

Supplementary Material

Planar Pentacoordinate Carbons in CBe_5^{4-} Derivatives

Rafael Grande-Aztatzi,¹ José Luis Cabellos,¹ Rafael Islas,² Ivan Infante,³

José M. Mercero,⁴ Albeiro Restrepo,⁵ and Gabriel Merino.^{1,}*

¹ *Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados,
Unidad Mérida, Km. 6 Antigua Carretera a Progreso, A.P. 73, Cordemex, Mérida
97310, Yucatán, México.*

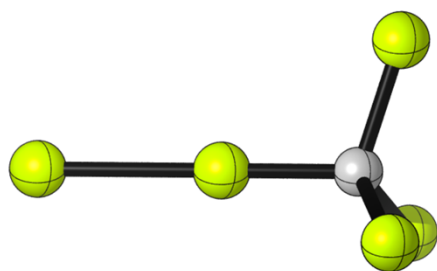
² *Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad
Andres Bello, Avenida República 275, Santiago, Chile.*

³ *Department of Theoretical Chemistry, Faculty of Sciences, Vrije Universiteit
Amsterdam De Boelelaan 1083 1081 HV Amsterdam*

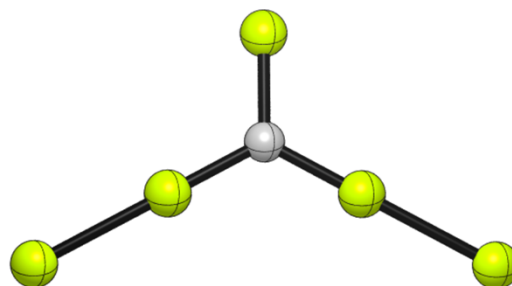
⁴ *IZO-SGI Sgiker, Euskal Herriko Unibertsitatea (UPV/EHU), Spain.*

⁵ *Instituto de Química, Universidad de Antioquia UdeA, Calle 70 No 52-21, Medellín,
Colombia.*

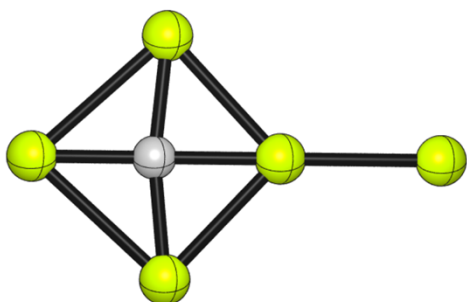
e-mail: gmerino@mda.cinvestav.mx



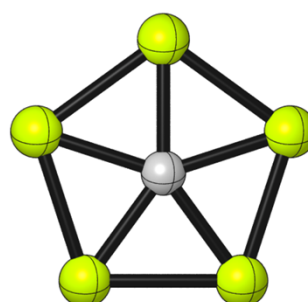
1-A, C_{3v}
0.0



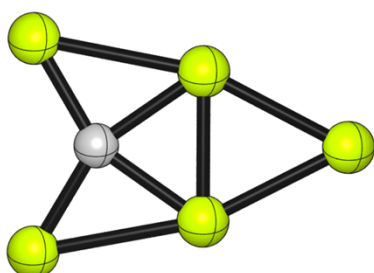
1-B, C_{2v}
6.7



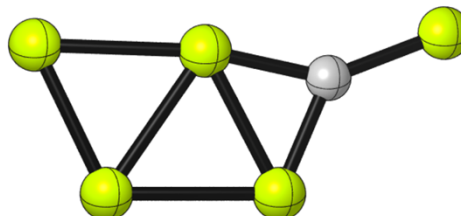
1-C, C_{2v}
9.0



1-D, D_{5h}
9.7



1-E, C_{2v}
15.2



1-F, C_s
22.6

Figure 1-SI. The lowest lying structure of the CBe_5^{4+} tetraanion (**1**). Relative energies are in $\text{kcal}\cdot\text{mol}^{-1}$.

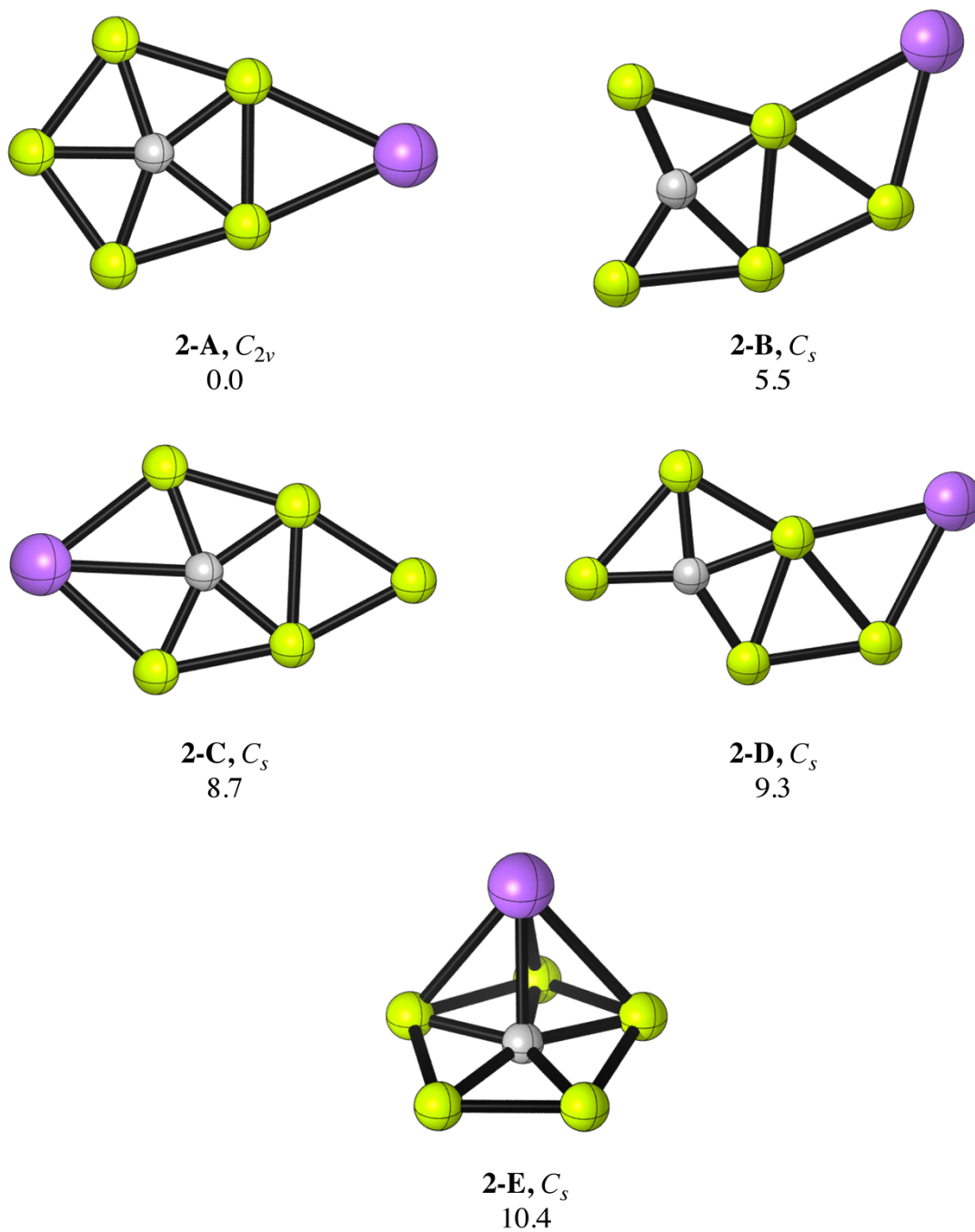
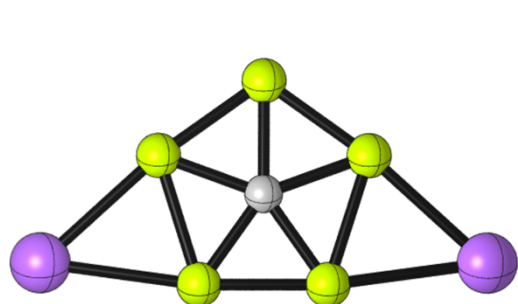
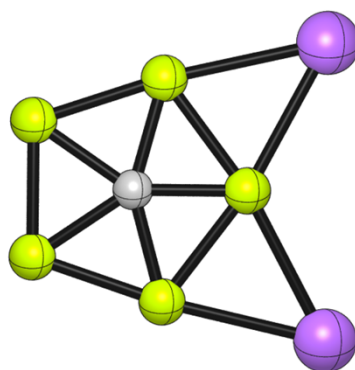


