0.9389732319 3.9807107958

H 3.0441006641 -0.8347941525 3.8514150946

H -2.6412418922 -2.6281675498 6.1410373939

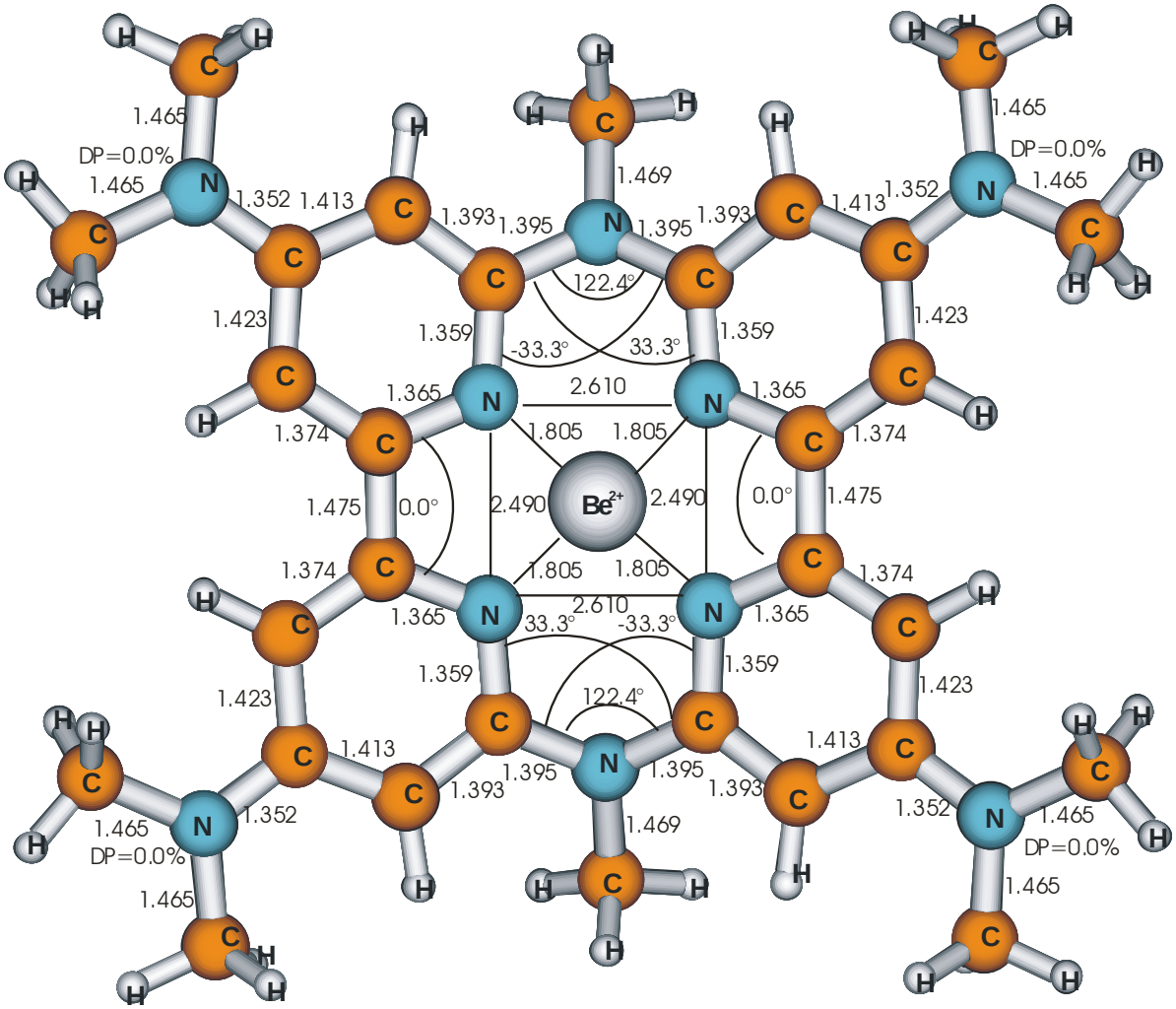
H -1.7367741261 -2.9554102317 4.6504699221

H -1.4340099782 -1.4669365772 5.5803312804

H -4.6953787899 -2.2416299698 5.8274716786

H -5.2130104369 -0.7901347933 4.9639952958

H -5.1613792713 -2.3573710005 4.1194854825



1b$_{Be2+}$

Figure S26 *The structure and Cartesian coordinates of molecule* ***1b$_{Be2+}$***

	X	Y	Z
N	-0.0095438892	0.0298164722	-0.0152723919
C	-0.0032560449	0.0714565773	1.3489342665
C	1.1317162304	0.1641632418	2.1178133873
C	2.4059068867	0.229654295	1.4873992028

C 2.3961269876 0.2243430928 0.0744296068

C 1.197542702 0.1356695922 -0.6306208306

C -1.3699357117 0.0764323225 1.9039383379

N -2.3168195819 0.0382499887 0.9217027674

C -3.6104740068 0.1532216153 1.3218984525

C -3.9775544783 0.2475636438 2.6627617334

C -2.9994043879 0.2493041654 3.6824806843

C -1.6468897706 0.174241209 3.2461982498

N -4.6037260952 0.194925821 0.3426244992

C -5.9011205576 0.7893923251 0.6912234586

N 1.2270572346 0.1735958663 -2.0252374709

C 2.4038609517 0.7590003866 -2.6814215388

C -4.4986779877 -0.5061543071 -0.8593393537

N -3.2645056194 -0.6653135334 -1.4056008007

C -3.2111518155 -1.2904827005 -2.6176859899

C -4.3037140013 -1.7981286266 -3.2783938103

C -5.5967850057 -1.6788973171 -2.6961357125

C -5.6560098693 -0.9984462169 -1.4591697968

C -1.8444669038 -1.2955063784 -3.1726765033

C -1.5250890474 -1.8083794867 -4.4067313327

C -0.1914459033 -1.6987962244 -4.8911482954

C 0.7176936908 -1.0218592663 -4.0474484624

C 0.3093465144 -0.523780691 -2.811838364

N -0.9572279804 -0.6737618463 -2.3425718829

Be -1.644829486 -0.2413675049 -0.7303464877

N -3.3250866561 0.3146164543 4.9929480876

H -0.8400284908 0.2089428841 3.9621038622

H 1.0526688968 0.202141697 3.1934803228

N 3.5534420344 0.289637107 2.1995966538

H 3.3267483093 0.2415261226 -0.469095686

H -5.0235069965 0.271955974 2.9219135992

H 1.7515652018 -0.9280466922 -4.3374143645

N 0.1803047557 -2.214834572 -6.0841131565

H -2.2875196058 -2.2777900476 -5.009312086

H -4.1802418985 -2.2707544891 -4.2407500243

N -6.6982641493 -2.1894869958 -3.2908642425

H -6.5987174397 -0.8973787484 -0.9464723235

H -6.3704879899 1.1625902149 -0.2195048551

H -6.5803161505 0.0809336438 1.1819448482

H -5.7297930913 1.6382085102 1.3539195831

H 2.1077060796 1.1315105925 -3.6625110461

H 2.7483908002 1.6072185916 -2.0891094194

H 3.2284369936 0.0450502959 -2.8013283186

C 1.5503927658 -2.0393080967 -6.5709214526

C -0.7804477832 -2.9500981773 -6.9105773609

C -6.5903989674 -2.9286108551 -4.5513254513

C -8.0187122249 -2.0040576794 -2.6850882251

C -4.7259576445 0.4402856484 5.4012380846

C -2.2844156221 0.2679724296 6.0232534953

C 4.84309198 0.4055528343 1.5152726343

C 3.5254891721 0.2469153078 3.6638692478

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H -1.5850218833 -2.2964762771 -7.2686807424

H -7.5689454791 -3.3296215081 -4.8118437058

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H -5.896403917 -3.7710226082 -4.4559019457

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H -8.0877340975 -2.5110368584 -1.7149475635

H -8.2434940941 -0.939849065 -2.549870054

H -4.7739225304 0.5435724579 6.4843445966

H -5.1874779212 1.3287505629 4.955167508

H -5.3059065654 -0.446048716 5.1165701047

H -2.7575466329 0.2421748446 7.0039236052

H -1.6703401381 -0.6337695357 5.922427639

H -1.6370244354 1.152195998 5.980445658

H 4.5482171861 0.2155961793 4.0370708875

H 3.0371595194 1.1353173567 4.0822906716

H 3.0092954932 -0.6506674496 4.0220320406

H 5.6332613117 0.505853074 2.2580115001

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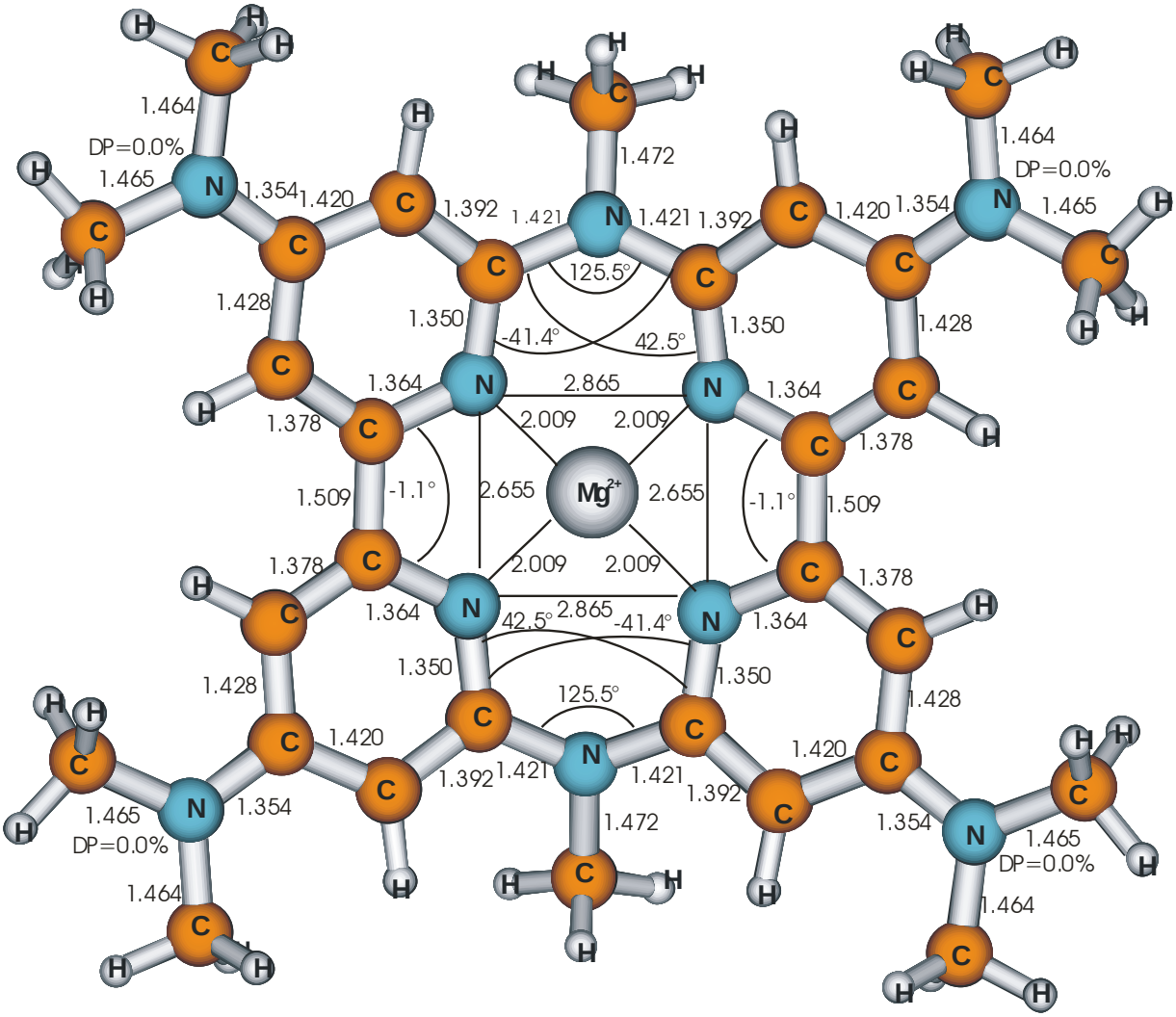
H 4.8684376404 1.2922254674 0.8714412849



$1b_{Mg2+}$

Figure S27 *The structure and Cartesian coordinates of molecule* ***$1b_{Mg2+}$***

	X	Y	Z
N	-0.0109879614	-0.099041645	-0.0560787662
C	0.0006304015	-0.0347220045	1.3059499412
C	1.1812066139	0.0066376584	2.0147442552
C	2.4247409629	0.0223314522	1.3130326574

C 2.3696131823 0.0418233308 -0.1060121663

C 1.1410224762 -0.0246669978 -0.7563960668

C -1.3623077771 0.0254115149 1.9502627916

N -2.4091025276 0.0309721649 1.0764559366

C -3.6721363223 0.2102525218 1.5188015152

C -3.9431196737 0.3206926198 2.8796579142

C -2.8864028664 0.2325571833 3.8243379075

C -1.5601608303 0.1015460336 3.3113894933

N -4.7265093896 0.2408155349 0.5668942694

C -6.0646600378 -0.1142906341 1.0662586286

Mg -1.8565904563 -0.1068830693 -0.8497515735

N -3.5575657861 0.786795099 -1.4364805464

C -3.4564749089 1.4250439239 -2.637235787

C -4.5199923406 2.1133662003 -3.178533564

C -5.7474285675 2.1980217049 -2.453787593

C -5.7860457664 1.5941768036 -1.1688801365

C -4.6802933871 0.8949591292 -0.6942626271

C -2.0966943479 1.3452257505 -3.2860667166

N -1.1578856936 0.6665464619 -2.5667746672

C 0.1284134388 0.6322872681 -2.9758302318

C 0.5122612587 1.2253745602 -4.175191393

C -0.4557230096 1.8666140596 -4.9929059027

C -1.7926740821 1.930871491 -4.4952809378

N 1.0765436836 -0.060528435 -2.1759428633

C 2.2792793132 -0.5495215112 -2.8690698103

N -6.8176730932 2.857304596 -2.9577912134

H -4.4227034181 2.6025371728 -4.1359509989

H -2.5554731105 2.4464865634 -5.0588871579

N -0.1202210254 2.4236873602 -6.1808814181

H 1.5505467527 1.232163457 -4.4664141015

H -6.6583547663 1.7119278578 -0.5457439003

H 3.2778770342 0.1481964108 -0.6777014458

N 3.6056304346 0.0527504871 1.9753556454

H 1.1687112524 0.0460254217 3.0934907484

H -0.7188569526 0.0752812196 3.9873267514

N -3.1212853436 0.3026837366 5.1562878777

H -4.9497173687 0.5114259673 3.2162220008

H -5.9691755061 -0.9423521293 1.77009713

H -6.5759628379 0.7191588117 1.5653006677

H -6.674773627 -0.4516977524 0.2273180126

H 2.7025934059 -1.3765171171 -2.2974169644

H 1.9900583737 -0.9291013141 -3.8501214033

H 3.0482250728 0.2230283899 -2.9994561717

C -8.0655463043 2.9367117775 -2.1957030328

C -6.7369586711 3.5256901374 -4.2586037897

C 1.2562997952 2.3446962371 -6.6738785313

C -1.1203821768 3.1344030699 -6.9808317526

C 4.8696146542 0.0737839763 1.2363204913

C 3.6387857425 0.0941521321 3.4391022038

C -4.4892757405 0.4348495021 5.6614906346

C -2.0120438209 0.2719089996 6.1123191749

H -7.6966485933 3.9912673237 -4.4782662907

H -5.9721191319 4.3114891306 -4.2573424081

H -6.5168165333 2.8107368472 -5.0598096194

H -8.8211542273 3.4358975425 -2.8006392191

H -8.4380522758 1.9364425708 -1.947364351

H -7.9354132188 3.5102725353 -1.2696068577

H -0.6471673254 3.5121374888 -7.8860678276

H -1.9382357813 2.4682402128 -7.2792937327

H -1.5344293158 3.9898506628 -6.4339718178

H 1.3029375427 2.7787730312 -7.6716269938

H 1.9475639329 2.8995046099 -6.0273968692

H 1.5893951779 1.302891762 -6.742514249

H -4.4726837139 0.3949088342 6.7497135864

H -4.9383264965 1.3898401068 5.3615850384

H -5.1211175692 -0.3855374181 5.3026576182

H -2.4121132262 0.3501176913 7.1222180881

H -1.4518039015 -0.6677432383 6.0421631181

H -1.3259010021 1.1125497711 5.9547990022

H 5.6963613162 0.0180542683 1.9430464903

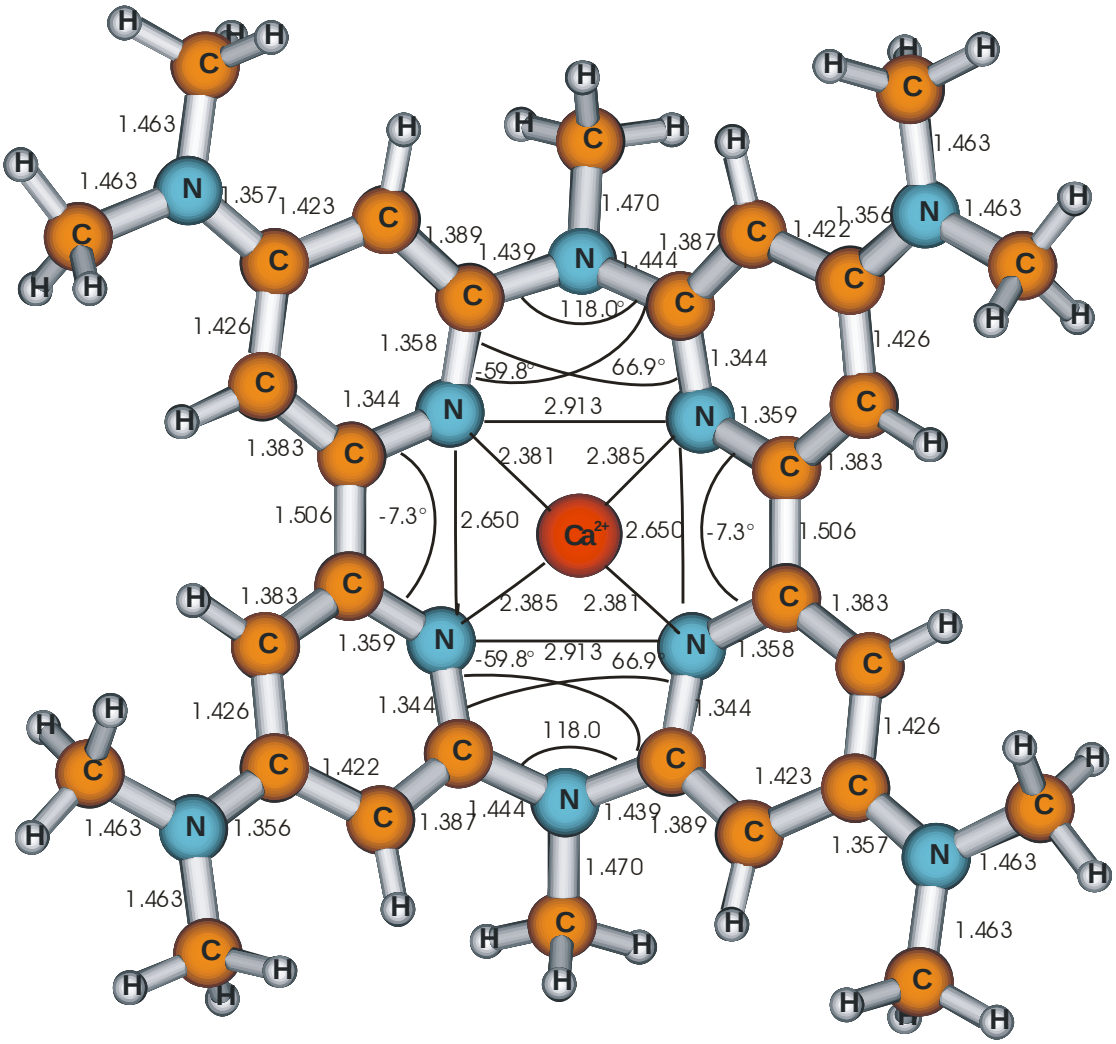
H 4.9437195494 -0.7861097488 0.5609961853

