10.1071/CH11334_AC

Australian Journal of Chemistry 2012, 65(2), 138-144

Supplementary Material

Structural Characteristics and Large Nonlinear Optical Responses of New Alkaline Earth-Based Alkalides

Li-Tao Fan, Ying Li, Di Wu*, Zhi-Ru Li, Chia-Chung Sun

Institute of Theoretical Chemistry, State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, Changchun 130023, P. R. China

*Email: wud@mail.jlu.edu.cn

Optimized Geometries (in Cartesian Coordinates) and Total Energies of the $M^{2+}(H_5Aza222)M'^{-}$ Alkalides

$Be^{2+}(H_5Aza222)^{-}Li^{-}$ (E = -1361.907984 au.)

N	-3.1102540	-0.3513110	0.9418570
C	-3.5440720	0.8527760	1.6454690
C	-2.3963430	1.5219970	2.3932280
N	-1.3564400	1.9710720	1.4632440
C	-0.0579630	2.1087190	2.1230490
C	1.0185560	2.7143050	1.2302400
N	1.1356740	2.0633370	-0.0819940
C	2.3956960	2.3836040	-0.7565360
C	3.6069200	1.5925860	-0.2540370
N	3.4751270	0.1453930	-0.3252300
C	3.3299220	-0.4299320	-1.6526350
C	2.1571820	-1.4144090	-1.6807360
N	0.8436640	-0.7345290	-1.5612700
C	0.3899170	-0.1867270	-2.8645250
C	-0.9976120	0.4023200	-2.6646350
N	-1.6909290	-0.4192780	-1.6975950

C	-3.0317500	0.0698050	-1.4990660
C	-3.7687480	-0.5830340	-0.3394330
C	-2.9938670	-1.5388230	1.7700830
C	-1.9920590	-2.5277400	1.1775620
N	-0.7469040	-1.8185180	0.7470500
C	0.5045750	-2.4501110	1.2605830
C	1.4913790	-1.3830740	1.7047850
N	2.8275950	-1.9421920	1.8528990
C	3.8795490	-0.9308990	1.9238760
C	4.4200460	-0.5686900	0.5408240
H	-4.3662000	0.6401480	2.3487310
H	-3.9297280	1.5567380	0.9013830
H	-2.7828560	2.3851390	2.9477970
H	-1.9899030	0.8246650	3.1436130
H	0.2919140	1.1446830	2.5215790
H	-0.1853170	2.7678280	2.9892190
H	0.8311810	3.7922060	1.1009320
H	1.9702340	2.6209040	1.7621660
H	0.3848410	2.4583250	-0.6536370
H	2.6493380	3.4536160	-0.6658070
H	2.2526720	2.2032470	-1.8272560
H	4.4951950	1.9542140	-0.8074770
H	3.7824980	1.8453220	0.7955460
H	4.2432060	-0.9545490	-1.9720540
H	3.1646130	0.3623530	-2.3886250
H	2.1635470	-1.9872480	-2.6162020
H	2.2825900	-2.1126500	-0.8496680
H	0.9695390	0.0651340	-0.9161880
H	0.3505760	-1.0259890	-3.5686490
H	1.0955590	0.5474630	-3.2683980
H	-0.9161060	1.4524200	-2.3291650
H	-1.5092310	0.4417300	-3.6445890
H	-3.6517850	-0.0635490	-2.4075390
H	-3.0203720	1.1627900	-1.3192960
H	-4.8102520	-0.2242860	-0.3217690
H	-3.8271660	-1.6610730	-0.5188540
H	-3.9576660	-2.0551600	1.9250440
H	-2.6280970	-1.2534120	2.7620900
H	-1.7482150	-3.2688450	1.9449580
H	-2.4221590	-3.0579060	0.3217890
H	-0.8221850	-0.8898650	1.1647440
H	0.9518670	-3.0766820	0.4827440
H	0.2707530	-3.0940400	2.1181680
H	1.5471600	-0.5741590	0.9756280
H	1.1181220	-0.9569670	2.6529020
H	2.8451870	-2.5175740	2.6930750

H	4.7119020	-1.3430450	2.5036290
H	3.5475350	-0.0229870	2.4538550
H	5.3462120	0.0195420	0.6555580
H	4.6982090	-1.5082200	0.0548880
N	-0.6929930	-3.1719050	-1.7119880
H	0.1930680	-3.3067700	-2.1962290
H	-0.6959230	-3.8786050	-0.9774890
C	-1.8006040	-3.4468880	-2.6552130
H	-2.7473120	-3.3948500	-2.1171440
H	-1.8163500	-2.6673070	-3.4158540
H	-1.7047690	-4.4309700	-3.1221710
C	-1.1029790	5.3262830	-0.9700200
H	-0.3336770	5.5581550	-0.2282040
H	-2.0098060	5.8838700	-0.6963400
H	-0.7497190	5.7058720	-1.9330230
N	-1.2827530	3.8769650	-1.0449580
H	-1.5781760	3.4892470	-0.1459230
H	-1.9979380	3.6422330	-1.7259090
Be	-0.6989630	-1.4711530	-0.9873230
Li	-0.2464520	-2.8130340	5.3206120
H	-1.2804060	1.2669190	0.7295980

$Be^{2+}(H_5Aza222)^-Na^-$ (E = -1516.699754 au.)