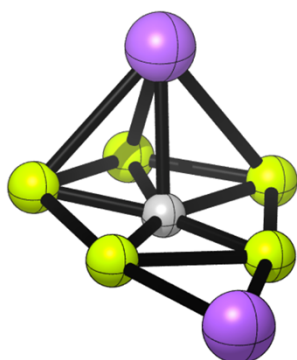
Figure 2-SI. The lowest lying structure of $\text{CBe}_5\text{Li}^{3-}$ (2). Relative energies are in $\text{kcal}\cdot\text{mol}^{-1}$.



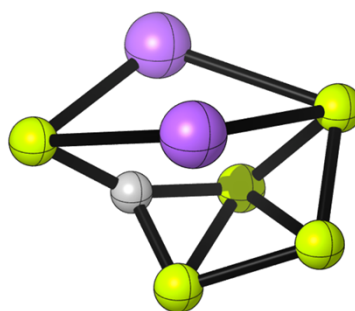
3-A, C_{2v}
0.0



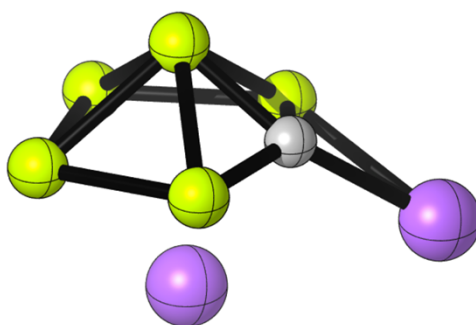
3-B, C_{2v}
0.6



3-C, C_s
3.0



3-D, C_s
10.5



3-E, C_1
14.2

Figure 3-SI. The lowest lying structure of $\text{CBe}_5\text{Li}_2^{2-}$ (**3**). Relative energies are in $\text{kcal}\cdot\text{mol}^{-1}$.

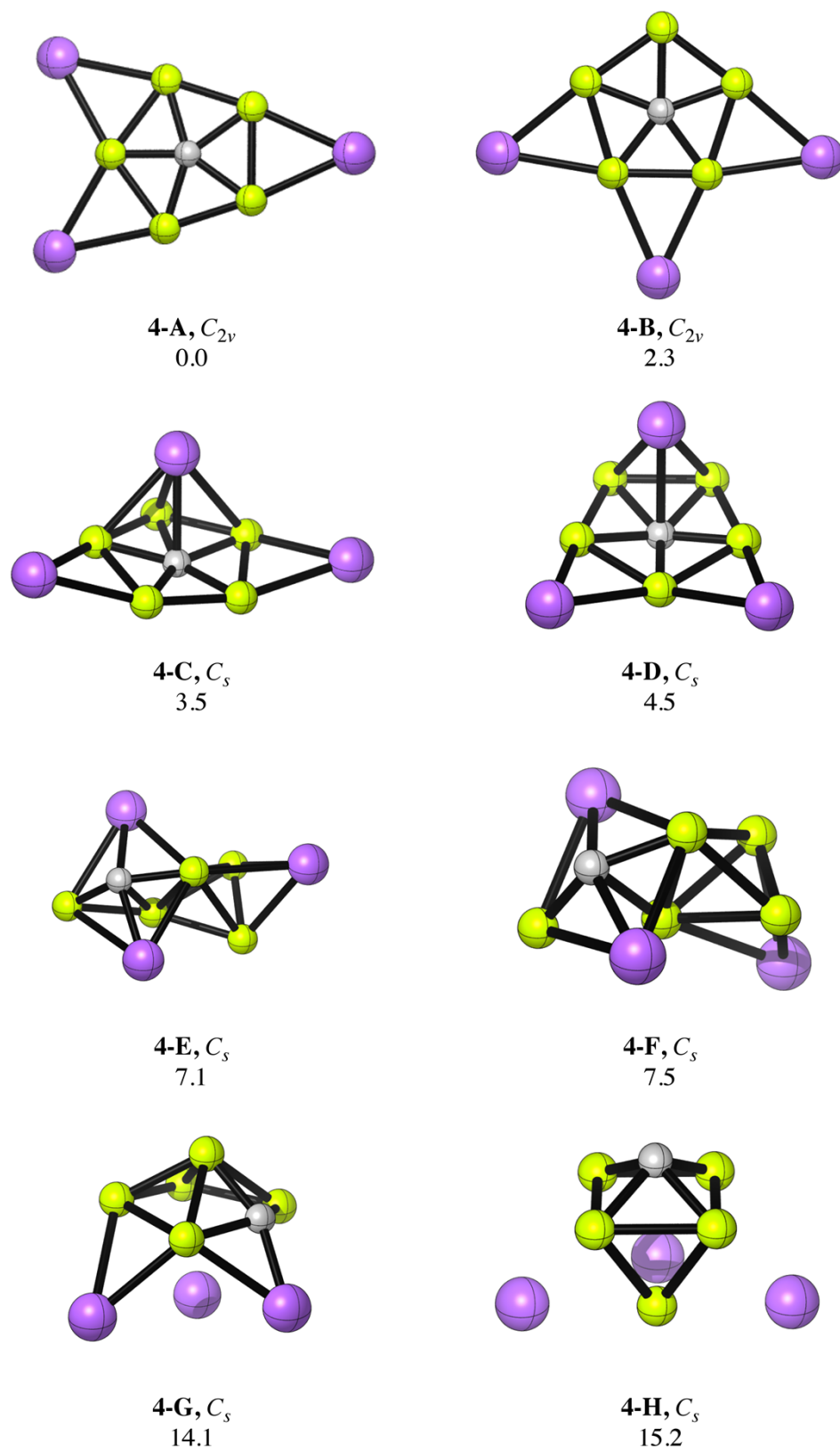
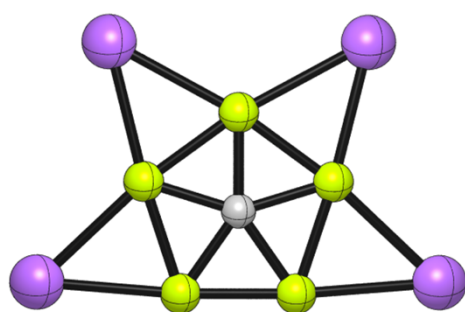
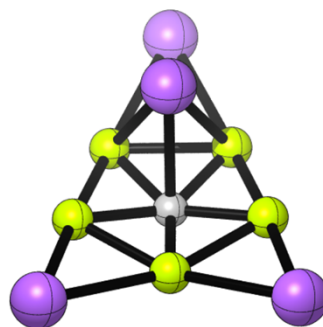