H 4.9795678205 0.99687935 0.6537695436

H 4.676185689 0.1129641279 3.7699585447

H 3.1443319605 0.9937460174 3.8247285364

H 3.1617159495 -0.7923964982 3.8726772555



1b$_{Ca2}$

Figure S28 *The structure and Cartesian coordinates of molecule* ***1b$_{Ca2+}$***

	X	Y	Z
N	0.073994206	0.6819749895	0.0055823986
C	-0.0094352324	0.2793039423	1.299528223
C	1.0788082084	-0.2579431197	1.9621980554
C	2.3063550044	-0.4510253486	1.2621138013

C 2.3152575309 -0.14281048 -0.1267873727

C 1.1831533273 0.4158536678 -0.7047576174

C -1.3830571021 0.4024100338 1.9054365086

N -2.2991826086 1.0386939646 1.1295665468

C -3.5993873322 0.9794692675 1.4632734235

C -4.0358471281 0.4239971379 2.6569957691

C -3.0830471972 -0.1210225311 3.5615621909

C -1.7288541379 -0.1648955672 3.118390894

N -4.5207905974 1.5482430467 0.5086905098

C -5.7479662199 2.1266594323 1.0747066683

N -3.4528321307 -0.622993398 4.7660339668

C -4.8572398973 -0.6028183157 5.1761673927

N 3.4054518153 -0.9457160923 1.8845464158

C 3.3542227368 -1.3203213751 3.2983416571

N 1.1282945566 0.7778168645 -2.096045744

C 2.4227883055 1.0052504801 -2.7544223024

C -4.6602933006 0.8969297929 -0.7664713999

N -3.5360537655 0.8112760409 -1.4974880663

C -3.5440064021 0.1200889908 -2.6660757479

C -4.7177941791 -0.3666087429 -3.2114075403

C -5.9470298603 -0.1937131542 -2.5090136504

C -5.8792598833 0.4158689723 -1.2252928068

C -2.1803878292 -0.1227948016 -3.2582470439

C -1.95500254 -0.9969579121 -4.3059634435

C -0.6204702392 -1.2762039466 -4.7221474116

C 0.4255347064 -0.7054477612 -3.9454712181

C 0.1084278033 0.1678721175 -2.915532405

N -1.158023392 0.5127123405 -2.6281524098

N -0.3605648859 -2.0896263494 -5.7758362903

C 1.0202344291 -2.3924425812 -6.1535574234

N -7.1237967947 -0.6287178157 -3.0249069857

C -7.161161669 -1.3145968597 -4.3171702442

C -2.4647290957 -1.2466266806 5.6470997223

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C -1.4538252852 -2.7248317524 -6.5126121116

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Ca -1.6188030249 2.0901087128 -0.8999273058

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H 3.1830020687 -0.3664641949 -0.7285835632

H -5.0912813688 0.3744449209 2.8795375629

H 1.4542359925 -0.9759223352 -4.1313185588

H -2.7850921908 -1.4953021056 -4.7846602759

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H -5.4771123925 2.7659194893 1.917382901

H 2.2445195569 1.4743136058 -3.7241225578

H 3.0146069146 1.6875793494 -2.1403085089

H 3.0077405155 0.089055512 -2.9148711473

H 1.0179524157 -2.9862206009 -7.0667791918

H 1.5834762727 -1.4732681849 -6.3502772168

H 1.5370238917 -2.9670183833 -5.3741853156

H -1.0393101489 -3.2858905325 -7.3492196424

H -2.0158916271 -3.4233479396 -5.8798987411

H -2.1436277871 -1.9759029296 -6.9180090827

H -8.1921223876 -1.577606267 -4.5501502795

H -6.786628588 -0.6698106346 -5.120944052

H -6.5722534115 -2.2398641615 -4.2977304353

H -9.2042520502 -0.7868201268 -2.8926018861

H -8.3717490259 -1.0355600419 -1.3501869003

H -8.534104883 0.6050770269 -2.0341829977

H 5.4290562687 -1.4680840453 1.830215556

H 4.5382434388 -1.91720848 0.3677805388

H 4.9799505157 -0.2141785529 0.6685861446

H 4.3323701177 -1.6894791301 3.6037657475

H 3.1055165399 -0.4590210448 3.9295178871

H 2.6214549216 -2.1170106954 3.4762407632

H -2.949755933 -1.5296649243 6.5804593628

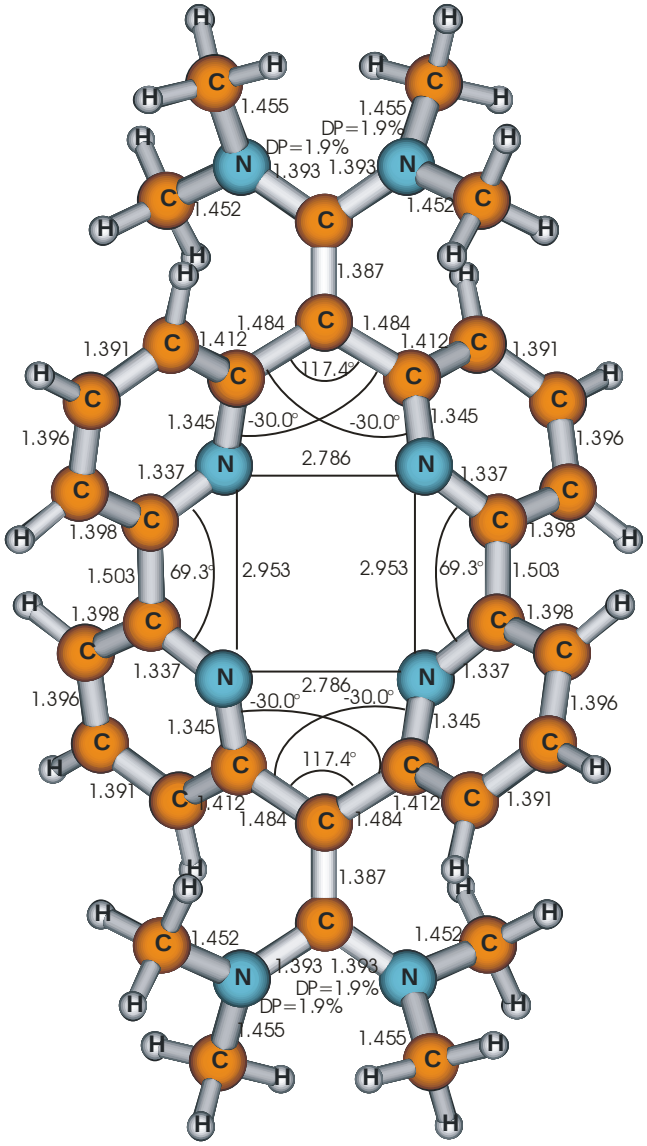
H -2.0366317894 -2.1518326393 5.1982074945

H -1.6540956185 -0.5491072352 5.8867018412

H -4.935087912 -0.9683165039 6.1993498727

H -5.2585306418 0.4165628495 5.1506787953

H -5.4757063184 -1.2452374204 4.5363030865



2a

Figure S29 *The structure and Cartesian coordinates of molecule* ***2a***

	X	Y	Z
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C	-1.734700754	-0.27691994	-2.3834944898

N -0.5810772592 0.2422346706 -1.9256122369

C 0.5827770871 -0.1824444756 -2.4280684064

C 0.6706278052 -1.086510444 -3.4912891083

C -0.5200748215 -1.6148887324 -3.9925123995

C 1.7966056073 0.3383921539 -1.710638768

N 1.9628354638 -0.1515823096 -0.4779011638

C 2.9223605745 0.3547673085 0.3176885604

C 3.7828335487 1.3703763766 -0.1526878724

C 3.6561848205 1.8202393727 -1.4622867408

C 2.6408811943 1.3034295312 -2.2686635801

C 2.9872262679 -0.1494786713 1.7118184261

C 4.1891854274 -0.2094267009 2.4004557217

N 5.4140600859 -0.4522949019 1.7832942573

C 5.5216824121 -1.2571503162 0.5800257481

H 4.3174823996 2.5970621119 -1.8395566807

C -2.9873373501 0.1495253254 -1.7117799943

C -4.1890188676 0.2100763786 -2.4008356445

N -4.2808399839 0.5280247575 -3.7539012075

C -3.3217582236 1.4024495689 -4.4041609305

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N 0.5866528704 0.0235082313 1.9386461139

C -0.5952435004 -0.3988897474 2.3991187882

C -0.7236922533 -1.3992005946 3.3678320538

C 0.4424108701 -2.0247956244 3.8116805966

C 1.6675946102 -1.6426733732 3.2765521218

C -1.7844512321 0.2417338031 1.7397791065

C -2.5887969723 1.1804271845 2.393530194

C -3.5798093716 1.8175932637 1.6451215912

C -3.7224237111 1.506977259 0.2973015715

C -2.9042672681 0.5084562948 -0.2743385086

N -1.9683931453 -0.1147444431 0.4644651122

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C 3.3704322889 0.8126727434 4.5152010965

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C -5.5694654505 -0.9567695275 -0.6920191398

C -6.5689044487 0.8288346571 -2.0327032376

C -5.1135322804 -0.2427035785 -4.6640503189

H 6.8599509906 0.9888649447 1.2392648422

H 6.3986452756 0.9705332912 2.9594390204

H 7.4587686181 -0.3011810149 2.3058401356

H 5.5943013949 -0.6444510851 -0.3305420199

H 6.4222629553 -1.8833844275 0.645606732

H 4.6445353451 -1.9000053615 0.4901611913

H 4.4427698595 -1.5536577434 5.2369561329

H 5.6933705645 -1.5745658608 3.9690137712

H 5.7589745446 -0.3590703554 5.2677041754

H 2.5769100745 0.2359318389 5.0126968939

H 3.9267648152 1.3661693261 5.2843846516

H 2.9001456138 1.5227897187 3.8330743609

H -2.5521878 0.8447280931 -4.9577979766

H -3.8517597267 2.0530969691 -5.1135580604

H -2.8235368342 2.0203020348 -3.6553292621

H -4.491456048 -0.832893423 -5.3562123496

H -5.7462480839 -0.9256129412 -4.0956534077

H -5.7550568338 0.4144012616 -5.2672342688

H -6.8092036631 1.3989124556 -1.1207637034

H -6.3449824772 1.533037456 -2.835026032

H -7.4598638988 0.248685029 -2.3098533845

H -5.6181468461 -0.4356447147 0.2753814943

H -6.4957387545 -1.5343448177 -0.8182674191

H -4.7207139661 -1.6421785903 -0.6685063654

H 2.4809463942 1.66296194 -3.2808072289

H 1.6366379512 -1.3932292922 -3.8811913085

H -0.5022047395 -2.3472898475 -4.7964831111

H -2.6588021431 -1.6896778859 -3.7487320968

H 4.5206826244 1.8114749253 0.5104419351

H -4.4397292179 2.0428628042 -0.3167193273

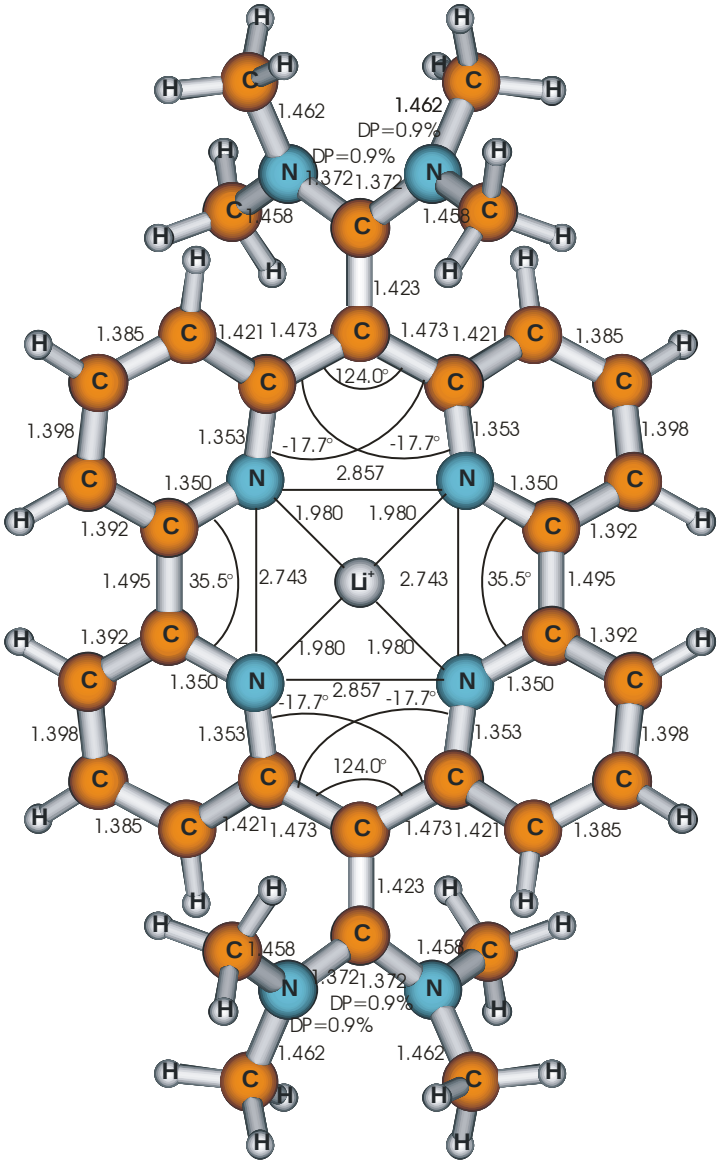
H -4.2087880008 2.5797032783 2.0997410109

H -2.4161345603 1.4296101226 3.4362995449

H -1.7026835809 -1.7016485255 3.7275227871

H 0.391740639 -2.8317887598 4.5392096155

H 2.5765259281 -2.1658770402 3.5573167837



2a$_{Li+}$

Figure S30 *The structure and Cartesian coordinates of molecule* ***2a$_{Li+}$***