N	3.1291360	-0.4229940	-0.5829190
C	3.5337430	0.4090020	-1.7132960
C	2.3775520	0.6696520	-2.6722140
N	1.3058010	1.4176560	-2.0097000
C	0.0158200	1.2243330	-2.6718330
C	-1.0952180	2.1019400	-2.1088890
N	-1.2213680	2.0328080	-0.6464160
C	-2.5083490	2.5441850	-0.1692820
C	-3.6769170	1.5660750	-0.3168610
N	-3.4950620	0.2791860	0.3373920
C	-3.3542770	0.2984900	1.7846510
C	-2.1481990	-0.5425190	2.2125720
N	-0.8572120	0.0832160	1.8331450
C	-0.4534270	1.1332200	2.8021830
C	0.9194690	1.6428060	2.3924670
N	1.6628440	0.5252760	1.8539740
C	2.9896960	0.9447680	1.4792180
C	3.7713730	-0.0901340	0.6844620
C	3.0724460	-1.8474990	-0.8596630
C	2.0917380	-2.5515760	0.0760760
N	0.8139580	-1.7796270	0.1749280
C	-0.4047890	-2.6147810	-0.0391430

C	-1.4188400	-1.8670700	-0.8899790
N	-2.7326170	-2.4865520	-0.7922240
C	-3.8183600	-1.6372540	-1.2764770
C	-4.3985210	-0.7615250	-0.1660910
H	4.3768190	-0.0369250	-2.2664630
H	3.8791830	1.3692470	-1.3179190
H	2.7439340	1.2457430	-3.5299730
H	2.0093540	-0.2883840	-3.0740600
H	-0.2957120	0.1694360	-2.6406660
H	0.1370760	1.4750440	-3.7317350
H	-0.9395540	3.1454690	-2.4253840
H	-2.0327310	1.7700300	-2.5652820
H	-0.4994280	2.6566030	-0.2775660
H	-2.7980090	3.4734680	-0.6886740
H	-2.3852800	2.8196540	0.8833900
H	-4.5912450	2.0823910	0.0344520
H	-3.8350950	1.3629770	-1.3799840
H	-4.2539080	-0.0880450	2.2870880
H	-3.2314060	1.3268370	2.1367120
H	-2.1522970	-0.6887700	3.2997290
H	-2.2332770	-1.5208490	1.7342210
H	-0.9978650	0.5457240	0.9176730
H	-0.4057720	0.6580120	3.7888930
H	-1.1916400	1.9402620	2.8626210
H	0.8130050	2.4598110	1.6554580
H	1.4045350	2.0997880	3.2752840
H	3.5966910	1.2142750	2.3659680
H	2.9436890	1.8708240	0.8731940
H	4.7990130	0.2737010	0.5255330
H	3.8668780	-1.0004960	1.2842000
H	4.0564330	-2.3430690	-0.7853160
H	2.7217160	-2.0013450	-1.8854660
H	1.8914680	-3.5502520	-0.3240450
H	2.5208510	-2.6719210	1.0758910
H	0.8639410	-1.0980430	-0.5836510
H	-0.8476690	-2.8806820	0.9254130
H	-0.1329450	-3.5476680	-0.5491200
H	-1.5138420	-0.8308100	-0.5635790
H	-1.0445030	-1.8590240	-1.9292600
H	-2.7187120	-3.3607690	-1.3147060
H	-4.6238860	-2.2844640	-1.6383840
H	-3.5083560	-1.0151560	-2.1322150
H	-5.3403180	-0.3068690	-0.5170940
H	-4.6570880	-1.4300400	0.6600290
N	0.7549880	-2.0199600	2.9734500
H	-0.1260470	-1.9601930	3.4814540

H	0.7697050	-2.9656820	2.5932240
C	1.8711160	-1.8662780	3.9344260
H	2.8144320	-2.0316450	3.4134450
H	1.8785850	-0.8411680	4.3026700
H	1.7922900	-2.5697860	4.7677080
C	0.8758010	5.4657760	-1.1439690
H	0.1106320	5.3475380	-1.9162960
H	1.7652440	5.9032070	-1.6189260
H	0.4923150	6.1855560	-0.4152580
N	1.1092210	4.1779010	-0.4916850
H	1.4356430	3.4743250	-1.1579770
H	1.8203870	4.2670360	0.2270630
Be	0.7202720	-0.7604460	1.6201690
H	1.2407360	1.0723020	-1.0525300
Na	0.3629070	-4.7248590	-3.6500220

$Be^{2+}(H_5Aza222)^-K^-$ (E = -1954.360990)

N	-0.6250370	-3.0746690	-0.3539840
C	-0.1810340	-3.5525160	-1.6604570
C	-0.0846320	-2.4209000	-2.6777140
N	0.9117430	-1.4296960	-2.2664390
C	0.6623780	-0.1202580	-2.8668650
C	1.7604620	0.8978300	-2.5850700
N	2.1093580	1.0097330	-1.1626520
C	2.8579110	2.2325840	-0.8625080
C	2.0002350	3.4964360	-0.7572700
N	0.9279540	3.4401930	0.2253720
C	1.3297180	3.2872080	1.6154760
C	0.5243870	2.1689660	2.2826410
N	0.8931000	0.8252500	1.7718200
C	2.1254290	0.3129080	2.4226670
C	2.3741250	-1.0963750	1.9081100
N	1.0878760	-1.7242010	1.7014840
C	1.2628160	-3.0821650	1.2530400
C	-0.0187920	-3.7558010	0.7861870
C	-2.0585600	-2.8779320	-0.2273770
C	-2.3779290	-1.8486930	0.8542440
N	-1.4978570	-0.6472430	0.7146620
C	-2.2458670	0.6444460	0.7188310
C	-1.6798700	1.5973680	-0.3235800
N	-2.0912060	2.9660940	-0.0512420
C	-1.3246120	3.9691600	-0.7862180
C	-0.1111990	4.4531460	0.0073740
H	-0.8408390	-4.3442290	-2.0522270
H	0.8132860	-3.9929900	-1.5383860