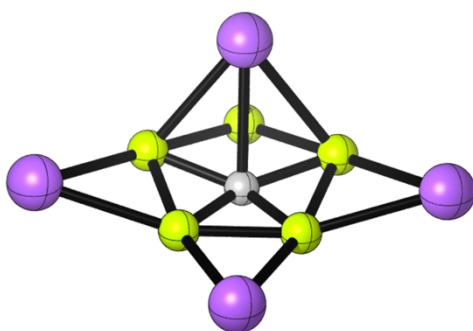
Figure 4-SI. The lowest lying structure of $\text{CBe}_5\text{Li}_3(4)$. Relative energies are in $\text{kcal}\cdot\text{mol}^{-1}$.



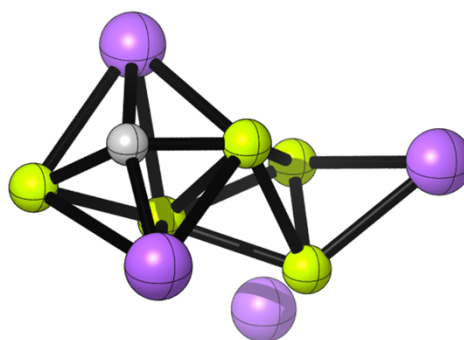
5-A, C_{2v}
0.0



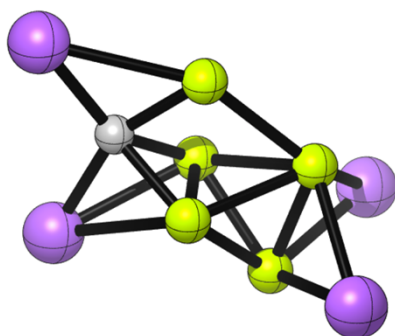
5-B, C_s
6.6



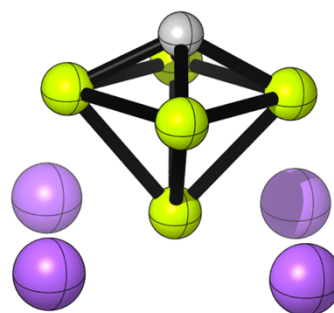
5-C, C_s
6.7



5-D, C_s
10.2

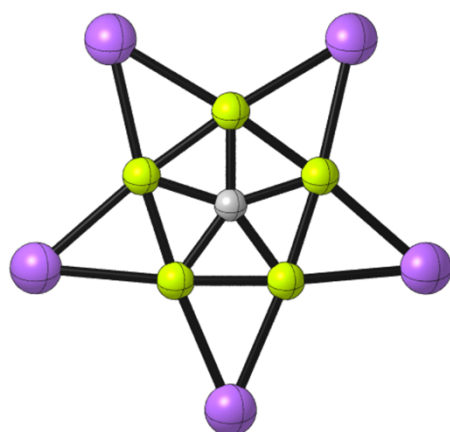


5-E, C_s
12.7

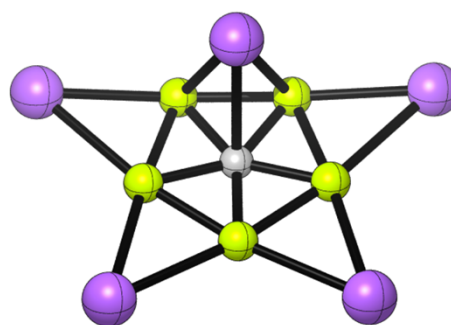


5-F, C_{4v}
15.3

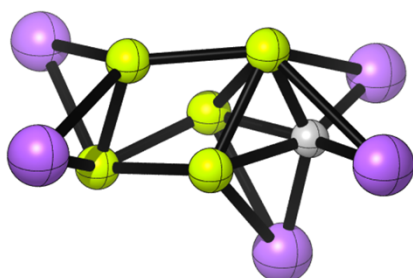
Figure 5-SI. The lowest lying structure of CBe_5Li_4 (**5**). Relative energies are in $\text{kcal}\cdot\text{mol}^{-1}$.