	X	Y	Z
N	-0.014324432	-0.0673950449	0.114109855
C	0.0164229536	0.2169104754	1.4331742338

C 1.1586943322 0.6845399945 2.0761805888

C 2.3269491253 0.7849761606 1.314128076

C 2.3052940585 0.4580181887 -0.0310535277

C 1.0909374345 0.0644199307 -0.6555890041

C -1.2568772144 -0.049145959 2.1693638729

N -1.9501741166 -1.1262777549 1.7441174016

C -3.1523738965 -1.4403855189 2.2802777326

C -3.6976360087 -0.5758720392 3.2676651346

C -2.9693231542 0.5073575901 3.7292447371

C -1.7084597989 0.7819296713 3.1902968618

C -3.8881475605 -2.6290764055 1.8161963652

C -4.9289271351 -3.1352822281 2.6432765152

N -4.7849768759 -3.2712189552 4.0009076269

C -5.867172003 -2.9910545166 4.9431603839

C 1.0357825498 -0.2341135289 -2.0969652042

C 2.0765278724 0.2721195479 -2.9240731562

N 2.5435699286 1.5570801415 -2.8095677412

C 3.9574124565 1.9006218713 -2.952770798

C -3.612060835 -3.325635161 0.5480056742

N -2.9075006557 -2.7123088427 -0.4311983618

C -2.6594798456 -3.3316178188 -1.6045058137

C -3.1271899149 -4.6098535941 -1.8948153806

C -3.8176714302 -5.284402907 -0.8829614749

C -4.0404191183 -4.6637387057 0.3344303094

C -1.8047314232 -2.5626104385 -2.5595367313

N -0.8326970378 -1.8204295731 -1.9885533654

C -0.0311936064 -1.0248128669 -2.7342102759

C -0.2718906007 -0.9448611673 -4.1325308314

C -1.2445763026 -1.7344352393 -4.7218851247

C -2.0276698143 -2.5831292278 -3.9331433089

N -6.1446200444 -3.5205991018 2.1373258265

C -6.8768164436 -4.6832665061 2.6368987341

C -6.6931652923 -2.9467825123 0.9142066996

N 2.6811931787 -0.4915487334 -3.8902788422

C 3.0816820491 0.0474286135 -5.1889677563

C 2.7624349247 -1.9441846592 -3.7931389726

C -3.4842966255 -3.4792204867 4.6263292378

C 1.7102152346 2.643879746 -2.3089942158

H -4.1491737687 -6.3076804212 -1.0372771047

H -7.0362093936 -5.3916222805 1.81280239

H -6.3028478802 -5.1815745954 3.4183071888

H -7.8582794593 -4.4020732126 3.0371407423

H -6.5651571957 -3.6221495341 0.0579205783

H -7.7652446748 -2.7668309362 1.0564105833

H -6.1964246086 -2.0016390812 0.6941206555

H -5.5461535765 -2.2041269381 5.6388612603

H -6.7509204322 -2.6433855675 4.4079352781

H -6.130616137 -3.8777517219 5.5321417635

H -3.0984230063 -2.5539147605 5.0742618936

H -3.5872956125 -4.2307204891 5.4179086203

H -2.7697937973 -3.8352255117 3.8838796911

H 2.0145438801 -2.4344925284 -4.4303123583

H 3.7588778061 -2.2663414566 -4.1176000486

H 2.6029885926 -2.2551277264 -2.7604835697

H 2.5686284245 -0.5087726127 -5.9850358646

H 2.8015689083 1.0983860073 -5.2622862014

H 4.1620974838 -0.047651833 -5.3508172391

H 4.3088672989 2.3782298745 -2.028282707

H 4.5472996499 1.0003413338 -3.125625637

H 4.1218373462 2.6012023086 -3.7802277596

H 1.944243951 2.8842480072 -1.2634386856

H 1.8887984064 3.5375873223 -2.9183823918

H 0.6584667294 2.365670259 -2.3790645599

H -2.9060560376 -5.0864447795 -2.8432933384

H -2.8213434908 -3.1831855769 -4.3640306466

H -1.4212754541 -1.6668269463 -5.791936648

H 0.2880564925 -0.2460354903 -4.7419565584

H -4.521864012 -5.2149542619 1.1329727996

H 3.2271997276 0.4799602853 -0.599302092

H 3.2601000454 1.0852721732 1.7830155544

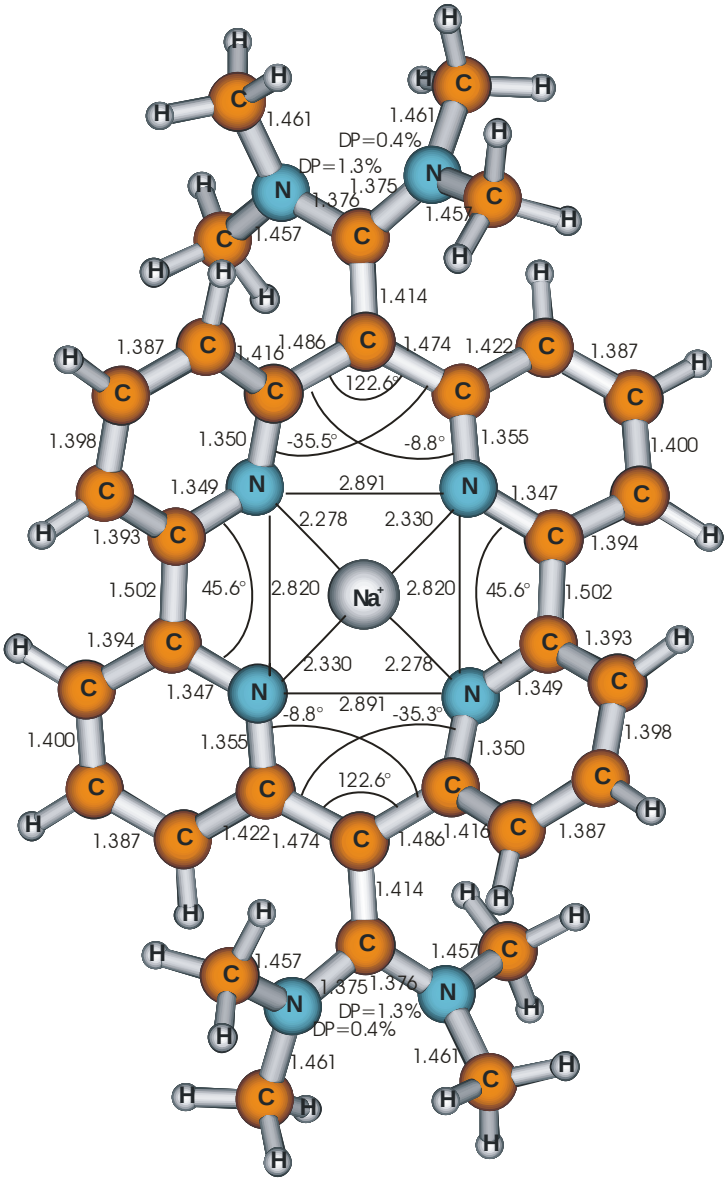
H 1.1568393336 0.8976188773 3.1393096636

H -1.1340380694 1.6454560473 3.5065427206

H -3.394243346 1.1626964188 4.4847432104

H -4.6980361314 -0.7454186368 3.6468095116

Li -1.4261618124 -1.4315825302 -0.1403946309



$2a_{Na+}$

Figure S31 *The structure and Cartesian coordinates of molecule* ***$2a_{Na+}$***

	X	Y	Z
N	-0.0090605544	-0.0578891032	0.1296439874
C	-0.0736580321	0.268434283	1.4352538337

C 1.0092441174 0.8030731239 2.1317935063

C 2.2196973849 0.9156268313 1.4371508009

C 2.2963643449 0.5525375608 0.1011812378

C 1.1328504191 0.102651585 -0.5810986613

C -1.4001902931 -0.004801411 2.0845616068

N -1.9555378097 -1.2046608817 1.8170107211

C -3.2249096529 -1.4771713882 2.1859642673

C -3.9471446259 -0.5097344244 2.9261551041

C -3.3431188847 0.6849277305 3.2890935326

C -2.0427950407 0.9603104031 2.8573345044

C -3.879714403 -2.7491626357 1.7845773598

C -4.8524932357 -3.2723951813 2.6676777733

N -4.6588598031 -3.2819676296 4.0302281505

C -5.7246263696 -2.9581104279 4.9759309966

C 1.1262812282 -0.2337160274 -2.0162054651

C 2.1850746673 0.1861600813 -2.8544186499

N 2.7965287879 1.4124680171 -2.7403138168

C 4.2317274036 1.6009226966 -2.9375286811

C -3.6273392095 -3.3965960759 0.4846325437

N -2.9111568587 -2.7246251922 -0.4483341493

C -2.6809196995 -3.2499342773 -1.6674806283

C -3.1715287012 -4.4961015887 -2.0548479105

C -3.8571393681 -5.2391592172 -1.0862421285

C -4.0696923461 -4.7128231376 0.1787947755

C -1.8399578545 -2.3933560023 -2.5702542696

N -0.7348826847 -1.8539289873 -2.0157410941

C -0.017382031 -0.9184090383 -2.6727704099

C -0.3984040959 -0.5604129353 -3.9888640295

C -1.4750401128 -1.1872891854 -4.5985118064

C -2.2273801836 -2.1210112468 -3.8807083183

N -6.0547311873 -3.7889450931 2.2451507391

C -6.6755433446 -4.9557906204 2.8674586183

C -6.7281229437 -3.3101160341 1.0454790404

N 2.666295712 -0.6150532074 -3.8646718943

C 3.0242065456 -0.0885554766 -5.1798889713

C 2.5933205576 -2.0689326518 -3.8008077643

C -3.3287936647 -3.3383370605 4.6226090219

C 2.0891989089 2.592420696 -2.2614164886

H -4.2044679528 -6.242964385 -1.3163388297

H -6.8331865824 -5.7353855923 2.1096412622

H -6.0258801064 -5.3534298622 3.6474313912

H -7.6509238147 -4.7101182354 3.3055930626

H -6.627264808 -4.0165445511 0.2106491117

H -7.7955015768 -3.1819662907 1.2624283725

H -6.3059676438 -2.3509603354 0.744103447

H -5.4397948154 -2.0703084602 5.557062666

H -6.6486055209 -2.7397749192 4.4402274507

H -5.9050381909 -3.7816356664 5.677514393

H -2.9747967303 -2.3454038899 4.9314370482

H -3.3619478667 -3.9844351799 5.507859302

H -2.6229808146 -3.7549327805 3.9030382439

H 1.7402431899 -2.4623067763 -4.3701236097

H 3.5139806809 -2.4890918697 -4.2227803074

H 2.4992696722 -2.387245409 -2.7618961251

H 2.3870489586 -0.5531092731 -5.9449089293

H 2.8686465221 0.9900600306 -5.2077385753

H 4.0700544439 -0.3047719121 -5.429716637

H 4.6716975928 2.0413770519 -2.0323586954

H 4.7121397494 0.6409096741 -3.1275702033

H 4.4398696073 2.276953797 -3.7761838834

H 2.366697378 2.8443404848 -1.2290961148

H 2.3405399059 3.44461249 -2.9043654439

H 1.0134806863 2.4184368346 -2.3011902022

H -2.9786529989 -4.8955469838 -3.0448299751

H -3.1170583301 -2.5756096618 -4.3033756809

H -1.763357093 -0.9137683047 -5.6098838896

H 0.1331666666 0.2280637343 -4.5100328418

H -4.5608142852 -5.3156349086 0.9334376653

H 3.2492295517 0.6006557064 -0.4124337777

H 3.1108763117 1.2660973176 1.9511323129

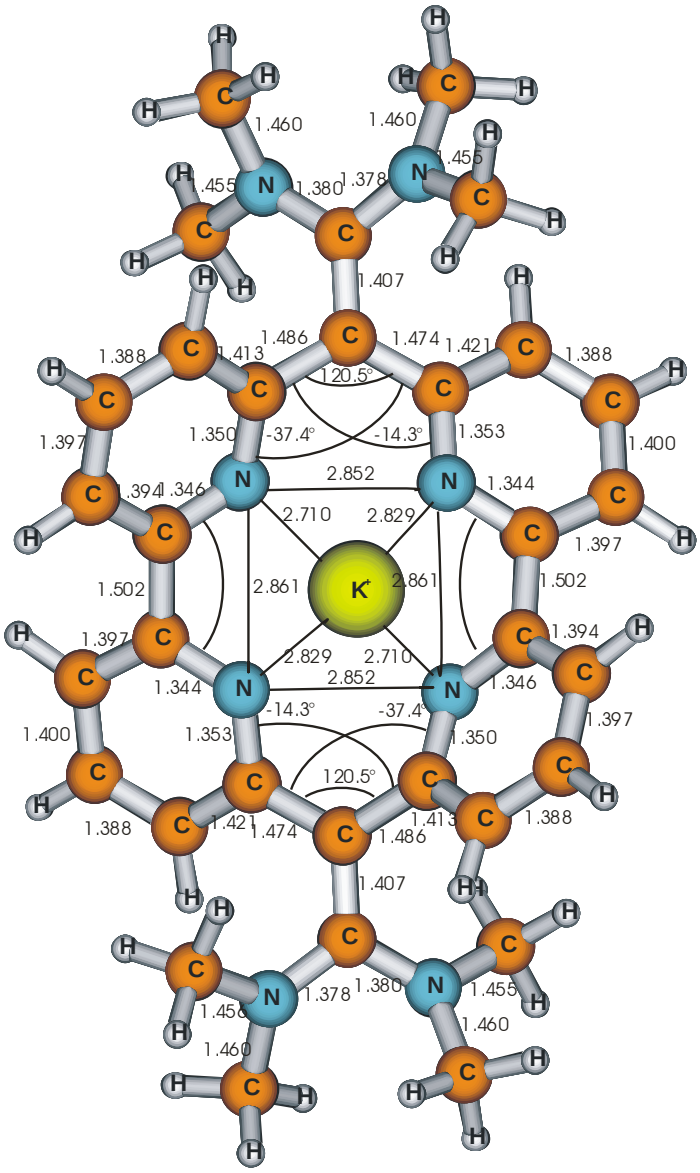
H 0.9312387922 1.0645268532 3.181735878

H -1.5685889937 1.9140486695 3.0631165021

H -3.8979105795 1.4243029599 3.8603590352

H -4.9851878462 -0.6897449334 3.1829472251

Na -0.7265981979 -2.2724590197 0.2235470449



$2a_{K+}$

Figure S32 *The structure and Cartesian coordinates of molecule* ***$2a_{K+}$***

	X	Y	Z
C	0.1564425487	0.6607615804	0.086207207
C	0.1182553873	0.2187036449	1.4077385877

N 1.2283234531 -0.0662067385 2.1143825736

C 2.4469751962 0.1903806495 1.5943029354

C 2.5536763764 0.6932554032 0.277724757

C 1.4104384124 0.8919405748 -0.4843166817

C -1.1741032922 0.1019235893 2.1648140596

N -1.2194293903 0.832136747 3.2917701403

C -2.291189812 0.7705469007 4.1153738639

C -3.3510157264 -0.1224899428 3.8027806408

C -3.3173422038 -0.8452509489 2.6179657112

C -2.2193678002 -0.7297431346 1.7564635908

C -2.2765784469 1.6049389214 5.3307239055

C -3.4662365141 1.9094052746 6.0175057123

N -4.674552659 2.1079429586 5.3853524775

C -4.7716685296 2.6733928419 4.0473889105

C 3.6604338128 -0.0134103692 2.426668722

C 4.8436479811 -0.4278392361 1.787989415

N 4.8353502004 -1.3466296327 0.758531375

C 3.8156347423 -2.378728952 0.6476942658

C -1.0143795399 2.2327347549 5.7993091578

N 0.1497686263 1.5594174761 5.6860202319

C 1.3117342346 2.1599636483 6.0053193863

C 1.3738545418 3.4293290934 6.5781821132

C 0.1742371437 4.125929017 6.7428432249

C -1.0146248478 3.5461810133 6.3213282878

C 2.5527137257 1.4000981232 5.6317347731

N 2.6210477882 1.0625274119 4.333014911

C 3.6452626505 0.3127925504 3.8643270051

C 4.6248064341 -0.1641089037 4.7762040017

C 4.5712703618 0.2197060899 6.1092917796

C 3.5279100555 1.0361042514 6.5631301619

N -3.5039432664 2.0432372477 7.3903482215

C -2.5865896564 1.3288088994 8.2652124856

C -4.2632022357 3.1026653735 8.048990182

N 6.091622573 0.050321986 2.1241179336

C 6.3010709508 1.4016039902 2.623598265

C 7.2759012441 -0.8026343001 2.1553172895

C -5.9370371381 1.6264475494 5.9379096144

C 5.6659105349 -1.1894477289 -0.4323237929

K 0.5931143957 -0.8902320861 4.6162294564

H -4.1346124851 -1.5187565853 2.372694723

H -6.4216455441 0.9518181445 5.218403137

H -5.7542036203 1.0783309674 6.8625672687

H -6.6302743575 2.4517286698 6.1444027745

H -4.9977377288 1.9076137631 3.2928338504

H -5.5759062574 3.4193564942 4.0317516073

H -3.831307368 3.1574525335 3.7814647364

H -3.578044758 3.7558166426 8.6073895668

H -4.7874704138 3.7049452658 7.3067728071

H -4.9949333547 2.6932300895 8.7565950171

H -1.7443873806 1.9580532125 8.5843093672

H -3.1301066618 1.0000867074 9.1594103438

H -2.1929879512 0.4540042813 7.745780237

H 3.0263102527 -2.1057054116 -0.0660990802

H 4.2854000708 -3.3083697753 0.3039689722

H 3.3607690339 -2.5493032216 1.6244321892

H 5.0248033732 -1.0909611533 -1.3195323505

H 6.2780995875 -0.2914914209 -0.346393916

H 6.322903069 -2.0553102425 -0.5820404266

H 7.7224250956 -0.7779496157 3.1591433185

H 7.0006658768 -1.8311779388 1.9203806742

H 8.0372479248 -0.4656779638 1.440392186

H 6.4830982068 1.4158861267 3.7068988108

H 7.1745360861 1.8368759982 2.1224980565

H 5.425015327 2.0147983438 2.409523957

H -2.1595720954 -1.2969792643 0.8332095142

H -0.7603051546 0.8665607728 -0.4567151666

H 1.4897328749 1.2720988075 -1.4992549053

H 3.5277418529 0.9480420637 -0.1259950459

H -4.1812814396 -0.2492052475 4.4887353772

H 5.408432472 -0.8332500351 4.4383993329

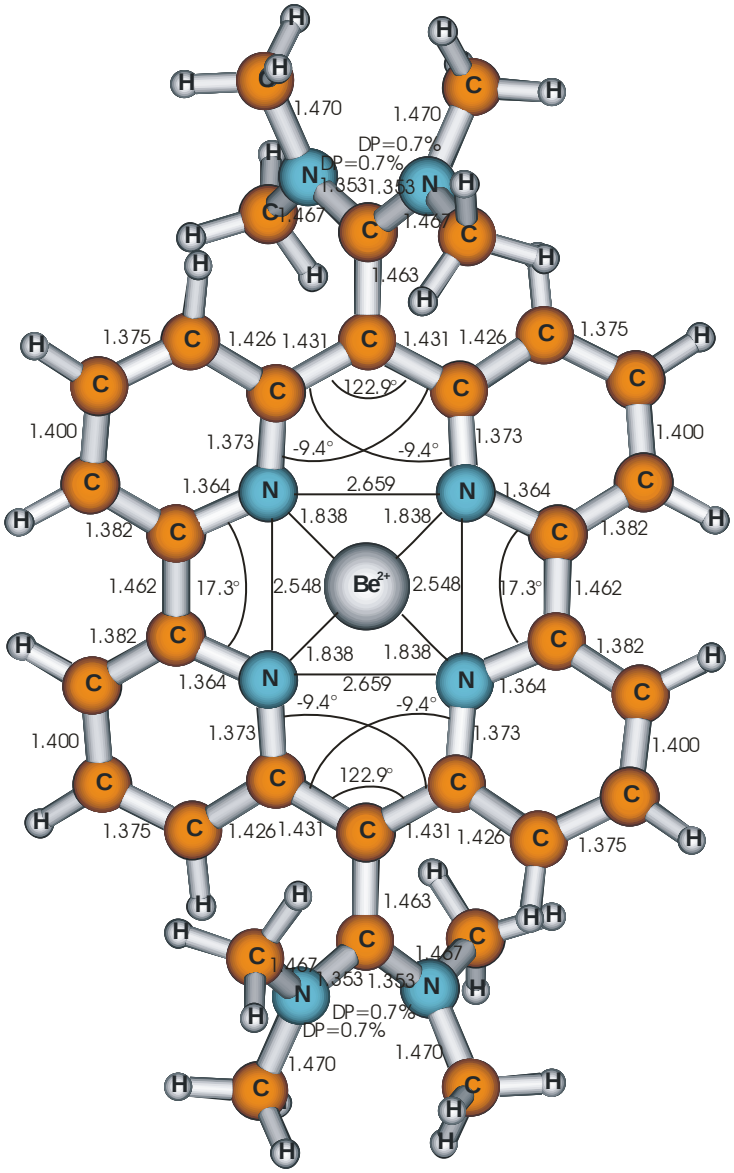
H 5.3282989089 -0.1347526994 6.8042486991

H 3.4524358245 1.3357639128 7.6034369127

H 2.3288230888 3.875640026 6.8358370239

H 0.1762565098 5.1331057686 7.1508852764

H -1.9407649291 4.1090810005 6.3673445963



2a$_{Be2+}$

Figure S33 *The structure and Cartesian coordinates of molecule* ***2a$_{Be2+}$***