H	0.1963240	-2.8351500	-3.6530340
H	-1.0776580	-1.9603380	-2.8094990
H	-0.3080630	0.2884610	-2.5452550
H	0.5950350	-0.2509280	-3.9528420
H	2.6559820	0.6504900	-3.1770180
H	1.4031340	1.8678790	-2.9436400
H	2.7360330	0.2245370	-0.9688660
H	3.6354790	2.4328830	-1.6192230
H	3.3955610	2.0686760	0.0772260
H	2.6831660	4.3485050	-0.5746320
H	1.5333170	3.6876090	-1.7278670
H	1.1867730	4.2175580	2.1852810
H	2.3979480	3.0593000	1.6745640
H	0.6832950	2.1793550	3.3678770
H	-0.5341500	2.3556350	2.0888210
H	1.0951900	0.9269590	0.7620490
H	1.9340400	0.2969240	3.5017280
H	2.9834010	0.9720670	2.2517210
H	2.9679730	-1.0579540	0.9764470
H	3.0046550	-1.6336360	2.6410050
H	1.7057960	-3.7188860	2.0440300
H	1.9885370	-3.1209380	0.4168690
H	0.1890490	-4.8118470	0.5524220
H	-0.7343590	-3.7686330	1.6137850
H	-2.6074180	-3.8100060	-0.0064210
H	-2.4525560	-2.5027720	-1.1771020
H	-3.4280660	-1.5558800	0.7585880
H	-2.2490170	-2.2783090	1.8524260
H	-1.0493970	-0.7537080	-0.1963100
H	-2.1894920	1.1027140	1.7105540
H	-3.3066090	0.4635790	0.5076580
H	-0.5888740	1.5729330	-0.3174490
H	-2.0134600	1.2550910	-1.3191890
H	-3.0836280	3.0633310	-0.2565780
H	-1.9701260	4.8359830	-0.9614050
H	-1.0128690	3.6056680	-1.7791590
H	0.3206190	5.3366830	-0.4918200
H	-0.4834320	4.7887730	0.9794710
N	-0.9558270	-0.5998700	3.4721890
H	-0.6879150	0.2708240	3.9288060
H	-1.9685490	-0.5331970	3.3697680
C	-0.6360950	-1.7291490	4.3758360
H	-1.0109800	-2.6538290	3.9364460
H	0.4464410	-1.8211540	4.4554110
H	-1.0801190	-1.5965040	5.3660450
C	5.0697510	-1.3939770	-2.5399200

H	4.8148230	-0.6206130	-3.2697900
H	5.2834620	-2.3189590	-3.0936780
H	5.9899170	-1.0779180	-2.0404760
N	3.9901160	-1.5107070	-1.5601550
H	3.1075490	-1.7709550	-2.0053340
H	4.2073900	-2.2281060	-0.8757420
Be	-0.1193400	-0.6651000	1.8297890
H	0.8568310	-1.3441210	-1.2518020
K	-6.2315450	0.1721920	-1.8313340

$Mg^{2+}(H_5Aza222)^-Li^-$ (E = -1547.244940 au.)

N	-3.2381670	-0.1272820	-0.0650900
C	-3.7689490	1.1411090	0.4422480
C	-2.9307820	1.6931820	1.5857830
N	-1.6155190	2.1166160	1.0985050
C	-0.6251700	2.1769460	2.1723240
C	0.6684530	2.8595490	1.7486540
N	1.2387580	2.3048950	0.5168430
C	2.6547880	2.6178280	0.3545150
C	3.5673990	1.6425270	1.1041100
N	3.4318360	0.2673440	0.6523140
C	4.0573490	-0.0815330	-0.6044970
C	3.1457670	-1.0432860	-1.3690830
N	1.7781310	-0.5004460	-1.4340980
C	1.4085680	-0.0433030	-2.7829070
C	0.0631380	0.6561910	-2.7422210
N	-0.9040070	-0.1058350	-1.9846850
C	-2.2070380	0.4636350	-2.2364780
C	-3.3347070	-0.2525190	-1.5149660
C	-3.7764540	-1.2749240	0.6457550
C	-2.8974030	-2.5145600	0.5397600
N	-1.5068740	-2.2119840	0.9356910
C	-0.7886290	-3.4145850	1.3936410
C	0.4814300	-2.9729580	2.0855660
N	1.3052090	-2.0395440	1.2743900
C	2.1197670	-1.2095310	2.2080740
C	3.4761250	-0.7611860	1.6753010
H	-4.8161930	1.0281050	0.7671840
H	-3.7664440	1.8712540	-0.3724760
H	-3.4415070	2.5566420	2.0296300
H	-2.8438740	0.9334120	2.3789470
H	-0.4086830	1.1736680	2.5741820
H	-1.0559700	2.7473260	3.0030410
H	0.4954180	3.9425040	1.6382900
H	1.3887280	2.7383430	2.5652010