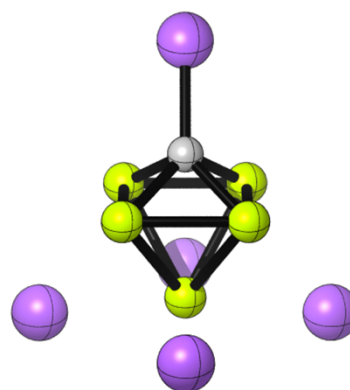
6-A, D_{5h}
0.0



6-B, C_s
11.4



6-C, C_s
22.2



6-D, C_{4v}
26.3

Figure 6-SI. The lowest lying structure of $\text{CBe}_5\text{Li}_5^+$ (**6**). Relative energies are in $\text{kcal}\cdot\text{mol}^{-1}$.

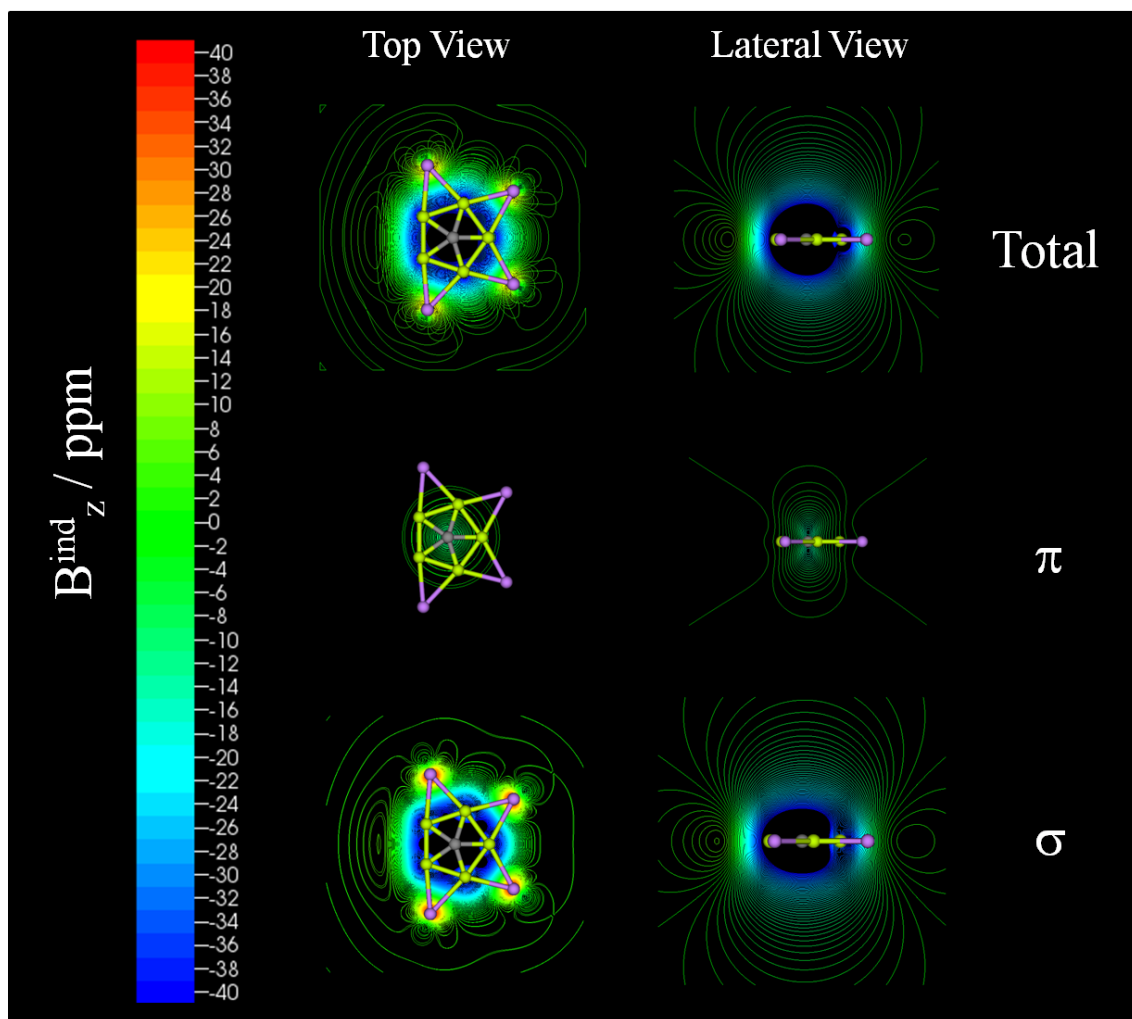


Figure 7-SI. Contour lines of B_z^{ind} of **5** in the molecular plane and perpendicular to the molecular plane through the origin. The scale is given in ppm (or μT for an external field of 1 T).