	X	Y	Z
C	0.0156545095	-0.1858845736	0.0506325527
C	-0.0021055691	0.008676741	1.4189427817

N 1.1097240363 0.2088671235 2.1833142296

C 2.3344789007 0.0640423722 1.5799359141

C 2.3980903407 -0.0410178578 0.159167472

C 1.2567262712 -0.1613358006 -0.5975339116

C -1.2393514837 0.0515327032 2.1962422693

N -1.0776057058 0.6412424977 3.4154997187

C -2.1999354683 0.8496020131 4.1784069785

C -3.4258095331 0.2338101533 3.7889184409

C -3.541250076 -0.4253740272 2.5881130636

C -2.429688714 -0.4811604525 1.738229247

C -2.1430001055 1.6678594873 5.3514842617

C -3.3968347448 2.0309411348 6.0119192781

N -4.3725205315 2.6749655612 5.33092208

C -4.0921838942 3.4571205526 4.1219894152

C 3.5327566284 0.0242935825 2.3618888947

C 4.7865911332 -0.3387873384 1.7014527709

N 4.9031251849 -1.5156731962 1.0443020353

C 4.0362592443 -2.6616030598 1.3397033934

C -0.9137894542 2.146653898 5.9070887018

N 0.2918199839 1.6808899549 5.443803132

C 1.4103579014 1.9935320808 6.159088367

C 1.4329412873 2.8643818142 7.2321928602

C 0.2299882683 3.4788322921 7.6014305408

C -0.9255538257 3.1208422154 6.9484750538

C 2.6106105705 1.3305450627 5.6524819419

N 2.4555733219 0.8532916882 4.3841361583

C 3.5587589113 0.3240077158 3.761315115

C 4.7327864975 0.0706834913 4.5301809562

C 4.8340477997 0.4921842668 5.8347372282

C 3.7606044305 1.1869539642 6.405699012

N -3.601602208 1.728747279 7.3146996472

C -2.867281105 0.6527711611 7.9891784534

C -4.410499768 2.5543713644 8.2232827806

N 5.8505089795 0.4962668397 1.7368192531

C 5.702716341 1.9360183436 1.9758719605

C 7.2463606405 0.0346823561 1.742430579

C -5.8064160252 2.4988010662 5.6036920409

C 5.750065626 -1.7035492841 -0.1426638521

Be 0.6948777855 0.8460730639 3.8566890944

H -4.4772935238 -0.8964964383 2.3044002953

H -6.3056023233 2.2598407881 4.6582725126

H -5.9628412639 1.6737050839 6.2977529112

H -6.2590376143 3.4091850094 6.0090844649

H -4.3649734841 2.8942024734 3.2217661666

H -4.6883163471 4.3740957396 4.1560289436

H -3.0358648052 3.7180121431 4.0795102083

H -3.8114174075 2.7644031566 9.1160839773

H -4.6699719413 3.4999021539 7.7482895823

H -5.3238957963 2.0395544162 8.5374156592

H -2.0591233834 1.0606595757 8.6074024775

H -3.5634345104 0.1100168586 8.6358345623

H -2.4498032249 -0.0349036444 7.2553565248

H 3.2467091204 -2.7575601226 0.5853190648

H 4.6458315713 -3.5702424936 1.326592207

H 3.5845657884 -2.5475017723 2.3238950238

H 5.1366001771 -2.1546756142 -0.930224764

H 6.1231793321 -0.7440590577 -0.4992273409

H 6.5928795802 -2.3719287915 0.0596767846

H 7.7599296269 0.5147364057 2.5826103752

H 7.2891453188 -1.0452422607 1.8799262591

H 7.7695630324 0.3074957568 0.8205627182

H 5.9568996075 2.1870085849 3.0122539632

H 6.385428404 2.4704410914 1.3082847698

H 4.6806118688 2.248692529 1.7679862591

H -2.4872730769 -0.9729411892 0.7758947646

H -0.903759538 -0.3000620157 -0.5087359552

H 1.3161888337 -0.2338813408 -1.6791197366

H 3.3627820205 -0.0146575593 -0.3302096369

H -4.2756540257 0.278692186 4.457173298

H 5.5529051145 -0.4725053726 4.0794415718

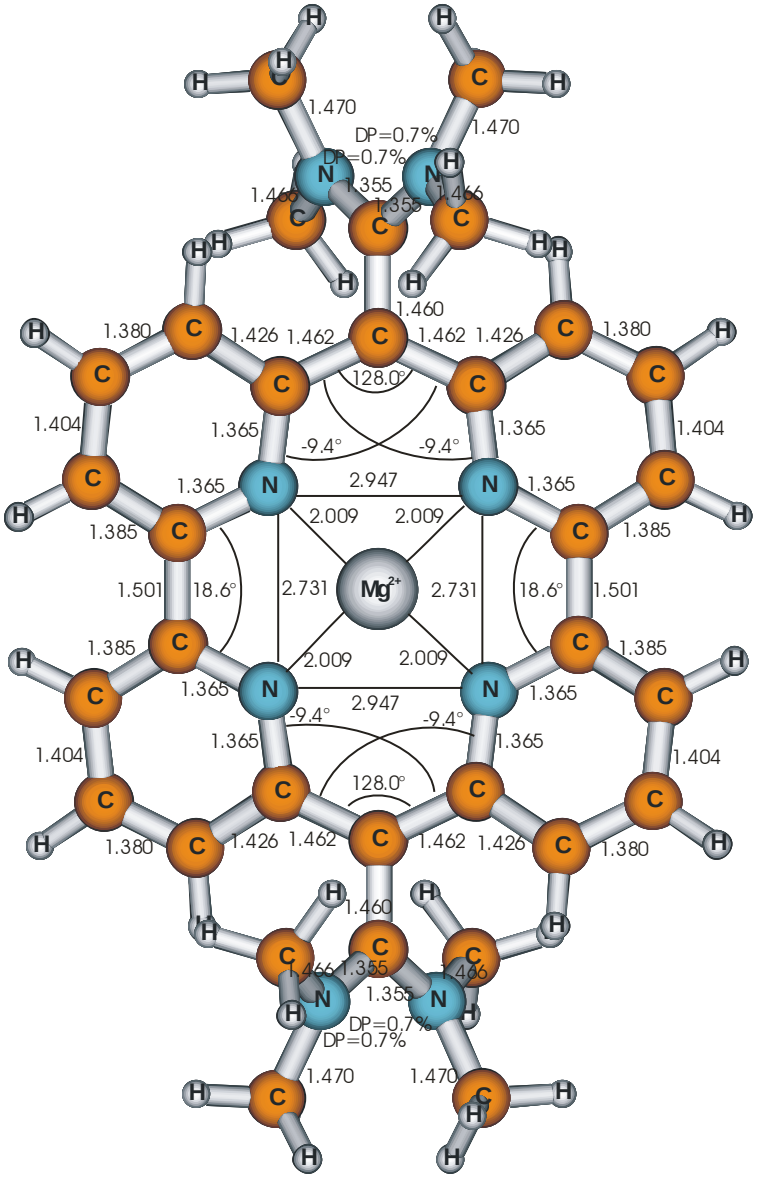
H 5.7298135881 0.2881225695 6.4131738687

H 3.8106800345 1.5528682543 7.4229752555

H 2.3598634814 3.1044200732 7.7366220077

H 0.210803703 4.2265706233 8.3882888579

H -1.8605180712 3.5928085554 7.2203284896



2a$_{Mg2+}$

Figure S34 *The structure and Cartesian coordinates of molecule* ***2a$_{Mg2+}$***

	X	Y	Z
C	-0.0261181391	-0.172831793	-0.0908564273
C	-0.0434130652	-0.1017076063	1.2917785369

N 1.108000293 -0.1824458566 2.0207094868

C 2.339498097 -0.3273942937 1.4502694205

C 2.3843177997 -0.3508130192 0.0250123695

C 1.2236884367 -0.2887409348 -0.7191720418

C -1.3081653696 0.0972101063 2.0745187839

N -1.1591514902 0.5637840944 3.3487704791

C -2.2116310947 0.7618465442 4.1949717386

C -3.5033028173 0.4153235126 3.6995715143

C -3.6652039644 -0.0391426581 2.4065241061

C -2.558456413 -0.197495948 1.5578394322

C -2.0254095523 1.2632421284 5.5552949116

C -3.242143192 1.6283444856 6.2748457426

N -4.1066734881 2.5380464343 5.763034266

C -5.5602202797 2.4837357731 5.9736199919

C 3.5577950456 -0.4120667361 2.2534758259

C 4.7745250489 -0.7771646099 1.5339164617

N 4.8398314038 -1.923996534 0.8145882449

C 5.6315393751 -2.0660472955 -0.4154988444

C -0.7713828883 1.4442254048 6.2841386247

N 0.4158523151 0.9702343466 5.8058075406

C 1.5991444626 1.126461274 6.4684015745

C 1.6599361763 1.7780899786 7.6885330057

C 0.4660943613 2.3100527284 8.2003833479

C -0.7225745305 2.1636812857 7.514552008

C 2.8172044809 0.5803840623 5.7828451624

C 3.9894092025 0.2945843488 6.4620293289

C 5.0401946101 -0.2798212608 5.7298123432

C 4.9063370108 -0.5258422912 4.3784132465

C 3.7082913797 -0.1763283709 3.688164972

N 2.7000743362 0.3507768435 4.4422568334

N -3.5372811665 1.0666229616 7.4724616951

C -4.2532283666 1.7719297926 8.5448683957

C -2.9899658933 -0.2306727978 7.8799495575

N 5.86888546 0.0216925279 1.5674345381

C 7.2466659673 -0.4872419841 1.5145111733

C 5.7781540326 1.4544566876 1.8632914627

C -3.6877054307 3.5453895079 4.7841051836

C 3.9642814751 -3.0668160657 1.0901830066

Mg 0.7662055036 0.4255889123 3.9043919042

H 0.4828681401 2.8687344484 9.1315002687

H -3.6627985569 1.6870857495 9.464049113

H -4.3629733422 2.8274893807 8.297840884

H -5.2399510393 1.3362183259 8.731544082

H -2.1557208652 -0.1026294392 8.5800244948

H -3.779642343 -0.8001904974 8.3798936248

H -2.6470858346 -0.783885984 7.0067234042

H -6.0502104184 2.5384395556 4.995041324

H -5.8399794271 1.5450545759 6.4509931014

H -5.9159008878 3.3222603686 6.5808116725

H -3.9915682447 3.2581935843 3.7703741165

H -4.1682859766 4.4960711478 5.0353621996

H -2.6063450921 3.6712338502 4.8150659639

H 6.0711576861 1.6608636693 2.899635937

H 6.4588731055 1.991656159 1.1955179092

H 4.7612342954 1.807677724 1.6982315645

H 7.8011277191 -0.0627101244 2.3589304497

H 7.2540819805 -1.5731645768 1.6038973037

H 7.7546403192 -0.1935680123 0.5903728468

H 4.9766399349 -2.4604454163 -1.200518558

H 6.013624648 -1.0970007009 -0.7352363945

H 6.4659655097 -2.7625233289 -0.2852370954

H 3.1408979419 -3.1140772196 0.3675000429

H 4.5538135893 -3.9851695519 1.0067440099

H 3.5569650128 -2.992676519 2.0975221117

H 2.5975923767 1.9248219694 8.2096118287

H 4.082625751 0.4537098359 7.5289137289

H 5.9577680621 -0.561282604 6.2379696465

H 5.7136711682 -1.0196398988 3.8540681604

H -1.614789284 2.6322952558 7.9081461682

H 3.3350317258 -0.3845350651 -0.4903209796

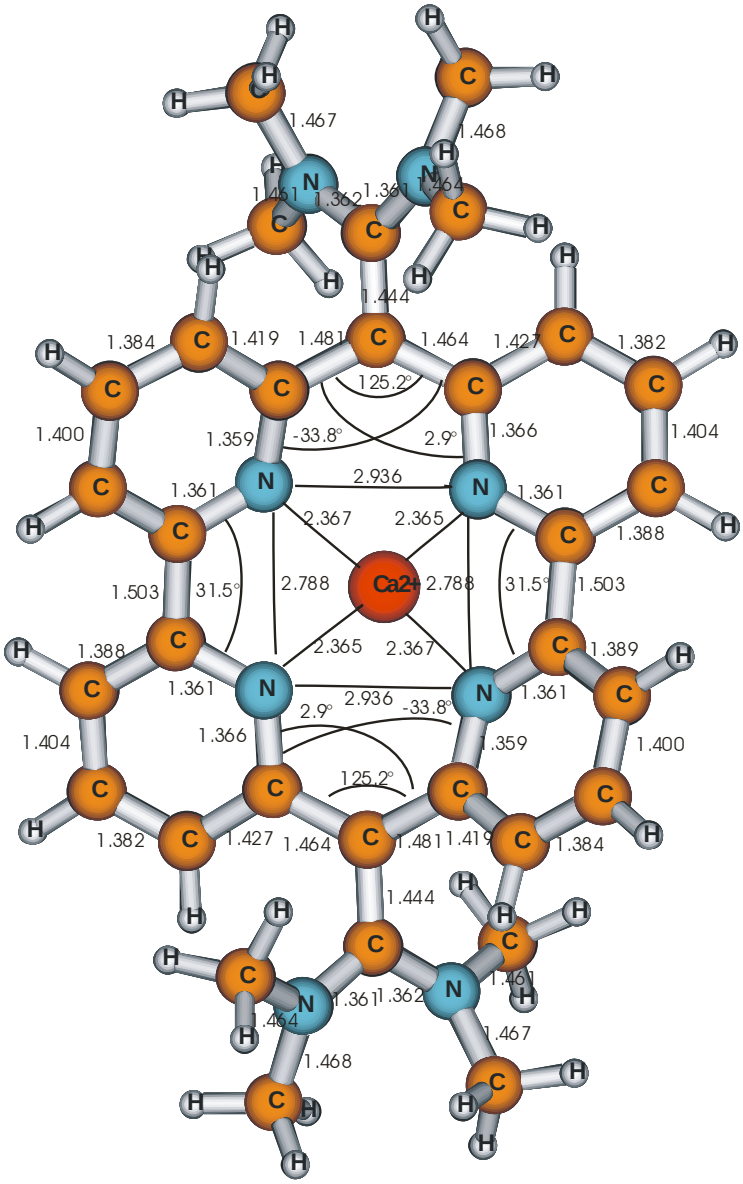
H 1.2805947024 -0.2996817712 -1.8036199796

H -0.9326155965 -0.0879260823 -0.6767795622

H -2.6828321462 -0.5882607155 0.5557984589

H -4.6564559603 -0.3054226813 2.0517005682

H -4.3691323706 0.4742298769 4.3456610637



$2a_{Ca2+}$

Figure S35 *The structure and Cartesian coordinates of molecule* ***$2a_{Ca2+}$***