H	0.7296460	2.7363180	-0.2570970
H	2.9006880	3.6396840	0.6918640
H	2.8892990	2.5896820	-0.7158250
H	4.6102310	1.9990220	1.0296960
H	3.3073620	1.6697410	2.1659450
H	5.0611530	-0.5246610	-0.4804570
H	4.1822920	0.8294960	-1.1974820
H	3.5321410	-1.2072120	-2.3806680
H	3.1489320	-2.0228130	-0.8764630
H	1.7572350	0.2996780	-0.7882060
H	1.3534110	-0.9259170	-3.4326300
H	2.1760770	0.6232360	-3.2051120
H	0.2070710	1.6801080	-2.3401760
H	-0.2580470	0.8032680	-3.7916330
H	-2.4460630	0.4396690	-3.3185540
H	-2.2468830	1.5391890	-1.9662360
H	-4.3098350	0.1151050	-1.8819910
H	-3.2853250	-1.3128550	-1.7814170
H	-4.7975100	-1.5339460	0.3078100
H	-3.8496140	-1.0232650	1.7092270
H	-3.3183200	-3.2768680	1.2081340
H	-2.9000130	-2.9322910	-0.4734960
H	-1.5908160	-1.6199360	1.7783950
H	-0.6011560	-4.0767150	0.5408560
H	-1.3914780	-3.9678480	2.1286540
H	0.1680920	-2.4409800	2.9937010
H	1.0693290	-3.8388340	2.4159080
H	1.9580380	-2.6034510	0.7328300
H	2.3088040	-1.7893980	3.1207550
H	1.5227900	-0.3423360	2.5025490
H	4.0626460	-0.4178680	2.5401850
H	4.0165650	-1.6357700	1.2877040
N	-0.2078370	-3.0498610	-1.8664610
H	-1.0312670	-3.6204510	-1.6890940
H	-0.4864700	-2.3784840	-2.5893530
C	0.9010550	-3.9051530	-2.3130460
H	1.7638500	-3.2808660	-2.5513950
H	1.1884680	-4.5856110	-1.5072020
H	0.6544650	-4.5037630	-3.1963220
C	-0.6726750	5.5876230	-0.9506540
H	-0.2376780	5.8145040	0.0269400
H	-1.6528370	6.0833290	-1.0026230
H	-0.0244950	6.0405910	-1.7065890
N	-0.7143900	4.1390410	-1.1362450
H	-1.2809730	3.6841680	-0.4159180
H	-1.1169770	3.9017490	-2.0370290

Mg	-0.1224570	-1.2819850	-0.5129720
Li	-2.2463200	-1.8004420	4.9903190
H	-1.3080390	1.4265940	0.4131060

$Mg^{2+}(H_5Aza222)^-Na^-$ (E = -1702.036215 au.)

N	-2.5200700	1.7709950	-0.7844570
C	-2.3548970	3.1007220	-0.1903650
C	-1.6376320	3.0396950	1.1500090
N	-0.2404030	2.6396110	0.9652420
C	0.3388080	2.0849050	2.1871510
C	1.8488460	1.9078260	2.1016850
N	2.2763640	1.1593340	0.9156450
C	3.6244940	0.6147290	1.0414430
C	3.6579420	-0.7206490	1.7907750
N	2.8823510	-1.7631700	1.1390150
C	3.4629340	-2.3910900	-0.0272590
C	2.3667540	-2.6358990	-1.0662560
N	1.5945840	-1.4018140	-1.2900770
C	1.8564780	-0.7945380	-2.6044710
C	1.1680490	0.5540120	-2.6965380
N	-0.2010470	0.4784470	-2.2376400
C	-0.8623430	1.7033000	-2.6232920
C	-2.3278280	1.7563600	-2.2304710
C	-3.7529310	1.1256200	-0.3651970
C	-3.7065440	-0.3921900	-0.4882090
N	-2.5163650	-0.9402160	0.1951150
C	-2.7137510	-2.3389150	0.6162280
C	-1.6083290	-2.7047640	1.5805150
N	-0.2478870	-2.4151150	1.0583810
C	0.6622990	-2.2191620	2.2232560
C	2.1114920	-2.6380190	2.0023480
H	-3.3286220	3.6028650	-0.0705910
H	-1.7619040	3.7170280	-0.8726850
H	-1.6665510	4.0273950	1.6261750
H	-2.1718520	2.3486460	1.8216730
H	-0.1378300	1.1284510	2.4578730
H	0.1218440	2.7729380	3.0119960
H	2.3383590	2.8949850	2.1314830
H	2.1697760	1.3712840	3.0012720
H	2.2770690	1.8237800	0.1391170
H	4.3123870	1.3093410	1.5540610
H	4.0311770	0.4776320	0.0328450
H	4.7102530	-1.0218860	1.9377600
H	3.2384510	-0.5704010	2.7894030
H	3.9860000	-3.3355970	0.2042100