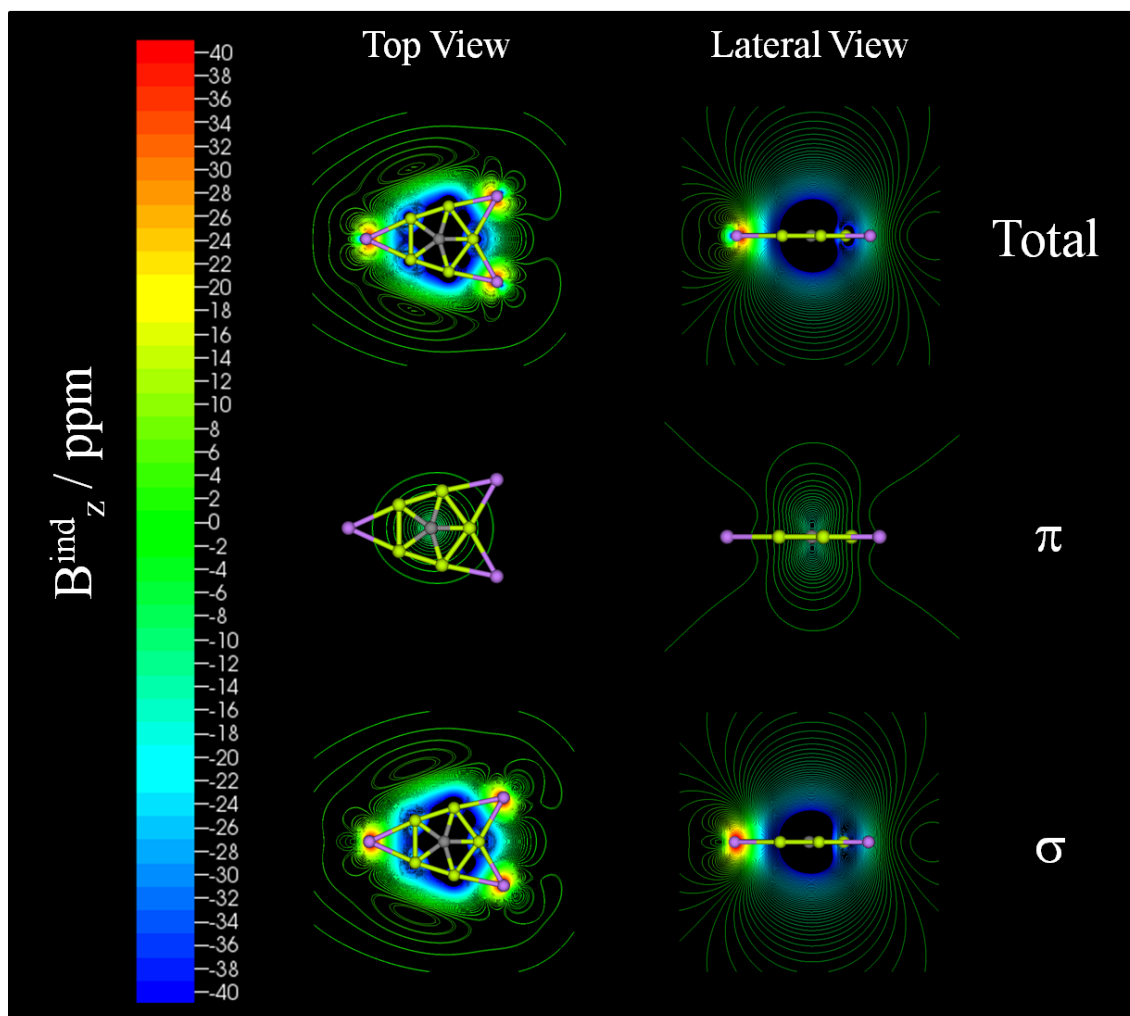


Figure 8-SI. Contour lines of B_z^{ind} of **4** in the molecular plane and perpendicular to the molecular plane through the origin. The scale is given in ppm (or μT for an external field of 1 T).

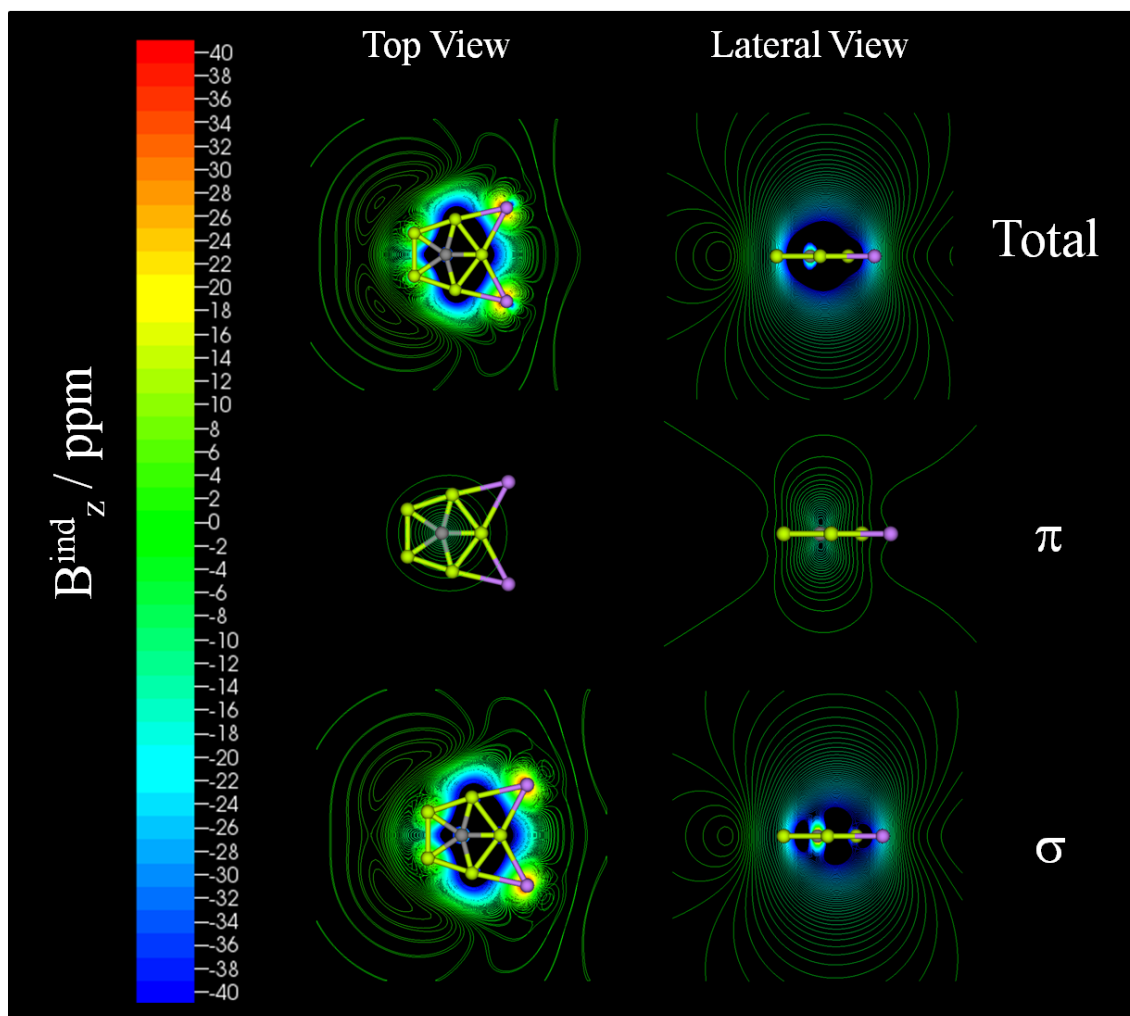


Figure 8-SI. Contour lines of B_z^{ind} of **3** in the molecular plane and perpendicular to the molecular plane through the origin. The scale is given in ppm (or μT for an external field of 1 T).