	X	Y	Z
C	0.1481501828	0.2869622285	-0.0080894132
C	0.0567978971	0.0539324141	1.3581397592

N 1.1621108777 -0.1706805596 2.1197987023

C 2.4158614736 -0.0420288484 1.6119722597

C 2.5471914081 0.2218117418 0.2240231783

C 1.4259763496 0.3506524666 -0.5771315316

C -1.2640048695 0.1261354267 2.0716942638

N -1.2169943976 0.6182698018 3.340102567

C -2.345886822 0.8348957994 4.077480219

C -3.5763706567 0.3523364252 3.538919005

C -3.6203219333 -0.1771786742 2.2627220863

C -2.4579364902 -0.262868248 1.4791733485

C -2.2501827879 1.5117257895 5.3724419606

C -3.4609151618 1.8558382273 6.0795806129

N -4.530542845 2.4335925485 5.4676544925

C -4.391349699 3.2800966934 4.2820044191

C 3.6220855109 -0.1117477512 2.4681648432

C 4.8289483752 -0.5191888044 1.7885986497

N 4.8454666743 -1.6548722976 1.0356253353

C 3.9470547056 -2.7777489219 1.2955725281

C -1.006187112 2.060189714 5.9594375397

N 0.2039000349 1.4742270575 5.7627979774

C 1.3592603634 2.0687300662 6.167769998

C 1.3532610988 3.2326772689 6.925676586

C 0.1153270276 3.8218740808 7.2104054004

C -1.0477883779 3.2649157815 6.7078799123

C 2.6473791421 1.461541017 5.6871824239

N 2.5944974857 0.8733078783 4.4606205174

C 3.7056326069 0.366023509 3.8498092178

C 4.9030320432 0.3069200085 4.6242414312

C 4.9493939437 0.875877093 5.8832624174

C 3.8204376709 1.5087969229 6.4285166036

N -3.560039344 1.6394113074 7.4213532134

C -2.7938055062 0.5987221901 8.1035699663

C -4.2739261289 2.5450845605 8.3287861737

N 5.9783215442 0.2084136394 1.8320826863

C 5.9795310521 1.6601508675 2.0169310954

C 7.3153020265 -0.3976877615 1.8106837694

C -5.9202626336 2.1764011532 5.8649767443

C 5.6071520586 -1.7780461668 -0.212563978

Ca 0.6173106271 -0.4235454383 4.4095484584

H -4.5649787865 -0.537238178 1.8653224979

H -6.4912041511 1.8906189879 4.9737864851

H -5.9621936821 1.3581092853 6.583669975

H -6.3917010561 3.0650990685 6.2980318481

H -4.7404394731 2.7636442003 3.3798831577

H -4.9975037093 4.1815643764 4.4212033103

H -3.348782289 3.5670752627 4.1475624349

H -3.5947457402 2.8318183473 9.1400866235

H -4.5806776488 3.446318814 7.7985094344

H -5.1552617125 2.0685112868 8.7711467528

H -1.9136945172 1.0139997526 8.6106849019

H -3.4339847665 0.1247694747 8.8549882405

H -2.474787002 -0.1551593214 7.3837250248

H 3.0923532459 -2.7770309375 0.6073130745

H 4.5011972035 -3.7120525294 1.1573955001

H 3.584946494 -2.7293103545 2.322615982

H 4.9254007636 -2.1067909823 -1.0055663669

H 6.0279024164 -0.8132749553 -0.4948732809

H 6.4144561656 -2.5132581477 -0.1272366505

H 7.8931522908 0.0010863498 2.6526659154

H 7.2411487282 -1.4796064266 1.9194649886

H 7.855466179 -0.1612988537 0.8876898319

H 6.3137941028 1.9336973903 3.0248248624

H 6.6679744878 2.1058387501 1.2910860434

H 4.9788585055 2.0589896484 1.8527365286

H -2.489030634 -0.6679464763 0.474503326

H -0.7370300333 0.4740877782 -0.6046764263

H 1.5378269862 0.561913146 -1.6365472945

H 3.529150384 0.3731581523 -0.2082632249

H -4.4836095962 0.3896308712 4.1275221863

H 5.7821762284 -0.1903136914 4.2359238997

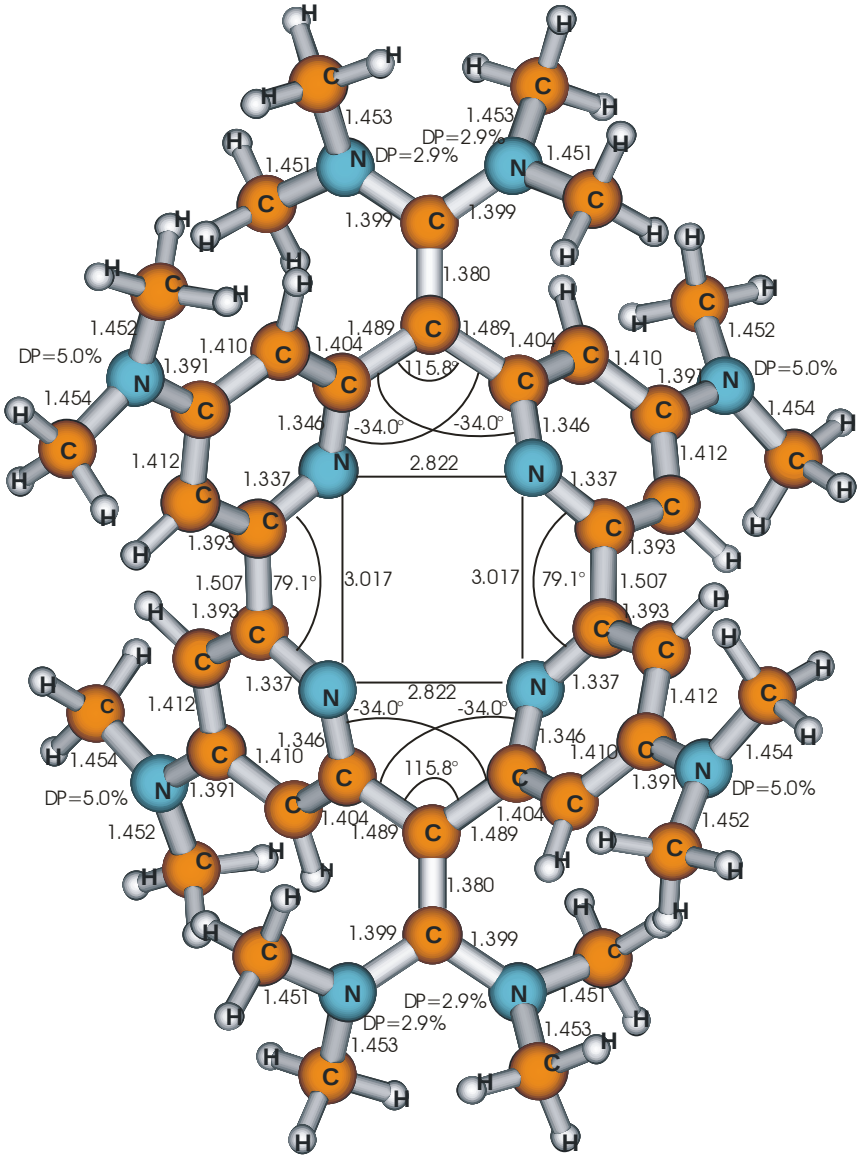
H 5.8689999215 0.8258160837 6.4592525519

H 3.8546621445 1.9650238156 7.4109130143

H 2.2786660595 3.7039095147 7.2355825418

H 0.0730503044 4.7492957994 7.7739700337

H -1.9888289802 3.7832590972 6.8485331378



2b

Figure S36 *The structure and Cartesian coordinates of molecule* ***2b***

	X	Y	Z
C	-1.6848440985	1.3920823486	-3.2994823235
C	-1.6591991031	1.520209989	-1.9014165877

N -0.5043933096 1.5832468652 -1.2133043879

C 0.6372767254 1.4374431579 -1.8926620466

C 0.7154026501 1.3447693692 -3.2802661986

C -0.480821841 1.3481905617 -4.0309265583

C 1.8495735198 1.2667748984 -1.0143137709

N 1.9896766742 0.0318313394 -0.5229060798

C 2.9083415114 -0.16189372 0.4412357367

C 3.7619762724 0.8666453603 0.8714361555

C 3.6914384583 2.1431134209 0.2779184564

C 2.6727672465 2.3395846359 -0.6802880563

C 2.9115452696 -1.4978694476 1.0974719919

C 4.0747001081 -2.0962563986 1.5358887121

N 5.3210989471 -1.9015088475 0.9322521595

C 5.4433223907 -1.6016921023 -0.4819551175

N 4.5603248208 3.1675394309 0.6388614976

C 5.3916317447 3.0072867941 1.8189537454

C -2.9116053958 1.4977645865 -1.0973987042

C -4.0747902016 2.0961184569 -1.5357911716

N -4.1017902828 3.2273880187 -2.3575614346

C -3.0398050011 4.2153654144 -2.3276326717

C 1.5813894089 -2.1479240141 1.2511111087

N 0.5355900033 -1.3310659012 1.4749194728

C -0.6900855272 -1.86338357 1.4514136577

C -0.9485762397 -3.2266826612 1.3300266288

C 0.1382305821 -4.113352485 1.1653622957

C 1.4196606834 -3.5323892289 1.0815385594

C -1.7968569653 -0.840971431 1.4556951063

C -2.4395189662 -0.457593001 2.6304884378

C -3.3487326341 0.6221931876 2.587558691

C -3.4967641137 1.2736953754 1.346492777

C -2.8306379775 0.7894393362 0.2092039863

N -2.0210703558 -0.2842947541 0.2615263067

N 4.1344196948 -2.962942898 2.6318389886

C 3.2087987091 -2.8494682087 3.7432180028

C 4.8158612451 -4.2429817932 2.5419722385

C 6.4965742331 -1.5767957746 1.7220356106

N -5.3539342424 1.6367405786 -1.2062861779

C -5.6125151536 0.2355024632 -0.933363517

C -6.3765838229 2.5457251273 -0.717533447

C -4.9361390166 3.2736926492 -3.5461135061

C 4.2668735122 4.5248773828 0.2089618725

H 6.7586082986 -0.5091855756 1.6230285919

H 6.3036027403 -1.7931014021 2.7738070646

H 7.3653421909 -2.1642177661 1.3940174909

H 6.3288507116 -2.1150922496 -0.8828521024

H 4.5548193261 -1.9553189586 -1.0079233298

H 5.5506212802 -0.5245290508 -0.6789791575

H 4.0924334167 -5.073213424 2.4669674418

H 5.4563939306 -4.256859858 1.6589237677

H 5.4360333594 -4.4216515586 3.4312864145

H 3.7429098144 -3.0664275599 4.6792265415

H 2.8108788931 -1.8340353501 3.7843017971

H 2.3606140386 -3.5454771049 3.66096146

H -2.2967467439 4.0629618702 -3.1246582843

H -3.4768444703 5.2164861674 -2.4509738104

H -2.5222245835 4.1655920002 -1.3680680153

H -4.3310377945 3.1491278777 -4.4607669368

H -5.6772960128 2.4741174359 -3.505933812

H -5.4592594871 4.2370130845 -3.6221239192

H -6.5202032179 2.4330576536 0.3710141802

H -6.0829391839 3.5754677348 -0.9264646508

H -7.3425964549 2.3483318353 -1.2025806672

H -6.5951891166 -0.0353320749 -1.3450169279

H -4.8436266558 -0.3765233469 -1.4080906168

H -5.6146525442 0.0068412982 0.1428892084

H 6.0412714085 3.8801508701 1.918234696

H 4.808970669 2.9011139162 2.7488197891

H 6.0356639423 2.1255955606 1.72269485

H 5.0754642376 5.1834499785 0.5348900889

H 4.2144823148 4.582285552 -0.8836613452

H 3.3184180833 4.9118242594 0.6157447109

H 2.4829775631 3.3095424774 -1.1223637088

H 1.6838682622 1.2215678099 -3.7484172965

N -0.4700260125 1.28037268 -5.4201603974

H -2.6412592599 1.2848235201 -3.7946815197

H 4.4398676011 0.6710451699 1.6922035061

H -4.0869673862 2.1766955153 1.2586987334

N -4.0388819301 1.0397248572 3.7207173972

H -2.191737542 -0.959949456 3.5570474253

H -1.9749593127 -3.5709739743 1.3136227003

N -0.0511854964 -5.487334227 1.0603913052

H 2.2884598532 -4.1324406351 0.8436693059

C -1.7084635485 0.9980191624 -6.1243721467

C 0.773056045 0.9556896679 -6.1003269643

H -1.5224778811 1.0338163126 -7.2004328549

H -2.1318655739 0.0102920975 -5.8783161366

H -2.4664045209 1.7558408417 -5.8948973088

H 0.6090084536 0.9979549959 -7.1797096612

H 1.5508639874 1.6871717033 -5.855752299

H 1.1561968301 -0.0460018839 -5.8461960201

C -1.3980644537 -6.0006986175 0.8714646085

C 1.049069414 -6.3206902899 0.6083530636

H -1.3641059719 -7.0927319881 0.862822804

H -2.0479098971 -5.6971885949 1.6993816036

H -1.8627962814 -5.6601918023 -0.0681339762

H 0.7378954808 -7.367663219 0.6366732432

H 1.3792981271 -6.0846765398 -0.4166670566

H 1.9139509832 -6.2151881076 1.2733824006

C -4.7320482035 2.315779221 3.6968122706

C -3.64138842 0.5207494051 5.0191674337

H -4.3197281034 0.9121138811 5.7810420377

H -3.7173560045 -0.5718118405 5.0393611094

H -2.6108953061 0.7952371199 5.2975599106

H -5.2563934998 2.4541358931 4.6453370036

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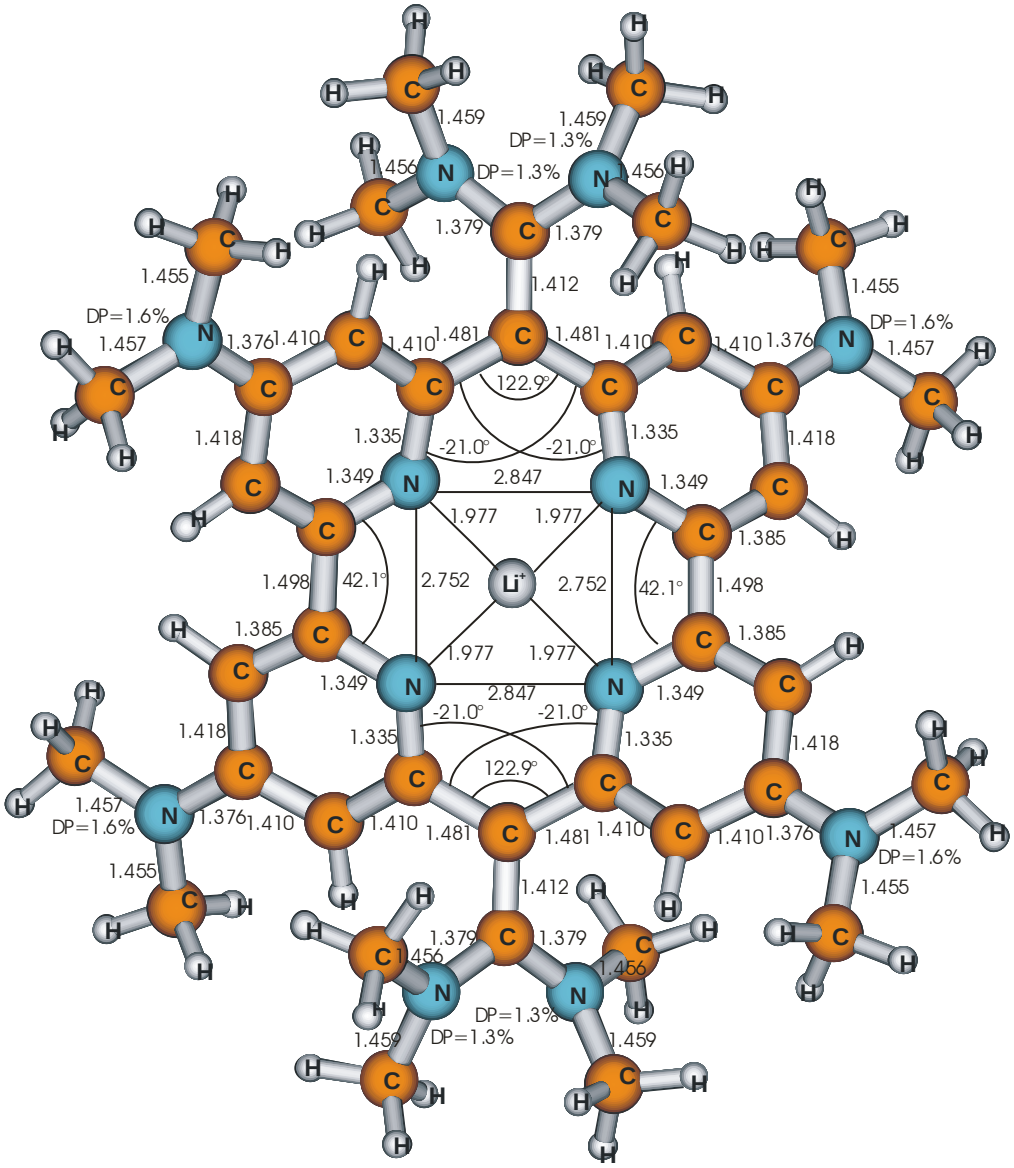
H -5.4830471944 2.3341366046 2.8986348813



$2b_{Li+}$

Figure S37 *The structure and Cartesian coordinates of molecule* ***$2b_{Li+}$***

	X	Y	Z
C	-0.1006962719	0.2949156862	-0.0270687545

C -0.0501346082 0.1930757558 1.353133549

N 1.0944401977 0.1202637455 2.0624080861

C 2.2820268185 0.2016207627 1.4159833641

C 2.3064101748 0.3878110582 0.018379162

C 1.1194701681 0.4043708377 -0.7416375742

C -1.2924325495 0.2191872577 2.1905179803

N -1.207542494 1.0051690858 3.2829689702

C -2.2301119192 1.0195445055 4.1712220574

C -3.3542216547 0.1954443387 3.9572256303

C -3.48248029 -0.584022851 2.7898748131

C -2.3980676997 -0.5533185491 1.8763643464

C -2.1315985658 1.8686240244 5.3806573242

C -3.3210879163 2.2312432117 6.0488206379

N -4.4576750813 2.632435649 5.3797644223

C -4.397411577 3.2535607908 4.0648387932

C 3.5402250816 0.1395285067 2.1947380791

C 4.7297132485 -0.2231110368 1.5265833253

N 4.7845794805 -1.2517856237 0.6104824973

C 3.8595517907 -2.3745082847 0.6581937819

C -0.8407325923 2.3542188584 5.920323431

N 0.3034587322 1.7080404317 5.5914989697

C 1.479419402 2.1614204957 6.0710681933

C 1.6000452788 3.2342311405 6.9384856752

C 0.4292470124 3.9524500642 7.2917394506

C -0.7854194511 3.504164806 6.7346472872

C 2.6804043707 1.4426834559 5.5360440812

N 2.6268973859 1.1828501224 4.2139070806

C 3.6060726533 0.4409516249 3.6432487303

C 4.6504891119 -0.0710388762 4.4405055356

C 4.7510235061 0.2436216016 5.8107643248

C 3.7159783325 1.0405874628 6.3629613425

N -3.438440462 2.2123169159 7.4222443545

C -2.6331663997 1.3273381559 8.2509813369

C -4.1545000698 3.2437817985 8.1643565548

N 5.9287850237 0.4232738106 1.7383272122

C 5.9882757013 1.80987583 2.1767940974

C 7.2015471402 -0.2852708262 1.8120296667

C -5.796851192 2.2275265906 5.7921322432

C 5.5670516958 -1.1698179198 -0.6176910696

Li 0.7043117742 1.0040529303 3.7877079485

N -4.5883143192 -1.3682444876 2.5574929521

H -6.2703780574 1.6453281256 4.9881423459

H -5.7423361202 1.6062989896 6.68657396

H -6.4357114052 3.0953623126 5.9993106076

H -4.6286080878 2.5367661364 3.2649559821

H -5.1287323489 4.0701734792 4.0218387372

H -3.3979713353 3.6547182216 3.8936975171

H -3.4600460218 3.7586386566 8.8442378808

H -4.576132506 3.9769179853 7.4761277311

H -4.9637290118 2.8174081357 8.770622023

H -1.7819551661 1.8551235164 8.7025794795

H -3.2595038377 0.9246194883 9.0566204203

H -2.2505711511 0.5048567159 7.6458014901

H 3.0464436482 -2.263474365 -0.072275589

H 4.4067902269 -3.2979024339 0.4314592431

H 3.4234631272 -2.4488722563 1.6548854372

H 4.8985197504 -1.2500788242 -1.487292053

H 6.0894265341 -0.213974389 -0.6667745696

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H 7.9142624577 0.0850991155 1.0643217797

H 6.1813701063 1.8878746906 3.2555385829

H 6.7986935974 2.3193583373 1.640896945

H 5.0423299562 2.3055761293 1.9564185906

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H 5.3691248472 -0.7405919753 3.990093587

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H 3.6731316704 1.2686435928 7.4194084154

H 2.5829579281 3.5515066869 7.2596470677

N 0.489638847 5.0553965644 8.111335059

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C -5.5897162999 -1.5410901461 3.5983168019

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H -6.0460039142 -0.5814246337 3.8723770143

H -5.6019022297 -2.7287235674 1.3440870336

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H -3.8584147722 -3.0445155129 1.4544220524