H	4.2068040	-1.7119380	-0.4550230
H	2.8087330	-2.9771040	-2.0084350
H	1.7098050	-3.4446840	-0.7250350
H	1.8816660	-0.7447850	-0.5526160
H	1.4607100	-1.4713440	-3.3721230
H	2.9362790	-0.6889050	-2.7893760
H	1.7663050	1.2970690	-2.1300870
H	1.2314220	0.8800340	-3.7527470
H	-0.8150760	1.8478600	-3.7211460
H	-0.3557310	2.5965080	-2.2027450
H	-2.8123150	2.6288670	-2.7042060
H	-2.8200920	0.8699120	-2.6423790
H	-4.6316940	1.5005440	-0.9224140
H	-3.9272840	1.3579260	0.6909250
H	-4.6193320	-0.7907380	-0.0269080
H	-3.7011250	-0.7164620	-1.5348480
H	-2.4423620	-0.4063460	1.0746230
H	-2.7367690	-2.9864700	-0.2673690
H	-3.6701700	-2.4525590	1.1474560
H	-1.7606080	-2.0906060	2.4775790
H	-1.6986850	-3.7505780	1.9006920
H	0.0719380	-3.2493160	0.5689740
H	0.2824110	-2.8063870	3.0692220
H	0.6147020	-1.1678080	2.5191110
H	2.5796280	-2.7087430	2.9952250
H	2.1331520	-3.6595320	1.5985600
N	-1.3245910	-2.3289550	-2.4224370
H	-2.3411570	-2.3255090	-2.4647990
H	-1.0173790	-1.6031460	-3.0782810
C	-0.8191390	-3.6562860	-2.8019920
H	0.2719660	-3.6384730	-2.8092920
H	-1.1403240	-4.3970550	-2.0650940
H	-1.1644300	-3.9818420	-3.7889120
C	2.9189920	4.9746120	-0.3684260
H	3.1780800	4.8898420	0.6908250
H	2.4308000	5.9487890	-0.5156460
H	3.8565620	4.9778290	-0.9320270
N	2.1084320	3.8240800	-0.7609360
H	1.2425350	3.7715590	-0.2188520
H	1.8522280	3.8805450	-1.7412310
Mg	-0.5630470	-0.9595650	-0.8372890
Na	-4.0074490	-0.2738690	4.1725570
H	-0.2229810	1.9199340	0.2426010

Mg^{2+}(H_5Aza222)$^-$$K^-$ (E = -2139.696114 au.)

N	1.8300890	1.9841080	1.5821660
C	1.7966520	3.2756760	0.8900530
C	1.5640720	3.1102440	-0.6045350
N	0.2088890	2.6183900	-0.8605710
C	0.0920370	1.9736910	-2.1664320
C	-1.3507100	1.6996030	-2.5691060
N	-2.1063240	0.9723990	-1.5447250
C	-3.3122180	0.3375410	-2.0678220
C	-3.0359640	-1.0209180	-2.7193740
N	-2.4546320	-1.9888510	-1.8035440
C	-3.3425610	-2.6228790	-0.8539920
C	-2.6227460	-2.7620700	0.4891810
N	-2.0384040	-1.4691920	0.8854860
C	-2.7536720	-0.8371630	2.0056610
C	-2.2129520	0.5607300	2.2422090
N	-0.7666960	0.5722640	2.2556070
C	-0.3427600	1.8551010	2.7667640
C	1.1640510	2.0019150	2.8799970
C	3.1655190	1.4135510	1.6345540
C	3.1564770	-0.1002460	1.8069770
N	2.2877750	-0.7365120	0.7937520
C	2.7067920	-2.1155400	0.4833970
C	2.0013310	-2.5558310	-0.7781770
N	0.5265020	-2.3905360	-0.7149560
C	0.0165720	-2.3080170	-2.1137880
C	-1.3982780	-2.8319400	-2.3310030
H	2.7257460	3.8418160	1.0639560
H	0.9786250	3.8727810	1.3037470
H	1.6955330	4.0765200	-1.1064850
H	2.3280570	2.4333980	-1.0210150
H	0.6743130	1.0376580	-2.2044360
H	0.5369610	2.6363110	-2.9171370
H	-1.8511550	2.6498750	-2.8167480
H	-1.3290640	1.1072300	-3.4903900
H	-2.3942320	1.6660280	-0.8512820
H	-3.8329460	0.9694470	-2.8080190
H	-4.0140840	0.2067050	-1.2361260
H	-3.9701960	-1.3949010	-3.1739760
H	-2.3306120	-0.8770810	-3.5425340
H	-3.7099630	-3.6068630	-1.1940920
H	-4.2208420	-1.9845430	-0.7171370
H	-3.3199890	-3.1092830	1.2589700
H	-1.8430930	-3.5287040	0.4113070
H	-2.1032910	-0.8616910	0.0577610
H	-2.5948650	-1.4568070	2.8972050
H	-3.8381640	-0.8041090	1.8214080

H	-2.6359120	1.2399600	1.4739070
H	-2.6366500	0.9144190	3.2019240
H	-0.7615340	2.0341940	3.7769560
H	-0.7305180	2.6938850	2.1521680
H	1.4107960	2.9215240	3.4398870
H	1.5390230	1.1660500	3.4784800
H	3.7826120	1.8605050	2.4358410
H	3.6756910	1.6300190	0.6896110
H	4.1881820	-0.4569770	1.6947220
H	2.8173200	-0.3924850	2.8067970
H	2.4432770	-0.2030290	-0.0706110
H	2.4816100	-2.7641470	1.3374480
H	3.7902020	-2.1643290	0.2980480
H	2.3750020	-1.9228300	-1.5933110
H	2.2783460	-3.5848460	-1.0404310
H	0.1470970	-3.2460500	-0.3118180
H	0.6808360	-2.8904490	-2.7655440
H	0.0853570	-1.2663570	-2.4384760
H	-1.5241700	-2.9759770	-3.4143580
H	-1.4814760	-3.8362990	-1.8942860
N	0.4047390	-2.1623470	2.9365090
H	1.3549190	-2.0979050	3.2945250
H	-0.1303540	-1.4483740	3.4407380
C	-0.1252240	-3.5114210	3.1865070
H	-1.1607330	-3.5609670	2.8459250
H	0.4535540	-4.2446430	2.6190040
H	-0.0959370	-3.7947390	4.2437420
C	-3.3375730	4.7702830	-0.7876260
H	-3.2208710	4.6213970	-1.8648880
H	-2.9834350	5.7837730	-0.5505010
H	-4.4084020	4.7266480	-0.5685400
N	-2.6412770	3.7018560	-0.0739890
H	-1.6423350	3.6936590	-0.2928640
H	-2.7333790	3.8189010	0.9298240
Mg	0.1067870	-0.8880780	1.1378890
K	5.5819090	-0.2162560	-2.9029630
H	-0.0102520	1.9325710	-0.1380710

$Ca^{2+}(H_5Aza222)^-Li^-$ (E = -2024.825161 au.)