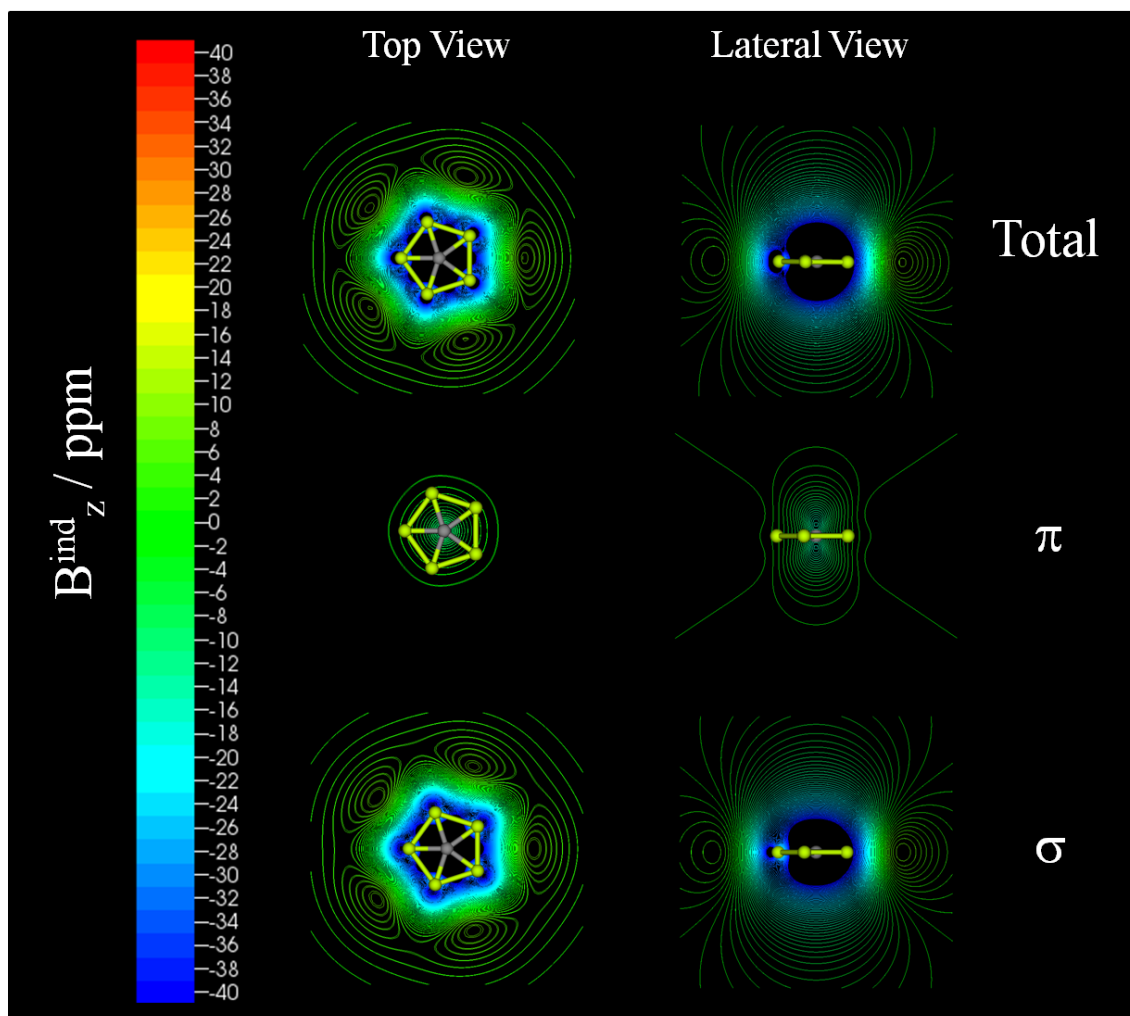


Figure 9-SI. Contour lines of B_z^{ind} of **1** in the molecular plane and perpendicular to the molecular plane through the origin. The scale is given in ppm (or μT for an external field of 1 T).

Cartesian coordinates (See Figures 1-6-SI)

CBe₅⁴⁻

1-A

C	0.3143640	-0.3839240	-0.3821060
Be	0.2447630	0.7108070	0.8595670
Be	1.9061120	-0.4883180	-0.8754190
Be	-0.2339080	-1.8503100	0.1987280
Be	-0.6629240	0.1793230	-1.6132390
Be	0.1503360	2.1876410	2.5366780

1-B

C	-0.1729070	0.1837330	-0.2564170
Be	3.2885210	-0.9220770	0.9433240
Be	1.2820580	-0.2936600	0.2552720
Be	-0.6107180	-0.1503970	-1.7921060
Be	-2.6775650	2.0230930	1.9919510
Be	-1.2237130	0.9586400	0.6951420

1-C

C	-0.0467080	-0.0049140	0.8360790
Be	0.3106220	0.6032450	-0.7268590
Be	-0.4934430	-0.6924770	2.2836090
Be	0.7754020	1.3881430	-2.7132040
Be	-1.0881140	-1.0057160	-0.0169180
Be	1.0553530	1.1051960	1.4098980

1-D

C	-0.1096740	0.0769330	0.1767130
Be	-1.7011630	0.4626530	-0.4799650
Be	-0.8120150	1.3580540	1.1662180
Be	1.3074310	-0.9541750	-0.0278850
Be	-0.3906990	-0.9652430	-1.2190120
Be	1.0470210	0.4818690	1.4459480

1-E

C	-0.6463670	0.0831620	0.3685350
Be	-1.5457950	1.4111370	0.7122490
Be	0.5968750	1.2058930	-0.0598640
Be	-1.3022460	-1.4054690	0.5796570
Be	2.4811630	0.4063710	-0.7487690
Be	0.7671700	-0.7657250	-0.1525990

1-F

C	1.1988300	0.3746500	-0.3679990
Be	-1.4840500	-1.4456510	0.0804330
Be	-2.2312960	0.1090910	1.3673910
Be	2.5974450	1.1485560	-0.6997540

Be	0.5450260	-1.0675550	-0.8212980
Be	-0.2345210	0.4149790	0.4424420

CBe₅Li³⁻

2-A

C	0.3599540	-0.2088390	0.1123630
Be	0.1986340	0.8283190	-1.2678960
Be	-0.8517070	-0.9581130	-0.8762090
Be	1.2498850	-0.3954570	1.6477150
Be	1.4645210	1.1251770	0.2981730
Be	-0.1746520	-1.6624710	0.9094320
Li	-1.4761350	0.1761630	-3.0555910

2-B

C	1.2322310	0.5144290	-0.4358160
Be	-0.0485020	-0.4276660	-1.0731010
Be	-0.1455140	1.1398970	0.3343060
Be	1.9639460	1.6739940	0.4806150
Be	2.0518710	-0.4911150	-1.4565270
Be	-1.9191890	0.1649790	-0.2557410
Li	-2.4326850	1.9706020	1.4280120

2-C

C	-0.1062880	0.1555510	-0.0222180
Be	-0.8042090	1.5059830	-0.7253120
Be	0.6348710	-1.4030140	-0.1758370
Be	0.7993290	-2.0189580	-2.1584610
Be	-0.0614090	-0.1731560	-1.7228890
Be	0.2216910	-0.3061040	1.5540210
Li	-0.8069080	1.8377820	1.6304470