C -0.1195801991 0.6948882502 -2.8378387687

C 2.3784552645 0.8694101305 -2.7931474802

H 0.0918333748 0.7235854877 -3.9077169122

H -0.7777368839 -0.1615410094 -2.6527236143

H -0.6631384878 1.6127775052 -2.5694334429

H 2.1879667049 0.9481861113 -3.8642502274

H 2.8159346998 1.8186508334 -2.4509683562

H 3.1229229035 0.0769101715 -2.6449016419

C 1.7813535222 5.5573635288 8.5605055122

C -0.6863110297 5.8920204318 8.2935355023

H -0.4423762079 6.7092897366 8.9734761732

H -1.0412774384 6.3261483951 7.3474570599

H -1.5119782948 5.3231736441 8.7395758225

H 1.620724461 6.3800913236 9.2587001407

H 2.3419572097 4.7782937591 9.0893558972

H 2.401665748 5.9262671552 7.7303606108

C 6.7148338177 -1.2038748916 6.052016134

C 5.776872723 0.0181618427 8.0267304651

H 6.7066132663 -0.3584017779 8.45561383

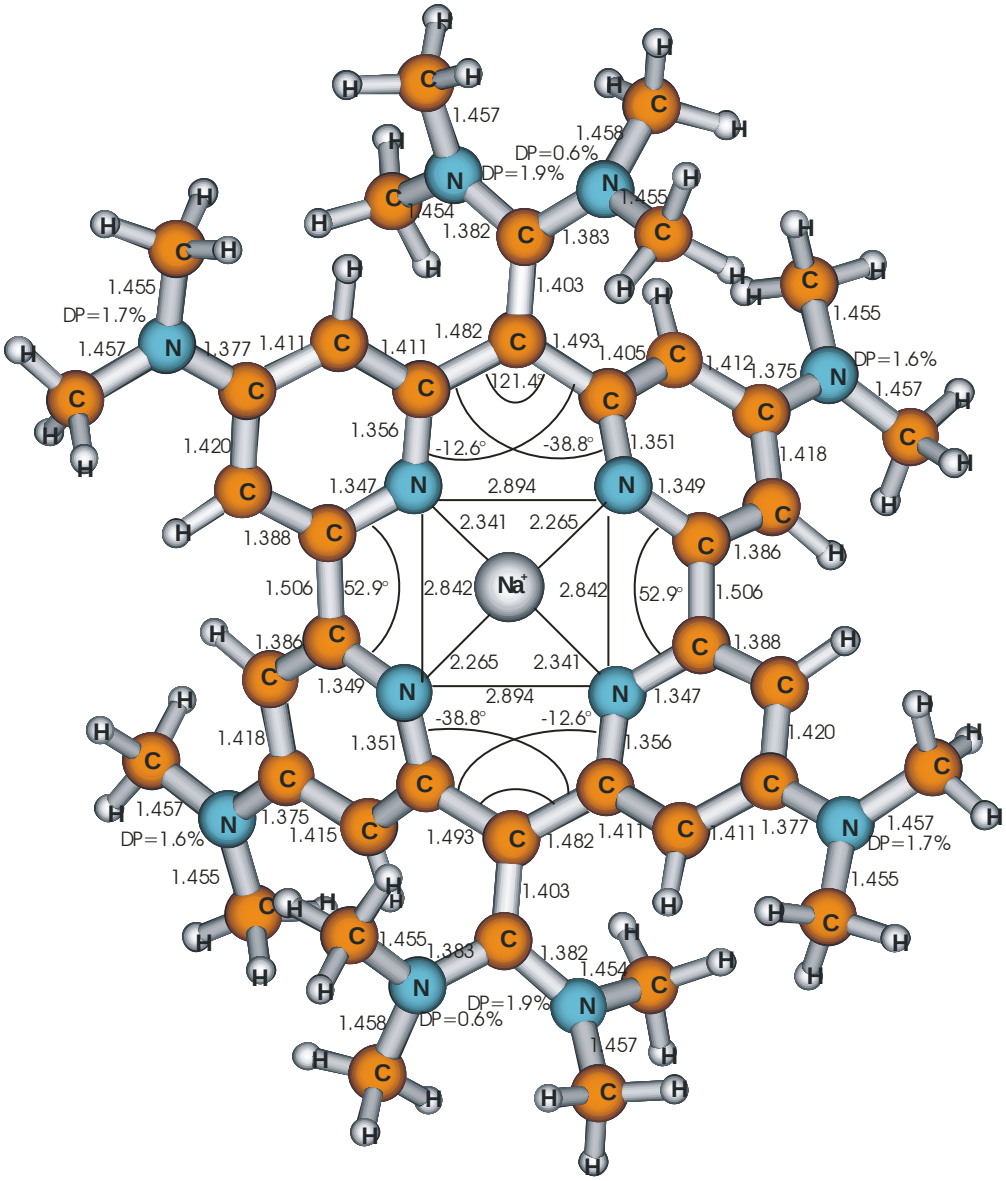
H 5.723532605 1.091497219 8.2412418017

H 4.9371556175 -0.4780203562 8.535352387

H 7.4550731872 -1.4502253496 6.8143214726

H 6.2147296925 -2.1340305988 5.7450329688

H 7.2523216259 -0.8021948566 5.1836698515



$2b_{Na+}$

Figure S38 *The structure and Cartesian coordinates of molecule* ***$2b_{Na+}$***

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C 2.2626221024 0.2704802055 1.3725115793

C 2.2904092862 0.4428922826 -0.0220133439

C 1.1056079908 0.3950126634 -0.7876366652

C -1.3154479609 0.2424680179 2.1432982918

N -1.2973087482 1.2162043065 3.0735281986

C -2.3335234832 1.3298432096 3.9405095831

C -3.3972807982 0.4039473119 3.8900370839

C -3.4558229144 -0.5831998227 2.8833495307

C -2.3656289308 -0.6486014715 1.9756119009

C -2.2681728208 2.4131042141 4.9496245695

C -3.4155775631 2.8313735846 5.6408822312

N -4.6710829657 2.9003070783 5.0675315145

C -4.8605817785 3.1852803024 3.6546041914

C 3.5364117106 0.3408149131 2.1477758508

C 4.685493601 -0.1993421151 1.5501427052

N 4.6543680369 -1.379301708 0.8297645427

C 3.6748799456 -2.4199719423 1.1007726501

C -1.0037758189 3.1659843331 5.2006093431

N 0.181794331 2.5185107423 5.1932964073

C 1.3193410757 3.2374901809 5.2803246808

C 1.3489850634 4.6002475503 5.5315721906

C 0.1220899627 5.3049554245 5.6221059959

C -1.0530795025 4.5571425522 5.3941182348

C 2.5841739129 2.4760589127 4.9812877326

N 2.5615528043 1.8280100646 3.8008894935

C 3.6070799537 1.0376647274 3.4537025382

C 4.6859380339 0.866232263 4.347059386

C 4.7481679342 1.5853877318 5.5595977831

C 3.6472977476 2.4266029933 5.8714143561

N -3.3736149355 3.2237716348 6.9662052959

C -2.3727464428 2.7107299518 7.8886408479

C -4.0862035044 4.4003013046 7.4495436114

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C 6.0976237581 1.8357513912 1.7013725107

C 7.1577966556 -0.3738723089 1.7922588429

C -5.8810525562 2.5097072062 5.7799051288

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H -6.3753822923 1.6799573491 5.252934274

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H -5.1004503724 2.2802887798 3.0790363755

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N 0.0882394285 6.6573981875 5.8685427484

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C -4.470184108 -2.5477618874 1.821343018

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H -3.6566106546 -3.2620655802 2.0179063506

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H 0.0755056154 0.625990178 -3.959850821

H -0.7888794808 -0.2325845785 -2.6822862233

H -0.6827233534 1.5437856711 -2.6426193703

H 2.1823655621 0.8075126858 -3.9262228392

H 2.7596503474 1.8051236882 -2.5756914733

H 3.1293389204 0.0654576662 -2.6328398619

C 6.8312909577 0.4493950019 6.17890569

C 5.7821713774 2.1226503303 7.7179480429

H 7.589828563 0.5097876769 6.9604470841

H 6.4160805367 -0.5694010132 6.1806499047

H 7.3321868807 0.6121650437 5.2163256907

H 6.7377353707 1.9680236572 8.2210202507

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C -1.1675078103 7.3843899406 5.7629141047

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H -1.5797341386 7.3671012962 4.7430382032

H -1.9199850033 6.9675998876 6.4433327272

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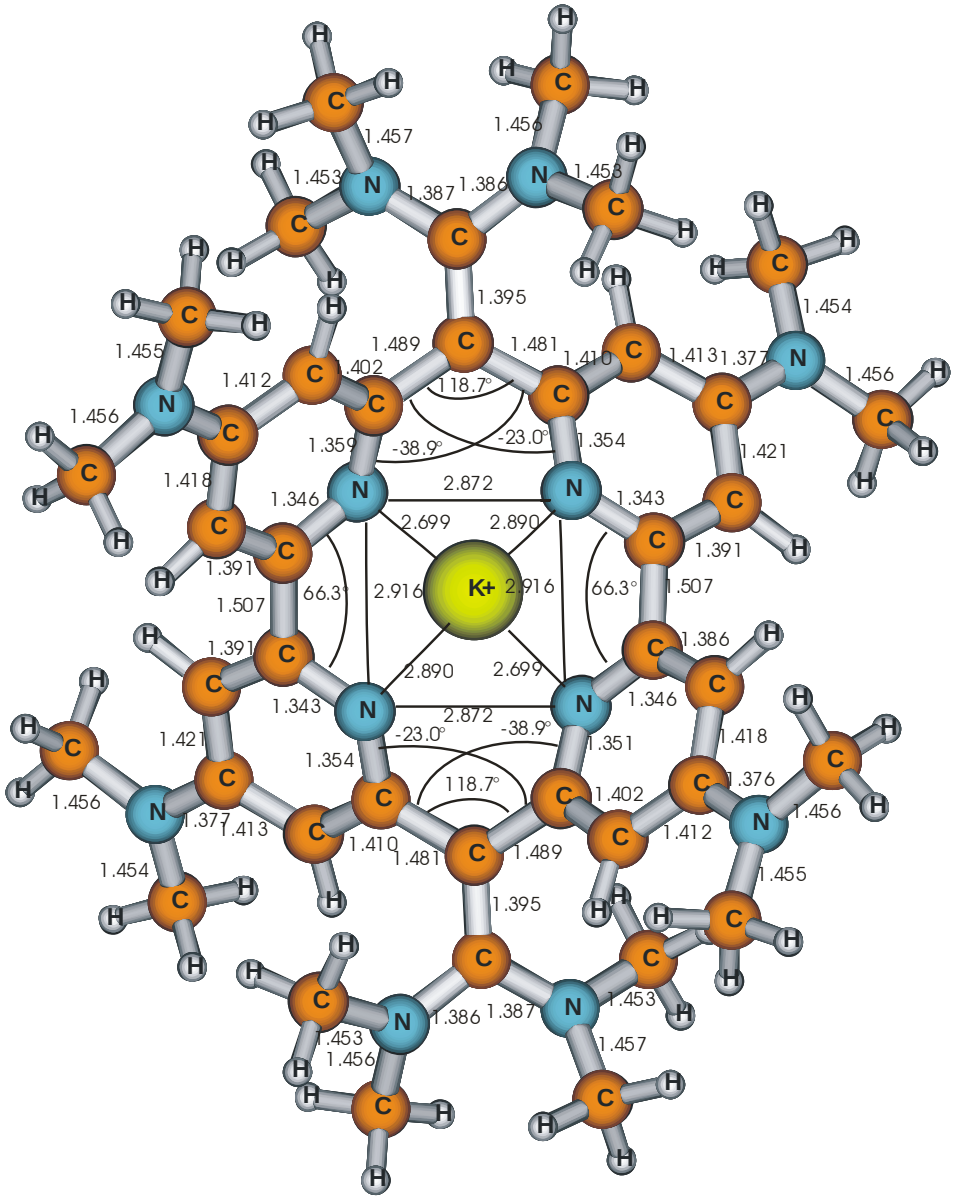

$2b_{K+}$

Figure S39 *The structure and Cartesian coordinates of molecule* ***$2b_{K+}$***

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C 1.1503575475 0.5576601443 -0.6440878125

C -1.1908702584 0.0053892593 2.324061392

N -1.3233064495 1.0478793185 3.1646129036

C -2.2427250435 0.9623303685 4.1510865513

C -3.1055876784 -0.1393589087 4.243619353

C -3.0575288267 -1.1796123507 3.2896724407

C -2.0324156065 -1.0959383206 2.3141825058

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C -3.5050822062 2.4546415725 5.701077467

N -4.6664127823 2.5019452783 4.9450136559

C -5.9361883963 2.0013619682 5.4556664694

N -3.9300381887 -2.242386563 3.3267272738

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C 3.5912063897 0.1643487924 2.2741005996

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N 4.9639710977 -1.0262915834 0.6334229096

C 5.8627965062 -0.7550951252 -0.4799195648

N 1.1376982978 0.8092643896 -1.9975168249

C -0.1309095382 0.9705806803 -2.6939499258

C -0.9988217955 2.6075639851 5.6597036292

N 0.1032470779 1.8325062495 5.5301136127

C 1.2934213212 2.3345395363 5.8968490981

C 1.4683797842 3.5890880674 6.4721775483

C 0.3303478522 4.4224612322 6.6420324172

C -0.9021607121 3.9193651313 6.1682400062

C 2.4565470605 1.4543221749 5.5170102981

C 3.1884251085 0.7596180954 6.4672531543

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C 1.7462047074 6.2130461257 7.5382698859

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H -5.4869960085 3.3730864915 3.2348200548

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H -1.7904424678 4.5362903546 6.1928565251

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H 2.3724940345 6.3751408687 6.6472626876

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H 3.6592928995 -1.1554032097 8.6318765308

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H 6.4709981346 -1.6405438932 5.7038504144

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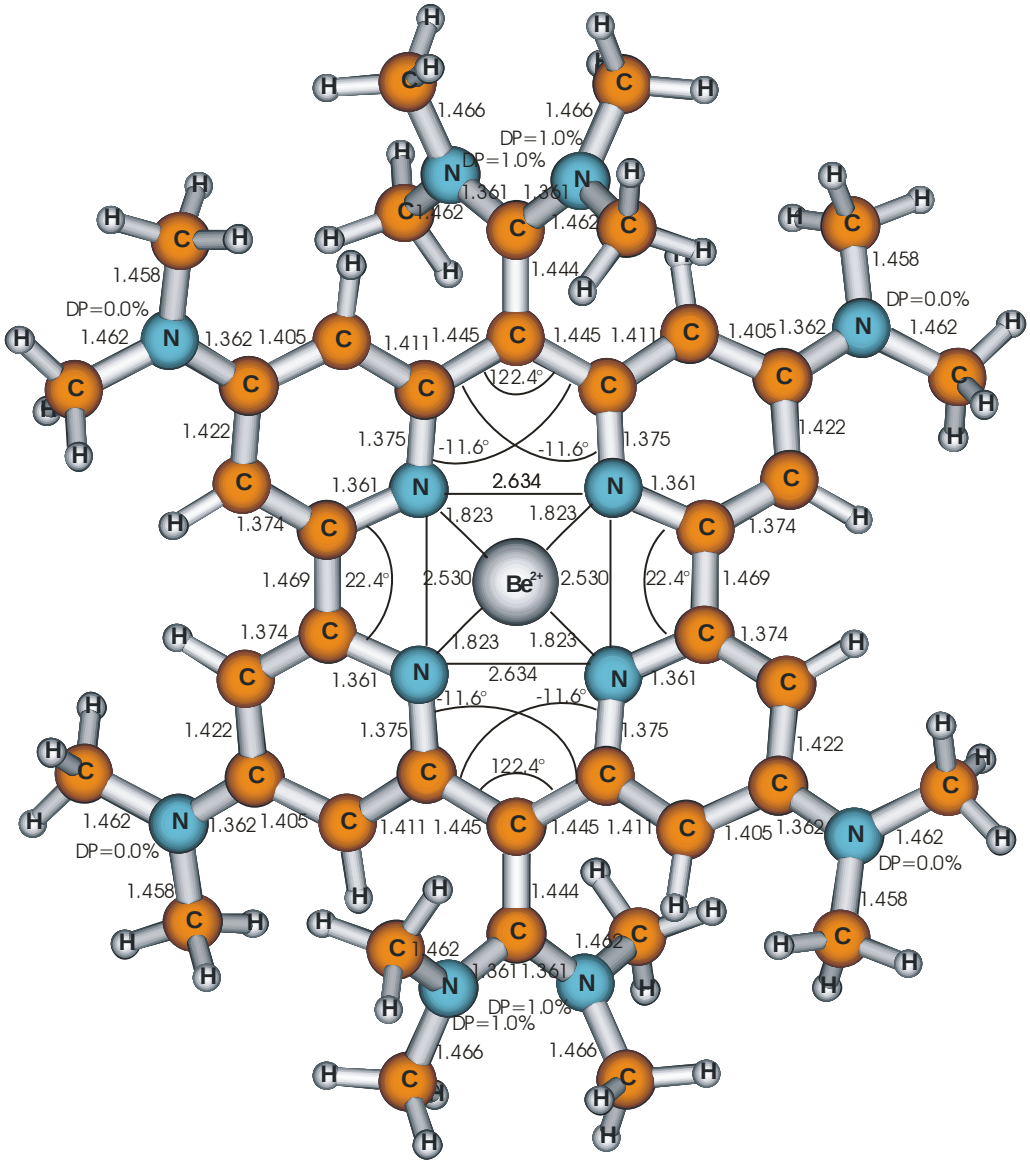

$2b_{Be2+}$

Figure S40 *The structure and Cartesian coordinates of molecule* ***$2b_{Be2+}$***

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C 0.7244270609 2.8618640685 7.8669125511

C -0.5000341762 2.6355440888 7.2156333756

C 2.7742552183 0.6163937039 5.6198746093

C 3.8744233301 0.192031495 6.3255042397

C 4.8638334154 -0.5772698513 5.6531817689

C 4.6828065779 -0.7319513337 4.268265654

C 3.5716298219 -0.1914160825 3.5877457006

N 2.5443442738 0.3807072912 4.2997215632

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C 3.6608819131 -2.6988446646 0.5636582424

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H -1.0454385447 0.4032026025 -0.5029583284

H -2.5469724335 -0.6071627782 0.7225056369

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H 2.5203282098 2.9661874009 9.9787378588

H 2.8981614508 4.3162873539 8.8758988917

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C 6.0685526765 -0.9138499246 7.7612422533

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H 6.1468207148 0.1530306115 8.0019076206

H 5.2306562821 -1.343014955 8.3248191749

H 7.5907357353 -2.3722727194 6.3353808861

H 6.3744293154 -2.8160624964 5.129375224

H 7.4316762086 -1.4056732972 4.8620532051

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C -4.9546892301 -1.3467977885 0.9185908319

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H -6.1943873627 0.0627193394 3.5608821319

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C 2.4163794122 0.7679279314 -2.7814077928