N	2.9304310	-1.1611130	0.5116470
C	4.1214240	-0.3929270	0.1297330
C	4.0357840	0.1513940	-1.2911150
N	2.8370370	0.9853950	-1.4322350
C	2.0524330	0.6264210	-2.6137080
C	0.8272880	1.5015360	-2.7800730

N	0.0370530	1.6548040	-1.5372780
C	-1.1523750	2.4791840	-1.8123650
C	-2.4088570	1.6673290	-2.0957810
N	-2.9234980	0.9958820	-0.8975320
C	-3.5125390	1.9454470	0.0548910
C	-3.1358700	1.6133550	1.4895530
N	-1.6833020	1.5372380	1.6160620
C	-1.2101490	1.4657830	3.0003980
C	0.3049950	1.3671450	3.0239920
N	0.7965770	0.2839580	2.2115150
C	2.1796220	0.0700550	2.5654770
C	2.7812110	-1.1935060	1.9691560
C	2.9879250	-2.5010580	-0.0671880
C	1.7037860	-3.3092580	0.0228470
N	0.5484320	-2.6696710	-0.6240590
C	-0.5358870	-3.6564060	-0.7505320
C	-1.7060440	-3.1036680	-1.5309100
N	-2.2610370	-1.8820180	-0.9353580
C	-3.2687690	-1.2988390	-1.8220360
C	-3.8911870	-0.0556640	-1.2175760
H	5.0372280	-0.9979640	0.2484910
H	4.2099770	0.4535600	0.8160370
H	4.9384080	0.7365750	-1.5032190
H	4.0195480	-0.6734940	-2.0145430
H	1.7510720	-0.4341280	-2.6027410
H	2.6746610	0.7422650	-3.5070800
H	1.1280750	2.4982560	-3.1368210
H	0.1943540	1.0499150	-3.5519890
H	0.6122470	2.2288470	-0.9064640
H	-0.9687400	3.1385000	-2.6723580
H	-1.3129960	3.1455830	-0.9599600
H	-3.1783720	2.3242720	-2.5387680
H	-2.1682360	0.9115080	-2.8471900
H	-4.6071350	1.9853580	-0.0486300
H	-3.1560530	2.9545160	-0.1686670
H	-3.5730320	2.3684830	2.1627740
H	-3.5565560	0.6444180	1.7844020
H	-1.2704880	2.3728110	1.2010640
H	-1.6496020	0.5749270	3.4612380
H	-1.5502660	2.3343680	3.5874910
H	0.7140120	2.3640190	2.7262260
H	0.6023390	1.2624570	4.0874810
H	2.3004920	-0.0296920	3.6645900
H	2.8238440	0.9393340	2.3051310
H	3.7558210	-1.4039250	2.4470290
H	2.1193250	-2.0209210	2.2343260

H	3.7933440	-3.0974300	0.4024150
H	3.2452060	-2.4108220	-1.1260510
H	1.9125920	-4.2815120	-0.4486310
H	1.4390250	-3.5238830	1.0643470
H	0.8307350	-2.4547260	-1.5942450
H	-0.8440000	-3.9750920	0.2532360
H	-0.1805060	-4.5549270	-1.2777910
H	-1.3563430	-2.8582330	-2.5418820
H	-2.4733620	-3.8857850	-1.6421590
H	-2.7023390	-2.1258350	-0.0486170
H	-4.0757790	-2.0139060	-2.0475060
H	-2.7814430	-1.0808610	-2.7770390
H	-4.6779040	0.3215690	-1.8945110
H	-4.3933010	-0.3377800	-0.2844770
N	-1.1873920	-1.9468370	2.2065050
H	-0.6752460	-2.8111290	2.0513370
H	-0.5161210	-1.3010130	2.6547780
C	-2.3628800	-2.2179390	3.0379280
H	-2.9192940	-1.2920660	3.2036840
H	-3.0330860	-2.9149190	2.5250880
H	-2.1227670	-2.6445450	4.0198850
C	1.9747070	4.9662470	0.0421970
H	1.8372070	5.2917940	-0.9925220
H	2.9466270	5.3441230	0.3878160
H	1.1947330	5.4438440	0.6420010
N	1.8347290	3.5120580	0.1155370
H	2.5416350	3.0375040	-0.4482340
H	1.9527230	3.1833430	1.0699460
Ca	-0.4533260	-0.3230080	0.2407840
Li	0.9193490	-2.9137510	-4.7955200
H	2.2652840	0.7581750	-0.6207940

$Ca^{2+}(H_5Aza222)^-Na^-$ (E = -2179.616474 au.)