2-D

C	-0.0886540	0.1266500	-1.2751100
Be	1.0343370	1.0702420	-0.5066910
Be	-1.3504340	-0.9424150	-1.2653720
Be	-0.1841680	0.0618330	-2.9106290
Be	-0.4126090	-0.1642710	0.3924510
Be	0.9627220	0.9890680	1.5919740
Li	-0.6427430	-0.3844790	2.9694740

2-E

C	1.3907390	0.0881360	0.9591710
Be	-0.0346160	0.1785840	-0.0480670
Be	0.0181080	-0.1047960	2.0268220
Be	1.9643000	0.1402850	2.6390050
Be	3.1604420	0.2345740	0.9549560
Be	1.9529230	0.0477220	-0.6971170
Li	0.5909550	-1.8835430	0.2810170

CBe₅Li₂²⁻**3-A**

C	1.3641460	0.0000000	0.9135120
Be	-0.0299200	0.0000000	-0.1264220
Be	-0.0006030	0.0000000	1.9742610
Be	1.9167820	0.0000000	2.5510130
Be	3.1021960	0.0000000	0.8181880
Be	1.8719980	0.0000000	-0.7684360
Li	-2.2637070	0.0000000	0.9395010
Li	4.3767870	0.0000000	2.9393450

3-B

C	-0.7456600	0.2289550	-0.4241580
Be	-1.4248600	-0.0679340	-2.0500850
Be	0.0700620	1.4609560	0.4412820
Be	-1.4259060	-1.3418210	-0.4700820
Be	-0.5129280	1.6406510	-1.4944570
Be	-0.4894780	-0.4103060	1.1212230
Li	0.6837510	1.0131460	2.7965410
Li	-1.3076620	-2.7181690	1.5832750

3-C

C	0.4015950	-0.1330770	-0.1768300
Be	-1.3403490	-0.2004740	-0.3582000
Be	-0.0949880	0.8677360	-1.5819690
Be	1.7538050	0.8494690	-0.7038250
Be	-0.2343240	-1.2098060	1.0076280
Be	1.7761540	-0.5275130	0.7830470
Li	1.3688320	-2.0240600	2.7298860
Li	-0.2430850	1.9324980	0.3325040

3-D

C	-0.2078700	1.2697830	0.3293170
Be	-1.6307190	0.4225480	0.1489580
Be	1.0925790	2.0568090	-0.2723760
Be	-0.9206290	-1.5347830	0.9214450
Be	-0.1237520	0.2690860	1.6427150
Be	-1.5720550	-1.2263180	-1.0272470
Li	-0.6341330	1.3057030	-1.7830860
Li	0.9095280	-0.5944560	-0.4533040

3-E

C	0.6308780	-0.0516630	-0.9377200
Be	-0.7515760	0.0175510	1.6248710
Be	1.1073630	1.5017660	-0.6963400
Be	-0.7762550	0.6169770	-0.2941670
Be	-0.0476440	-1.3081300	-0.0366370

Be	0.1755150	1.8223400	1.1944330
Li	1.7492870	-0.0545210	1.0933230
Li	1.8482320	-1.5508330	-1.5321480

CBe₅Li₃⁻

4-A

C	1.3849410	0.0000000	0.9401590
Be	0.0105310	0.0000000	-0.0841650
Be	0.0244330	0.0000000	1.9582230
Be	1.9793330	0.0000000	2.5479270
Be	3.1313540	0.0000000	0.9168440
Be	1.9010700	0.0000000	-0.7281260
Li	-2.2295780	0.0000000	0.9659090
Li	0.3397750	0.0000000	4.4007320
Li	4.3103160	0.0000000	-1.2496040

4-B

C	0.2358620	-0.1451980	0.9324660
Be	-0.2684280	-1.5735630	1.7678260
Be	-0.9676760	-0.8563600	-0.0188730
Be	1.1513100	-0.3344870	2.4561970
Be	1.3582980	1.1562220	1.1295890
Be	0.0520650	0.8540340	-0.4189520
Li	1.4940340	2.8988610	-0.5685450
Li	-1.6114920	0.2403400	-2.1341110
Li	-2.0098250	-2.9814170	0.8079690

4-C

C	0.3967800	-0.2711820	0.3053510
Be	-0.1760300	1.0068710	1.3326760
Be	1.4399730	1.1148030	0.1151560
Be	-0.9734580	-0.8954430	1.1595160
Be	-0.0301280	-1.8135190	-0.3552020
Be	1.3559550	-0.4839710	-1.1267500
Li	-0.3559220	1.3389660	-1.1409150
Li	0.8537390	-2.4250070	-2.5681570
Li	-2.3129820	0.6558530	2.5198530

4-D

C	-1.0624880	0.4717750	-0.1201860
Be	-2.3544430	0.9594790	1.0192130
Be	0.1523940	1.2278040	-1.0579800
Be	-1.4146570	-0.8276130	0.9335640
Be	-1.3520140	2.2415310	-0.1761900
Be	0.0229100	-0.7617320	-0.5395420
Li	-0.2754920	1.5250740	1.7493180
Li	0.1048140	-2.7715220	0.8887020
Li	2.1072760	-0.1248760	-1.7059370

4-E

C	0.0751710	-0.6887860	-1.1720670
Be	-1.8306440	0.3682880	1.2931950
Be	-0.7554610	0.8448140	-0.5563770
Be	-0.1040740	1.2183940	1.5033340
Be	-0.1187320	-0.7152210	0.5301070
Be	-0.1897370	0.1629330	-2.4534190
Li	1.6476460	0.4205570	-0.6363410
Li	-0.5381890	-0.5013850	3.1068060
Li	-1.8259710	-1.2911190	-1.0582310

4-F

C	-0.4541110	0.6286420	-1.5704240
Be	1.0053420	2.2267460	0.8846330
Be	0.1272600	0.3503960	0.1962580
Be	-0.1428190	-0.9015570	-1.5088020
Be	-0.8266160	1.8761120	1.4323070
Be	-0.4559330	2.0609440	-0.6594820
Li	0.8141700	0.6564790	2.6898210
Li	-2.1702470	0.3531290	-0.5705500
Li	1.5025530	1.0560710	-1.6684200

4-G

C	-0.8002320	-0.1578680	-1.4717640
Be	0.7535150	-0.6338270	-1.8665780
Be	-0.3300340	-1.1827800	-0.2134840
Be	-0.2389750	1.2696220	-2.0378350
Be	1.7646640	-0.5520760	-0.1274220
Be	1.7252440	1.1689480	-1.3004070
Li	0.0002910	1.2528780	0.3392380
Li	0.3778700	-0.9786370	2.0587590
Li	-2.4096890	-0.0898780	-0.3360430