H 2.2207951671 1.0063911082 -3.826481891

H 3.0148531485 1.5816511875 -2.3536114933

H 3.009407495 -0.156292498 -2.7510434997

H 0.1245216648 0.8746581414 -3.8796130708

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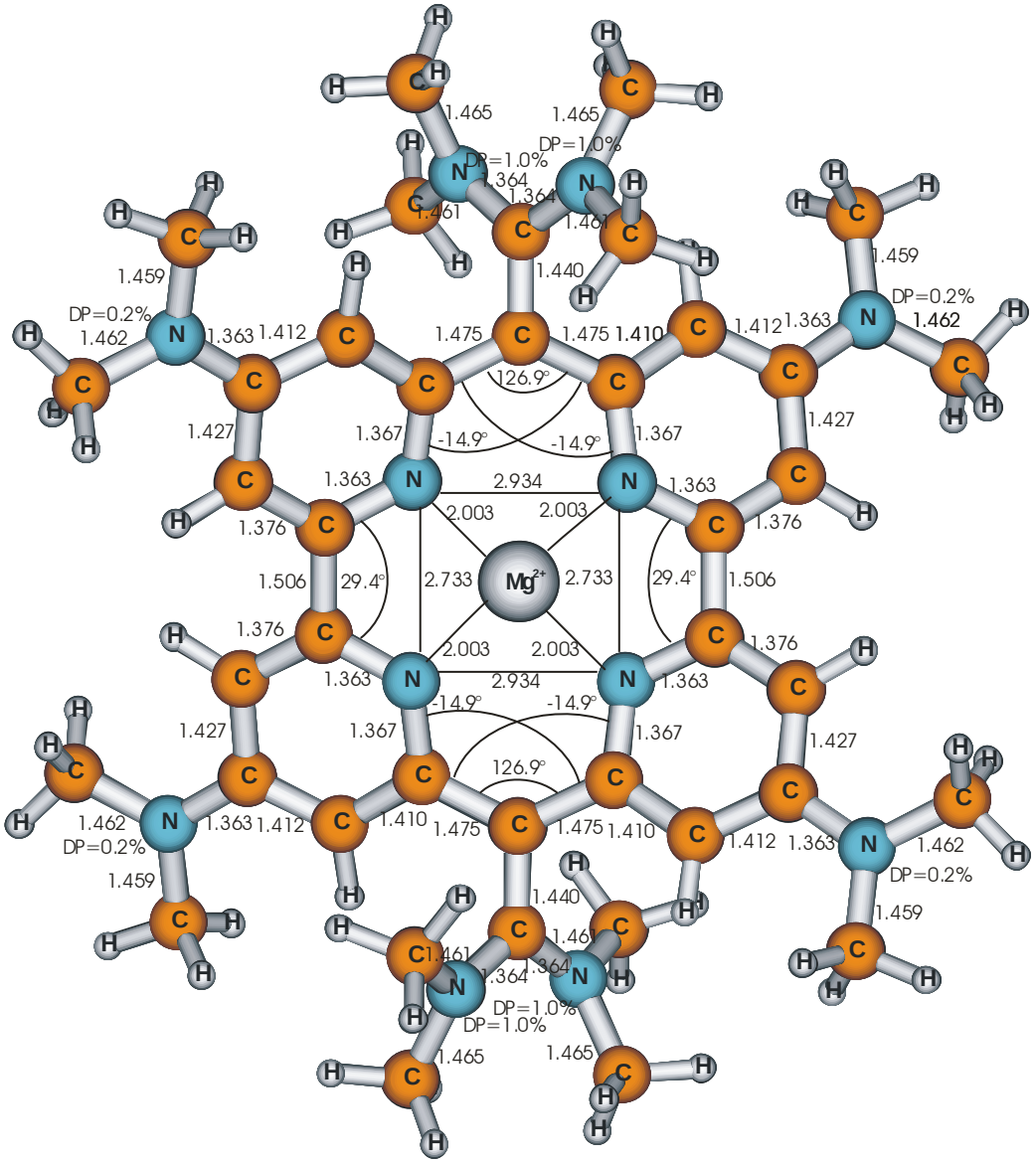

$2b_{Mg2+}$

Figure S41 *The structure and Cartesian coordinates of molecule* ***$2b_{Mg2+}$***

	X	Y	Z
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C	0.0442134968	0.0956730261	1.439243279

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C 1.2708655251 0.3233503915 -0.5846195625

C -1.329959705 -0.0958536403 2.0237995403

N -2.223835253 -0.7187870895 1.2053944244

C -3.5289466229 -0.8825607093 1.5787439043

C -3.9282245144 -0.3722013399 2.8306949812

C -3.0139086527 0.2360302614 3.7180327481

C -1.6636120424 0.3668471392 3.2762354851

C -4.4935433755 -1.5384051297 0.6757793033

C -5.7378777193 -1.9636579312 1.2621221761

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C -4.6463132933 -3.5890922899 2.7674312364

N -3.4011620619 0.7200813996 4.9321826276

C -4.8048374234 0.6839486371 5.3271963603

N 3.6023895108 0.1346439023 2.3065266755

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C 1.3009046084 0.4418841111 -2.0546449775

C 2.5452362406 0.8671382041 -2.6409925548

N 3.1879648803 1.9930642888 -2.2166386363

C 2.4768889826 3.0808582983 -1.5481637158

C -4.3179752601 -1.8045940475 -0.7644446888

N -3.3270552576 -1.1836836668 -1.4730179307

C -3.1436971466 -1.4384658891 -2.7990310141

C -3.953850324 -2.2920710059 -3.5124886402

C -4.9984382395 -2.9797235357 -2.8257807178

C -5.1358629631 -2.7309304954 -1.4428477887

C -1.9558339436 -0.7543985494 -3.4217426144

C -1.9460291714 -0.3609388637 -4.7404940236

C -0.8233436518 0.3716155909 -5.2288988834

C 0.2184677568 0.6427865558 -4.3154524134

C 0.190782111 0.1707626166 -2.9874098764

N -0.9161782228 -0.5168678516 -2.5734868828

N -0.7892966948 0.8213356168 -6.5153758777

C 0.3087497738 1.6654576421 -6.9729763494

N -5.7972103914 -3.8691092828 -3.4810567287

C -5.6031627369 -4.1312879425 -4.9063341518

N -6.9401717431 -1.6102329634 0.7231733019

C -7.0882377984 -0.4266688363 -0.1212412381

C -8.1117043758 -2.4896325098 0.7276849501

N 3.138735805 0.163697898 -3.6478769194

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C 3.8819551534 0.7968509867 -4.7399367232

C -6.8024933699 -2.6127700012 3.4167846122

C 4.646946995 2.1125223759 -2.1622906006

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C 4.8976960373 0.10846943 1.6363460034

C -1.902797867 0.5548865065 -7.4247315318

C -6.7868871585 -4.6509238 -2.748286625

Mg -1.5963108542 -0.548254401 -0.6894323218

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H -7.4576063263 -1.7698095384 3.197109367

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H -5.0370952775 -4.530510916 3.1676422265

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H 3.4465253501 0.4764317516 -5.694907127

H 3.8077587665 1.8820062093 -4.6696127103

H 4.9384002953 0.5065327625 -4.7359155259

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H -4.9720881457 -0.4162201157 3.1012193698

H 1.0451513592 1.2609647907 -4.6304477979

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H -3.7412513611 -2.4906283033 -4.5531292807

H -5.8642511878 -3.2925919071 -0.878260099

H -2.9215367496 1.6160351397 6.7572900031

H -1.5865085623 0.7209836096 6.0280849489

H -2.058200512 2.3136307942 5.3775849348

H -4.9094827837 1.1211029218 6.3197222924

H -5.4361292736 1.2560910221 4.6349671436

H -5.1793904439 -0.3467473241 5.3719932831

H 4.5701922448 0.0708676175 4.1566838006

H 2.970016129 0.8134731721 4.2126388095

H 3.1311536823 -0.9577246901 4.0745754661

H 5.6880972746 0.0655826055 2.3850708496

H 4.9992753872 -0.7682252161 0.9835476532

H 5.0528103517 1.0130007499 1.0343548632

H -7.3140377967 -5.3039993726 -3.4431008557

H -6.3192722646 -5.2790040247 -1.9789303492

H -7.529583942 -4.0020568423 -2.2666187674

H -6.3876657828 -4.8029435054 -5.2539376154

H -5.6720406032 -3.2070662191 -5.4910321546

H -4.6339900815 -4.6061553613 -5.1074055659

H 0.1501394934 1.9242667738 -8.019409766

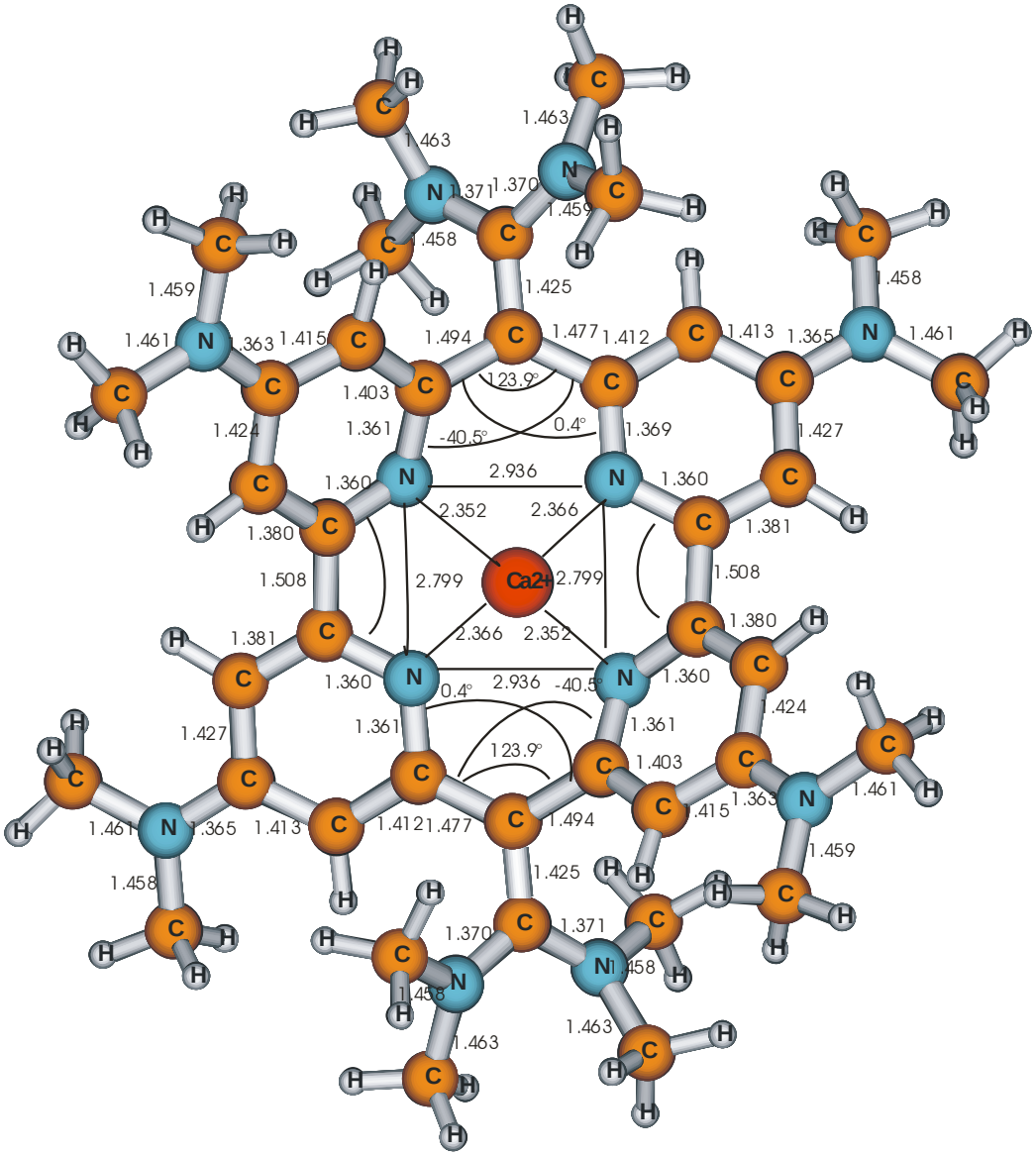
H 0.3708500893 2.5980894675 -6.3973037471

H 1.270887763 1.1427556426 -6.8974525418

H -1.6462770056 0.9229864586 -8.4177540865

H -2.0967547187 -0.5204489662 -7.5074123563

H -2.8242446365 1.0571927658 -7.1024759268



$2b_{Ca2+}$

Figure S42 *The structure and Cartesian coordinates of molecule* ***$2b_{Ca2+}$***

	X	Y	Z
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C	0.0280840326	-0.118474422	1.4473582272

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C 1.4010112998 0.2533895833 -0.5065892501

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N -1.2573803669 0.5896469318 3.3587174656

C -2.4013743889 0.7649978181 4.089226179

C -3.5883358166 0.1429646819 3.644521042

C -3.6472079807 -0.5421035386 2.4100741944

C -2.4506790626 -0.6025934845 1.6346174119

C -2.319921865 1.5637740838 5.3287168651

C -3.5045213533 1.9222246545 6.0354539371

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C -5.9913898644 2.0079860761 5.9119784331

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C -5.9843164528 -1.1573288899 2.815958701

C 3.5750804547 -0.2481975696 2.5884109125

C 4.7509804389 -0.7434825882 1.9534350884

N 4.7189741771 -1.8888399173 1.2000766577

C 5.4623424029 -2.0324218419 -0.0521531101

N 1.5400883437 0.5073942962 -1.8384103434

C 0.3623623069 0.7252386773 -2.6759012812

C -1.0640777123 2.1998318782 5.8281280874

N 0.1303650283 1.5514173286 5.7610476163

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C 1.2876811521 3.4900892312 6.5972274334

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C -1.1119845705 3.5070667692 6.3355640473

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C 3.6822115691 1.5467985024 6.4772580616

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C 4.7819935033 0.2057940742 4.779606728

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N 2.5251250505 0.9237864714 4.4546539371

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C -4.2349588979 2.9110112134 8.1984483353

C -2.6767187127 1.0206896364 8.1860499285

N 5.9667873793 -0.116582627 2.0286914351

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C 5.9693607576 1.3953499866 8.1491129738

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C -4.8256271586 -1.831364631 0.6865506429

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H -1.7795776388 1.5489626785 8.535414112

H -3.2292037702 0.6587938293 9.0600812269

H -2.3727575512 0.1677748572 7.5780318944

H -6.5693119616 1.5370156345 5.106205669

H -5.921770551 1.3096294626 6.746304158

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H 6.1728529854 -2.8657313689 -0.0079523189

H 2.8694484094 -2.8322716266 0.7445736718

H 4.194008725 -3.9084263361 1.2510554176

H 3.3714354491 -2.8847544356 2.453777366

H 2.2334679742 3.9794484489 6.7851302529

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H -2.0556068056 4.0340224697 6.3204109481

H 3.5063979296 0.3572917048 -0.0162235872

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H -2.4176527561 -1.1147510457 0.6828900751

H -4.4721809692 0.1990173727 4.2612069131

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H -1.6599225577 6.3786407082 6.4274305234

H -2.0036522804 5.5625097951 7.9743226315

H 0.9942589811 7.0488813025 8.1919491316

H 1.8386335764 5.5119851915 8.3982451671

H 1.8590312078 6.3381476578 6.8181375389

H 6.9513798382 1.2522101739 8.599301002

H 5.8002481046 2.4740225684 8.0516815228

H 5.2176605493 0.9823026975 8.8346143738

H 7.826532656 -0.0745565025 7.233706928

H 6.7809634057 -1.1290303291 6.2713682684

H 7.5466242164 0.2982491541 5.5279745846

H -6.7694898778 -1.7246037577 2.3167899636

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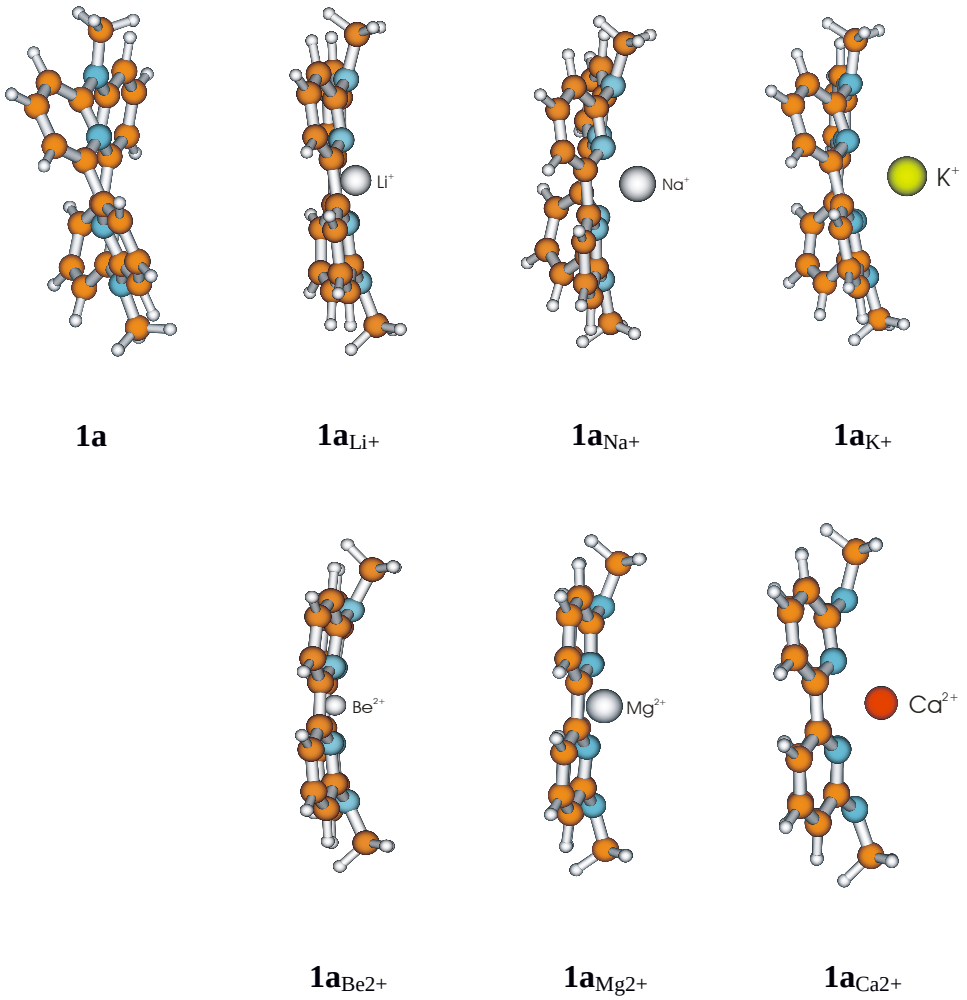

1a **1a**$_{Li+}$ **1a**$_{Na+}$ **1a**$_{K+}$

1a$_{Be2+}$ **1a**$_{Mg2+}$ **1a**$_{Ca2+}$

Figure S43 *The side view of the of the structures* ***1a, 1a***$_{Li+}$***, 1a***$_{Na+}$***, 1a***$_{K+}$***, 1a***$_{Be2+}$***, 1a***$_{Mg2+}$*, and* ***1a***$_{Ca2+}$.