N	-2.9293900	0.0983790	1.1964700
C	-4.0168660	-0.6785820	0.5897360
C	-4.0365660	-0.5725710	-0.9304130
N	-2.7476950	-1.0086110	-1.4795650
C	-2.1866960	-0.0318510	-2.4126270
C	-0.8716660	-0.4905580	-3.0070390
N	0.0918080	-0.9825740	-1.9962290
C	1.3533770	-1.3538130	-2.6603130
C	2.4082710	-0.2564130	-2.6271410
N	2.9567150	-0.0472740	-1.2825200
C	3.8158590	-1.1612220	-0.8612030
C	3.5807720	-1.5367270	0.5927140

N	2.1650440	-1.8216330	0.8089650
C	1.8724440	-2.4208740	2.1131710
C	0.3775140	-2.6473880	2.2555410
N	-0.3843340	-1.4500580	2.0068110
C	-1.7230070	-1.6788060	2.4959320
C	-2.5928110	-0.4308730	2.5210280
C	-3.2878000	1.5137210	1.2432530
C	-2.1594580	2.4639640	1.6091250
N	-1.0023140	2.3928920	0.7049060
C	-0.1173860	3.5392680	0.9656200
C	1.0155410	3.6087660	-0.0320320
N	1.8318920	2.3889770	-0.0508870
C	2.7963140	2.4418330	-1.1506330
C	3.6882960	1.2164370	-1.1680450
H	-4.9959070	-0.3775580	1.0019710
H	-3.8707770	-1.7284040	0.8580360
H	-4.8505900	-1.1957390	-1.3192320
H	-4.2572550	0.4572960	-1.2372380
H	-2.0557710	0.9575970	-1.9439830
H	-2.8919510	0.1273080	-3.2346510
H	-1.0561320	-1.2870460	-3.7435310
H	-0.4286990	0.3584670	-3.5396990
H	-0.2921220	-1.8713500	-1.6482910
H	1.1682460	-1.6196190	-3.7105650
H	1.7341240	-2.2648470	-2.1891900
H	3.2119440	-0.4977180	-3.3452420
H	1.9482170	0.6737820	-2.9693270
H	4.8785020	-0.9271840	-1.0234010
H	3.6069850	-2.0372200	-1.4810570
H	4.2225650	-2.3936340	0.8540840
H	3.8684940	-0.7113910	1.2551520
H	1.8475460	-2.4800860	0.0974210
H	2.2198230	-1.7284220	2.8870200
H	2.4220460	-3.3656100	2.2549010
H	0.0970700	-3.4968880	1.5855750
H	0.2105160	-3.0458880	3.2771330
H	-1.7085940	-2.0547800	3.5404110
H	-2.2494680	-2.4808120	1.9323380
H	-3.5152260	-0.6309890	3.0969400
H	-2.0410350	0.3335730	3.0724430
H	-4.1156770	1.6860090	1.9572680
H	-3.6607630	1.8098670	0.2588420
H	-2.5879170	3.4777020	1.5991180
H	-1.8062830	2.2906580	2.6316850
H	-1.3609190	2.5381700	-0.2511110
H	0.2636240	3.4650270	1.9918910

H	-0.6777220	4.4843820	0.8997980
H	0.5849660	3.7416410	-1.0325560
H	1.6259040	4.5027450	0.1700670
H	2.3393180	2.3260430	0.8318180
H	3.4378500	3.3350010	-1.0874740
H	2.2305850	2.5400730	-2.0820100
H	4.4306970	1.3201120	-1.9788490
H	4.2552830	1.1861800	-0.2299310
N	1.1892270	0.9333330	2.8631180
H	0.5267200	1.6599720	3.1208700
H	0.6947990	0.0381450	3.0166570
C	2.3995130	1.0651350	3.6784010
H	3.1177690	0.2894370	3.4014870
H	2.8753140	2.0328730	3.4913210
H	2.2182280	0.9834030	4.7574390
C	-1.0336660	-4.9781460	-1.8903340
H	-0.9684300	-4.8219880	-2.9705220
H	-1.8753230	-5.6573780	-1.6980330
H	-0.1153350	-5.4823590	-1.5763530
N	-1.1417470	-3.6828200	-1.2190360
H	-1.9866420	-3.1837250	-1.5008120
H	-1.1942060	-3.7996270	-0.2107940
Ca	0.4821960	0.1466850	0.4264480
Na	-1.8996150	4.2930380	-3.1363640
H	-2.1188600	-1.0444260	-0.6794680

$Ca^{2+}(H_5Aza222)^-K^-$ (E = -2617.276613 au.)

N	1.2098830	2.5586000	1.3924800
C	1.4934850	3.7619280	0.6007680
C	2.0874960	3.4309100	-0.7629870
N	1.1681060	2.5596120	-1.5017500
C	1.8467980	1.4145520	-2.1047480
C	0.8978080	0.5390480	-2.8985360
N	-0.3511110	0.2136000	-2.1733470
C	-1.1794600	-0.6833170	-2.9980630
C	-0.9974060	-2.1584180	-2.6683700
N	-1.5760060	-2.5168440	-1.3684350
C	-3.0442400	-2.5151800	-1.4024600
C	-3.6381890	-1.8936180	-0.1488550
N	-3.0938750	-0.5522020	0.0428970
C	-3.7721410	0.2253880	1.0827890
C	-3.1222250	1.5920670	1.2096100
N	-1.6994620	1.5061600	1.4242990
C	-1.2468440	2.8082800	1.8548160
C	0.1749340	2.8245290	2.3955450