4-H

C	-0.6334110	-0.3729390	-1.6184760
Be	0.9158820	-0.3758400	-1.0064980
Be	-0.6066500	-1.4578720	0.7761840
Be	-0.3801320	-1.9658610	-1.2772740
Be	-0.6276050	0.8139430	-0.4496530
Be	-1.9556930	-0.7511830	-0.7093820
Li	0.9899890	0.3002390	1.4435220
Li	-2.0870950	0.2039200	1.6518170
Li	1.4821120	-2.5480540	0.3650110

CBe₅Li₄**5-A**

C	0.3610400	-0.1460480	-0.2451920
Be	-0.8894020	-1.2816120	-0.0140740
Be	-0.0864060	-0.0717000	1.3813370
Be	0.0537850	-0.9140100	-1.7629810
Be	1.3462920	1.0318840	0.4952070
Be	1.4178910	0.4975070	-1.4522870
Li	1.1237410	1.5612110	2.8919480
Li	-1.6868420	-2.6559790	-1.9596080
Li	3.0591690	2.2526130	-0.8773400
Li	-1.9338270	-1.6011140	2.1950010

5-B

C	-0.1863980	-0.2152610	-0.0335280
Be	0.6829210	-0.0119410	-1.5255130
Be	-1.5670390	0.3447860	0.8232120
Be	0.0639210	-0.5416690	1.6369150
Be	1.4036520	-0.8783070	0.2012250
Be	-1.0715780	0.8214780	-1.0832590
Li	1.2743890	1.4734620	0.2060930
Li	3.1321700	-0.4941190	-1.5592580
Li	-3.0979480	1.9981380	-0.2604480
Li	-1.6049120	0.2026290	3.3191430

5-C

C	0.6139010	0.0428600	0.3370880
Be	-0.2536050	0.1531080	-1.1216150
Be	0.9973830	1.5690760	-0.3743200
Be	0.5669010	-0.5890530	1.9437050
Be	-0.5280040	-1.2175360	0.3517410
Be	1.7801040	0.8883920	1.3409560
Li	-2.1094540	-1.4579780	-1.5680550
Li	-1.0913040	-2.3025110	2.5590520
Li	-0.1318410	1.8508850	1.8825430
Li	-0.1677690	2.3218020	-2.4088570

5-D

C	1.6532070	-0.0540290	-0.7175800
Be	-1.4581450	-0.1462390	0.2071340
Be	0.3374200	-1.0662830	-0.4683540
Be	-0.4527950	-1.1339600	1.5056200
Be	0.5530360	0.5934670	0.6261310
Be	2.2967720	1.2759530	-0.2057250
Li	-1.4837250	0.8461690	2.3955240
Li	2.3984590	-1.0957910	0.8226680
Li	-1.9922930	-2.4834190	0.2572460
Li	0.3295360	0.9345270	-1.8503820

5-E

C	-1.5553290	1.1037650	1.0165590
Be	-1.6410940	-0.3427070	0.0061260

Be	-0.0788080	0.8186850	0.0897810
Be	-0.7383420	-0.0568880	1.8730210
Be	0.2495810	-1.2785490	0.3819440
Be	-0.1545120	-0.6071250	-1.3958700
Li	2.1678790	-0.6354430	-0.9302870
Li	-0.8244500	-2.8585770	-1.0890900
Li	-2.1225750	1.9856100	-0.6402970
Li	-2.2176980	1.8852830	2.6058090

5-F

C	-0.3547300	-1.7429510	-0.4267700
Be	0.0112320	0.4613720	0.5128410
Be	-1.5923590	-1.0454200	0.4081040
Be	-0.7275770	-0.4360530	-1.3589440
Be	0.2512490	-1.6469920	1.1026440
Be	1.1154440	-1.0380550	-0.6648670
Li	-2.0359950	1.4671230	-0.1441270
Li	2.1649410	0.0949680	1.4414380
Li	-0.9239710	0.0885710	2.6618830
Li	1.0507410	1.4753990	-1.3645550

CBe₅Li₅⁺

6-A

C	0.5536280	0.0756650	-0.0644060
Be	1.8459360	-1.0259460	-0.1164750
Be	0.1208540	1.6687050	0.3360890
Be	1.9437410	0.8698730	0.5043940
Be	-0.0375310	-1.3994710	-0.6653510
Be	-1.1040590	0.2656730	-0.3853670
Li	1.8437150	3.3032850	1.2448460
Li	-2.4843810	-1.6613390	-1.3099980
Li	4.1777870	-0.3421580	0.6339880
Li	-2.2682190	2.4884640	0.0431280
Li	1.5026390	-3.4054790	-0.9464100

6-B

C	-0.7382820	-0.3365090	-0.3060360
Be	0.6400010	0.5038370	0.2429690
Be	0.3757360	-0.2688670	-1.6007600
Be	-2.2614680	-0.9899960	0.1652450
Be	-1.4558760	-1.1155900	-1.6653040
Be	-0.9322230	-0.0647010	1.3704070
Li	0.8081360	1.1992000	2.7094200
Li	-0.1870020	-1.5176030	-3.7899630
Li	2.6006670	0.9197740	-1.3625970
Li	-0.6901300	-2.6864190	-0.1243120
Li	-2.9840100	-1.0802890	2.5645790

6-C

C	0.7270740	-0.1739760	0.5064730
Be	-2.4861000	0.6286840	0.2814640
Be	0.7070670	1.3263530	-0.2164720
Be	-1.3376770	1.9658390	-0.4216390
Be	-0.7569410	-0.0655100	-0.5548280
Be	-0.6683400	0.7811100	1.2000760
Li	-2.9250760	1.1047770	-2.0951540
Li	1.9259140	0.3960170	1.9136380
Li	-2.7473520	2.7987760	1.4171430
Li	1.7823680	-0.9662820	-0.9079350
Li	-0.4189850	-1.6713690	1.2869920

6-D

C	1.3552660	-0.9612360	0.9252810
Be	-0.1070460	-0.1631220	-0.9434830
Be	0.2273960	-2.0111320	0.2251700
Be	1.8428060	-1.1208770	-0.6574900
Be	-0.1663360	-0.3021230	1.2647060
Be	1.4414180	0.6143090	0.3973700
Li	1.5065460	-1.9431870	2.5975690
Li	-2.1961200	-1.1590890	-0.0977300
Li	0.1639770	-2.1252910	-2.3680270
Li	1.6150400	0.9992170	-2.1973010
Li	-0.7761250	1.9378850	0.1032970