Table S1 *The relevant interatomic distances describing the cavity of the neutral ligands* ***1a*** *–* ***2b*** *and their complexes with* Li^+, Na^+, K^+, Be^{2+}, Mg^{2+} *and* Ca^{2+} *in Å.*

System	N1··N2	N2··N3	N3··N4	N1··N4	N1-M	N2-M	N3-M	N4-M
1a	2.795	2.704	2.795	2.704	-	-	-	-
1a$_{Li+}$	2.622	2.794	2.622	2.794	1.964	1.966	1.964	1.966
1a$_{Na+}$	2.711	2.817	2.711	2.817	2.310	2.319	2.310	2.319
1a$_{K+}$	2.718	2.794	2.718	2.794	2.720	2.747	2.720	2.747
1a$_{Be2+}$	2.519	2.628	2.519	2.628	1.822	1.822	1.822	1.822
1a$_{Mg2+}$	2.685	2.874	2.685	2.874	2.021	2.021	2.021	2.021
1a$_{Ca2+}$	2.673	2.901	2.673	2.901	2.405	2.405	2.405	2.405
1b	2.816	2.705	2.816	2.705	-	-	-	-
1b$_{Li+}$	2.653	2.776	2.653	2.776	1.954	1.953	1.954	1.953
1b$_{Na+}$	2.707	2.814	2.707	2.814	2.295	2.305	2.295	2.305
1b$_{K+}$	2.713	2.795	2.713	2.795	2.693	2.729	2.693	2.729
1b$_{Be2+}$	2.490	2.610	2.490	2.610	1.805	1.805	1.805	1.805
1b$_{Mg2+}$	2.655	2.865	2.655	2.865	2.009	2.009	2.009	2.009
1b$_{Ca2+}$	2.650	2.913	2.650	2.913	2.385	2.381	2.385	2.381
2a	2.953	2.786	2.953	2.786	-	-	-	-
2a$_{Li+}$	2.743	2.857	2.743	2.857	1.980	1.980	1.980	1.980
2a$_{Na+}$	2.820	2.891	2.820	2.891	2.330	2.287	2.330	2.287
2a$_{K+}$	2.861	2.852	2.861	2.852	2.829	2.710	2.829	2.710
2a$_{Be2+}$	2.548	2.659	2.548	2.659	1.838	1.838	1.838	1.838
2a$_{Mg2+}$	2.731	2.947	2.731	2.947	2.009	2.009	2.009	2.009
2a$_{Ca2+}$	2.788	2.936	2.788	2.936	2.365	2.367	2.365	2.367
2b	3.017	2.822	3.017	2.822	-	-	-	-
2b$_{Li+}$	2.752	2.847	2.752	2.847	1.977	1.977	1.977	1.977
2b$_{Na+}$	2.842	2.894	2.842	2.894	2.265	2.341	2.265	2.341

2b$_{K+}$	2.916	2.872	2.916	2.872	2.699	2.890	2.699	2.890
2b$_{Be2+}$	2.530	2.634	2.530	2.634	1.823	1.823	1.823	1.823
2b$_{Mg2+}$	2.733	2.934	2.733	2.934	2.003	2.003	2.003	2.003
2b$_{Ca2+}$	2.799	2.936	2.799	2.936	2.352	2.366	2.352	2.366

Table S2 *Electronic energy, ΔE_{elect}, thermal correction to enthalpy, Enthalpy corr., thermal correction to Gibbs free energy, Gibbs corr., and basis set superposition error, BSSE.*

System	ΔE_{elect} [a]	Enthalpy corr.[b]	Gibbs corr.[b]	BSSE[a]
Py	-248.36897	0.09425	0.06229	-
Py_{Li+}	-255.72914	0.09825	0.06275	0.00037
Py_{Na+}	-410.50949	0.09775	0.05999	0.00087
Py_{K+}	-848.16635	0.09755	0.05828	0.00025
Py_{Be2+}	-262.37637	0.09859	0.06357	0.00040
Py_{Mg2+}	-447.81895	0.09781	0.06121	0.00076
Py_{Ca2+}	-925.41707	0.09771	0.05940	0.00025
DMAP	-382.38720	0.17222	0.12894	-
$DMAP_{Li+}$	-389.76484	0.17651	0.12989	0.00035
$DMAP_{Na+}$	-544.54207	0.17592	0.12700	0.00091
$DMAP_{K+}$	-982.19660	0.17567	0.12520	0.00027
$DMAP_{Be2+}$	-396.46305	0.17681	0.13023	0.00036
$DMAP_{Mg2+}$	-581.88609	0.17583	0.12655	0.00074
$DMAP_{Ca2+}$	-1059.47687	0.17596	0.12595	0.00023
$[Li(Py)_4]^+$	-1000.95655	0.388577	0.30124	0.00221
$[Na(Py)_4]^+$	-1155.71360	0.38741	0.29121	0.00289
$[K(Py)_4]^+$	-1593.34596	0.38698	0.28709	0.00116
$[Be(Py)_4]^{2+}$	-1007.91385	0.39291	0.31817	0.00298
$[Mg(Py)_4]^{2+}$	-1193.25765	0.38964	0.30518	0.00274
$[Ca(Py)_4]^{2+}$	-1670.77754	0.38831	0.29566	0.00145
$[Li(DMAP)_4]^+$	-1537.05938	0.70085	0.57084	0.00199
$[Na(DMAP)_4]^+$	-1691.81456	0.69978	0.56267	0.00275
$[K(DMAP)_4]^+$	-2129.44487	0.69934	0.55673	0.00107
$[Be(DMAP)_4]^{2+}$	-1544.07839	0.70587	0.58887	0.00264

$[Mg(DMAP)_4]^{2+}$	-1729.41593	0.70263	0.57653	0.00250
$[Ca(DMAP)_4]^{2+}$	-2206.92957	0.70120	0.56691	0.00129
1a	-1178.05120	0.38687	0.31449	-
$1a_{Li+}$	-1185.53773	0.39362	0.32181	0.00103
$1a_{Na+}$	-1340.27538	0.39169	0.31863	0.00202
$1a_{K+}$	-1777.90803	0.39106	0.31644	0.00076
$1a_{Be2+}$	-1192.48490	0.39678	0.32729	0.00096
$1a_{Mg2+}$	-1377.82712	0.39415	0.32298	0.00166
$1a_{Ca2+}$	-1855.33919	0.39231	0.31914	0.00076
1b	-1714.11305	0.69882	0.58612	-
$1b_{Li+}$	-1721.63092	0.70583	0.59283	0.00096
$1b_{Na+}$	-1876.36622	0.70386	0.58947	0.00195
$1b_{K+}$	-2313.99621	0.70316	0.58688	0.00077
$1b_{Be2+}$	-1728.63602	0.70967	0.59859	0.00089
$1b_{Mg2+}$	-1913.97081	0.70695	0.59424	0.00161
$1b_{Ca2+}$	-2391.47651	0.70507	0.59118	0.00074
2a	-1679.55594	0.67285	0.56739	-
$2a_{Li+}$	-1687.05896	0.68000	0.57562	0.00114
$2a_{Na+}$	-1841.79191	0.67800	0.57141	0.00208
$2a_{K+}$	-2279.42278	0.67737	0.56835	0.00082
$2a_{Be2+}$	-1694.04938	0.68366	0.57982	0.00095
$2a_{Mg2+}$	-1879.39698	0.68129	0.57604	0.00170
$2a_{Ca2+}$	-2356.88830	0.67948	0.57355	0.00085
2b	-2215.61532	0.98465	0.83925	-
$2b_{Li+}$	-2223.13575	0.99187	0.84804	0.00120
$2b_{Na+}$	-2377.86872	0.98984	0.84268	0.00226
$2b_{K+}$	-2815.49929	0.98919	0.83934	0.00094

$2b_{Be2+}$	-2230.16020	0.99552	0.85000	0.00092
$2b_{Mg2+}$	-2415.50361	0.99340	0.84806	0.00174
$2b_{Ca2+}$	-2892.99299	0.99140	0.84454	0.00100
Li^+	-7.28492	0.00236	-0.01275	-
Na^+	-162.08757	0.00236	-0.01443	-
K^+	-599.76105	0.00236	-0.01518	-
Be^{2+}	-13.65289	0.00236	-0.01310	-
Mg^{2+}	-199.24100	0.00236	-0.01449	-
Ca^{2+}	-676.90578	0.00236	-0.01521	-
$[Li(CH_3CN)_4]^+$	-538.69696	0.20967	0.12967	0.00114
$[Na(CH_3CN)_4]^+$	-693.46031	0.20792	0.12647	0.00225
$[K(CH_3CN)_4]^+$	-1131.09739	0.20764	0.12021	0.00066
$[Be(CH_3CN)_4]^{2+}$	-545.61870	0.21155	0.14038	0.00162
$[Mg(CH_3CN)_4]^{2+}$	-730.98177	0.20913	0.13499	0.00185
$[Ca(CH_3CN)_4]^{2+}$	-1208.51590	0.20668	0.13156	0.00073
CH_3CN	-132.80467	0.05018	0.02163	-

[a]Calculated at the B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d) level of theory (in a.u.)
[b]Calculated at the B3LYP/6-31G(d) level of theory (in a.u.)

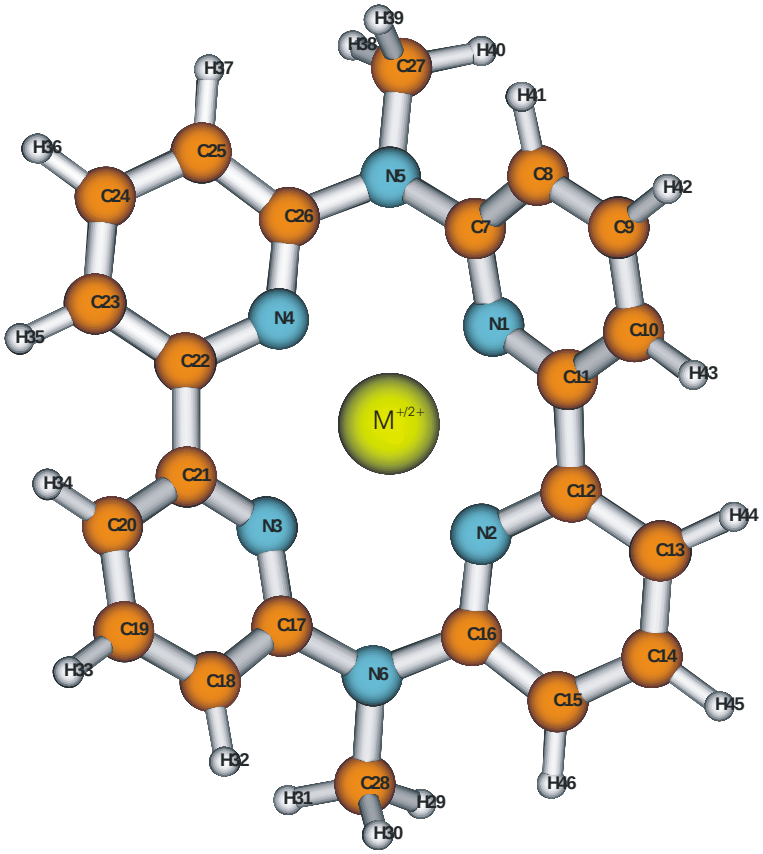

Table S3 *Atomic populations obtained by the Hirshfeld population analysis (in* e*) of* ***1a, 1a$_{Li+}$, 1a$_{Na+}$, 1a$_{K+}$, 1a$_{Be2+}$, 1a$_{Mg2+}$*** *and* ***1a$_{Ca2+}$****.*

Atom	1a	1a$_{Li+}$	1a$_{Na+}$	1a$_{K+}$	1a$_{Be2+}$	1a$_{Mg2+}$	1a$_{Ca2+}$
N1	7.17	7.17	7.17	7.19	7.14	7.18	7.18
N2	7.18	7.18	7.18	7.21	7.14	7.18	7.18
N3	7.17	7.17	7.17	7.19	7.14	7.18	7.18
N4	7.18	7.18	7.18	7.21	7.14	7.18	7.18
N5	7.09	7.07	7.08	7.12	7.06	7.06	7.12
N6	7.09	7.07	7.08	7.12	7.06	7.06	7.12
C7	5.86	5.83	5.84	5.84	5.81	5.82	5.83
C8	6.07	6.05	6.05	6.05	6.04	6.03	6.03
C9	6.02	5.98	5.98	5.99	5.94	5.94	5.96
C10	6.07	6.05	6.04	6.04	6.02	6.02	6.02
C11	5.92	5.90	5.91	5.90	5.90	5.90	5.89
C12	5.92	5.90	5.91	5.90	5.90	5.90	5.89
C13	6.08	6.05	6.05	6.05	6.03	6.03	6.03
C14	6.01	5.98	5.98	5.99	5.94	5.94	5.96
C15	6.09	6.06	6.06	6.06	6.04	6.04	6.04
C16	5.86	5.83	5.84	5.84	5.81	5.82	5.83
C17	5.86	5.83	5.84	5.84	5.81	5.82	5.83
C18	6.07	6.05	6.05	6.05	6.04	6.04	6.04

C19	6.02	5.98	5.98	5.99	5.94	5.94	5.96
C20	6.07	6.04	6.04	6.04	6.02	6.02	6.03
C21	5.92	5.90	5.91	5.91	5.90	5.90	5.90
C22	5.92	5.90	5.91	5.91	5.90	5.90	5.90
C23	6.08	6.05	6.05	6.05	6.02	6.02	6.02
C24	6.01	5.98	5.98	5.99	5.94	5.94	5.96
C25	6.09	6.06	6.06	6.06	6.04	6.04	6.04
C26	5.86	5.83	5.84	5.84	5.81	5.82	5.83
C27	6.01	6.00	6.00	6.00	5.98	5.99	6.00
C28	6.01	6.00	6.00	6.00	5.98	5.99	6.00
H29	0.97	0.95	0.95	0.95	0.94	0.94	0.94
H30	0.97	0.96	0.96	0.96	0.94	0.95	0.95
H31	0.96	0.95	0.95	0.94	0.94	0.94	0.94
H32	0.96	0.95	0.94	0.94	0.93	0.93	0.93
H33	0.95	0.93	0.93	0.93	0.90	0.91	0.91
H34	0.96	0.95	0.94	0.94	0.92	0.92	0.92
H35	0.96	0.95	0.94	0.94	0.92	0.92	0.92
H36	0.95	0.93	0.93	0.93	0.90	0.91	0.91
H37	0.97	0.95	0.94	0.94	0.93	0.93	0.93
H38	0.97	0.95	0.95	0.95	0.94	0.94	0.94
H39	0.97	0.96	0.96	0.96	0.94	0.95	0.95
H40	0.96	0.95	0.95	0.94	0.94	0.94	0.94
H41	0.96	0.95	0.94	0.94	0.93	0.93	0.93
H42	0.95	0.93	0.93	0.93	0.90	0.91	0.91
H43	0.96	0.95	0.94	0.94	0.92	0.92	0.92
H44	0.95	0.95	0.94	0.94	0.92	0.92	0.92
H45	0.95	0.93	0.93	0.93	0.90	0.91	0.91
H46	0.95	0.95	0.94	0.94	0.93	0.93	0.93
M	-	2.79	10.65	18.53	3.66	11.41	19.24

Table S4 *The continuum solvation free energy in CH_3CN, ΔG_{sol}*.*

System	ΔG_{sol}*[a]	System	ΔG_{sol}*[a]
1a	0.3	**[2a$_{Be2+}$(AN)]**	-70.3
[1a$_{Li+}$(AN)]	-13.3	**[2a$_{Mg2+}$(AN)]**	-67.9
[1a$_{Na+}$(AN)]	-12.3	**[2a$_{Ca2+}$(AN)]**	-67.3
[1a$_{K+}$(AN)]	-14.0	**2b**	32.2
[1a$_{Be2+}$(AN)]	-102.7	**[2b$_{Li+}$(AN)]**	27.4
[1a$_{Mg2+}$(AN)]	-99.2	**[2b$_{Na+}$(AN)]**	27.7
[1a$_{Ca2+}$(AN)]	-101.2	**[2b$_{K+}$(AN)]**	25.1
1b	15.0	**[2b$_{Be2+}$(AN)]**	-37.3
[1b$_{Li+}$(AN)]	13.2	**[2b$_{Mg2+}$(AN)]**	-35.3
[1b$_{Na+}$(AN)]	13.7	**[2b$_{Ca2+}$(AN)]**	-59.8
[1b$_{K+}$(AN)]	12.5	**[Li(CH$_3$CN)$_4$]$^+$**	-11.1
[1b$_{Be2+}$(AN)]	-56.9	**[Na(CH$_3$CN)$_4$]$^+$**	-9.6
[1b$_{Mg2+}$(AN)]	-54.4	**[K(CH$_3$CN)$_4$]$^+$**	-11.0
[1b$_{Ca2+}$(AN)]	-56.1	**[Be(CH$_3$CN)$_4$]$^{2+}$**	-113.0
2a	13.9	**[Mg(CH$_3$CN)$_4$]$^{2+}$**	-108.6
[2a$_{Li+}$(AN)]	4.7	**[Ca(CH$_3$CN)$_4$]$^{2+}$**	-113.0
[2a$_{Na+}$(AN)]	4.9	**CH$_3$CN**	-0.1
[2a$_{K+}$(AN)]	4.9		

[a]Calculated at the B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level of theory (in kcal mol^{-1})

Table S5 *The gas phase Gibbs free energy of complexation, $\Delta_r G°_{(g)}$, and Gibbs free energy of complexation in acetonitrile solvent, $\Delta_r G*_{(AN)}$ for reaction $[M(AN)_4]^{+/2+} + L \rightarrow [L_{M+/2+}(AN)] + 3AN$.*

Host compound	$\Delta_r G°_{(g)}$					
	Li^+	**Na^+**	**K^+**	**Be^{2+}**	**Mg^{2+}**	**Ca^{2+}**
1a	-29.9	-18.7	-11.9	-65.5	-61.6	-46.9
1b	-46.5	-34.6	-26.8	-112.0	-105.2	-87.0
2a	-33.5	-23.4	-16.9	-89.0	-87.0	-67.2
2b	-43.5	-32.1	-21.6	-117.8	-114.9	-92.5
	$\Delta_r G*_{(AN)}$					
1a	-28.7	-18.2	-11.7	-51.8	-49.0	-31.8
1b	-33.5	-22.8	-14.9	-67.5	-62.5	-41.6
2a	-27.9	-19.4	-11.4	-56.7	-56.7	-31.2
2b	-33.5	-23.5	-14.2	-70.7	-70.3	-43.7