C	2.4376920	2.0486050	1.9968360
C	2.3417460	0.6456630	2.5727740
N	1.9421380	-0.3716460	1.5881060
C	2.2196520	-1.7098690	2.1340160
C	1.9354280	-2.7968170	1.1242250
N	0.5407280	-2.7898090	0.6659500
C	0.3497060	-3.7762680	-0.3986050
C	-1.0888770	-3.8074890	-0.8762210
H	2.1610150	4.4492360	1.1486820
H	0.5504490	4.2931210	0.4450360
H	2.2604500	4.3622450	-1.3148400
H	3.0675480	2.9507540	-0.6442510
H	2.3748410	0.8064990	-1.3505910
H	2.6256700	1.7739130	-2.7851190
H	0.6420790	1.0370280	-3.8455960
H	1.4209640	-0.3913480	-3.1461970
H	-0.8865480	1.0913600	-2.1241390
H	-0.9543220	-0.5386860	-4.0640800
H	-2.2266660	-0.3911180	-2.8757440
H	-1.4342990	-2.7725920	-3.4753420
H	0.0728840	-2.3774280	-2.6505190
H	-3.4397690	-3.5319050	-1.5441540
H	-3.3873620	-1.9396900	-2.2666550
H	-4.7369500	-1.8887550	-0.2320960
H	-3.3899360	-2.4940650	0.7346010
H	-3.1865130	-0.0311330	-0.8292710
H	-3.6799560	-0.3210650	2.0271620
H	-4.8488590	0.3272640	0.8715710
H	-3.3992300	2.1820520	0.3013790
H	-3.6398010	2.1175830	2.0376990
H	-1.8818500	3.1992340	2.6767110
H	-1.3413540	3.5784880	1.0568170
H	0.3712380	3.7902100	2.8965630
H	0.2332320	2.0550560	3.1687280
H	2.7904650	2.7210550	2.8014920
H	3.2235390	2.0395160	1.2361210
H	3.3324880	0.4059000	2.9874610
H	1.6386490	0.6064420	3.4121010
H	2.5707340	-0.2670450	0.7805880
H	1.6172920	-1.8510780	3.0399750
H	3.2749100	-1.7969240	2.4344290
H	2.5797080	-2.6410440	0.2498640
H	2.2196840	-3.7719310	1.5493050
H	-0.0572800	-3.0375660	1.4543970
H	0.6283740	-4.7895710	-0.0695870
H	1.0367240	-3.5240010	-1.2119070

H	-1.1984510	-4.5929090	-1.6444330
H	-1.7278970	-4.1032400	-0.0356500
N	-1.0948560	-0.9990450	2.9579160
H	-0.2396660	-0.8311370	3.4812430
H	-1.5333010	-0.0712090	2.8397170
C	-1.9406270	-1.9406900	3.6969210
H	-2.8629420	-2.1245470	3.1404800
H	-1.4269290	-2.9008890	3.8054340
H	-2.2181090	-1.5931390	4.6997500
C	-2.7359750	3.4748210	-3.2239660
H	-2.3616670	3.2275250	-4.2209960
H	-2.8153900	4.5682340	-3.1548430
H	-3.7435450	3.0579180	-3.1397190
N	-1.8651030	2.8713830	-2.2152050
H	-0.9120310	3.2311510	-2.2772350
H	-2.1948760	3.0821790	-1.2771060
Ca	-0.5254600	-0.3604520	0.4537200
K	5.8227080	-1.4538970	-1.3778630
H	0.5346510	2.1897260	-0.7955350

Table S1. Main geometrical parameters of the $Be^{2+}(H_5Aza222)^{-}Li'^{-}$ complex from the B3LYP and CAM-B3LYP computational methods.

Method	M-M'/Å	M-N1/Å	M-N2/Å	M-N3/Å
B3LYP	6.497	3.325	4.563	1.618
CAM-B3LYP	6.465	3.283	4.525	1.611

Table S2. The polarizabilities components (au.) of the $M^{2+}(H_5Aza222)^{-}M'^{-}$ complexes at the CAM-B3LYP level.

Species (M;M')	α_{xx}	α_{yy}	α_{zz}
Be; Li	680.05	669.53	729.73
Be; Na	715.30	722.00	774.12
Be; K	1085.29	982.46	1228.95
Mg; Li	638.30	622.47	626.73

Mg; Na	700.01	660.80	671.24
Mg; K	1020.27	957.38	934.21
Ca; Li	639.64	637.95	667.68
Ca; Na	683.71	698.20	662.56
Ca; K	1031.72	908.08	885.96

Table S3. The hyperpolarizabilities components (au.) of the $M^{2+}(H_5Aza222)^{-}M'^{-}$ complexes at the CAM-B3LYP level.

Species(M;M')	β_{xxx}	β_{xxy}	β_{xyy}	β_{yyy}	β_{xxz}	β_{xyz}	β_{yyz}	β_{xzz}	β_{yzz}	β_{zzz}
Be; Li	-2301	-6363	-1670	-18589	2577	-2081	-6611	-3884	-32199	-28038
Be; Na	3492	-7091	757	-21070	1382	-373	-4836	6342	-4424	81958
Be; K	-18235	2737	-5893	-4285	74287	3311	7177	135064	-4147	230047
Mg; Li	834	-5984	1783	-15126	6710	778	5388	-127	-3179	22507
Mg; Na	-12794	-4851	-2454	-21007	6265	124	1088	-4896	-5805	21123
Mg; K	23298	-35273	-31736	-69751	-7181	18101	23008	2788	-32953	12406
Ca; Li	-4245	-3749	-3170	-12504	-6828	-728	-7000	-182	-2102	-22404
Ca; Na	1149	6362	1794	22521	-5165	888	-3980	-1634	7073	-18895
Ca; K	35771	-21692	3175	-31252	-11686	1536	2184	10636	-12186	-7981