Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Solvent induced ion separation of a beryllium scorpionate complex

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Content

Fig. S1. ^{1}H NMR spectrum of **2** in thf-d_8

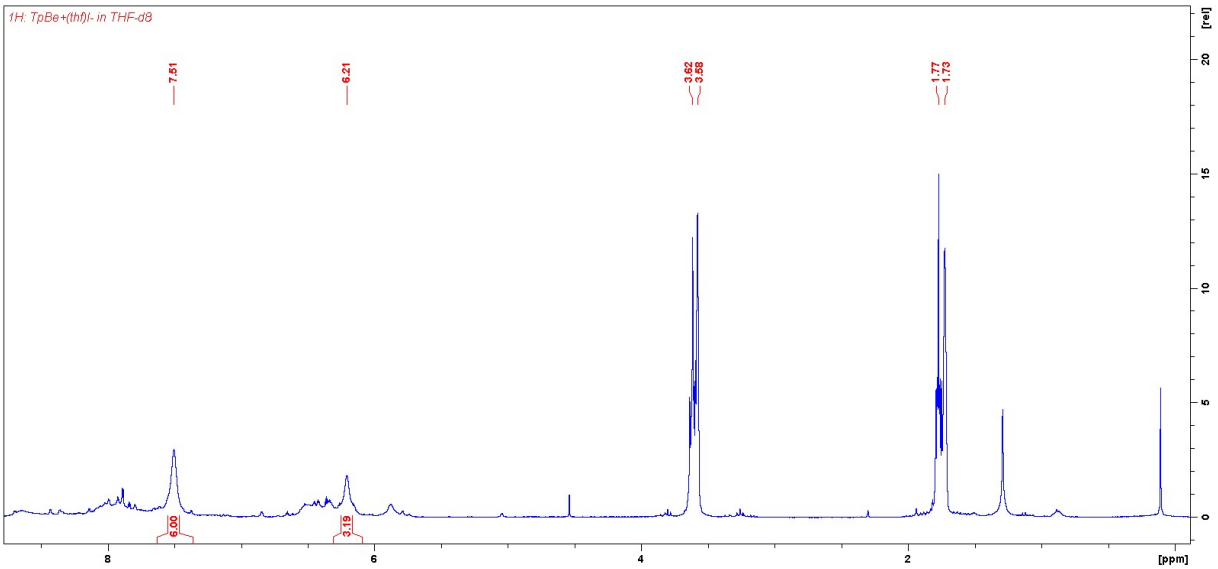


Fig. S2. ^{9}Be NMR spectrum of **2** in thf-d_8

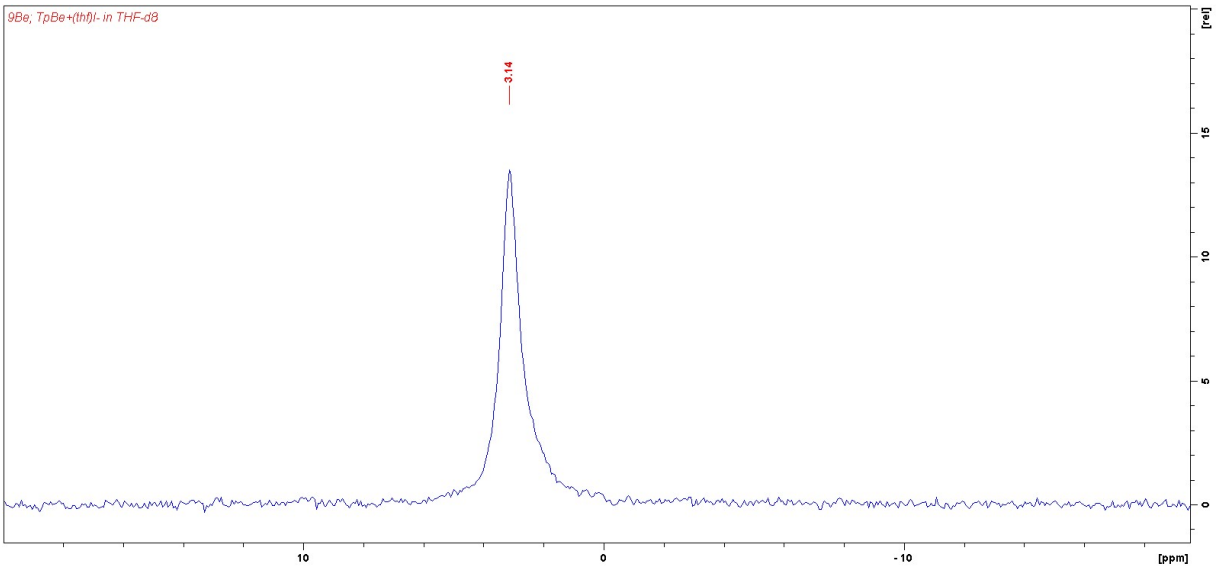


Fig. S3. ^{13}C NMR spectrum of **2** in thf-d_8

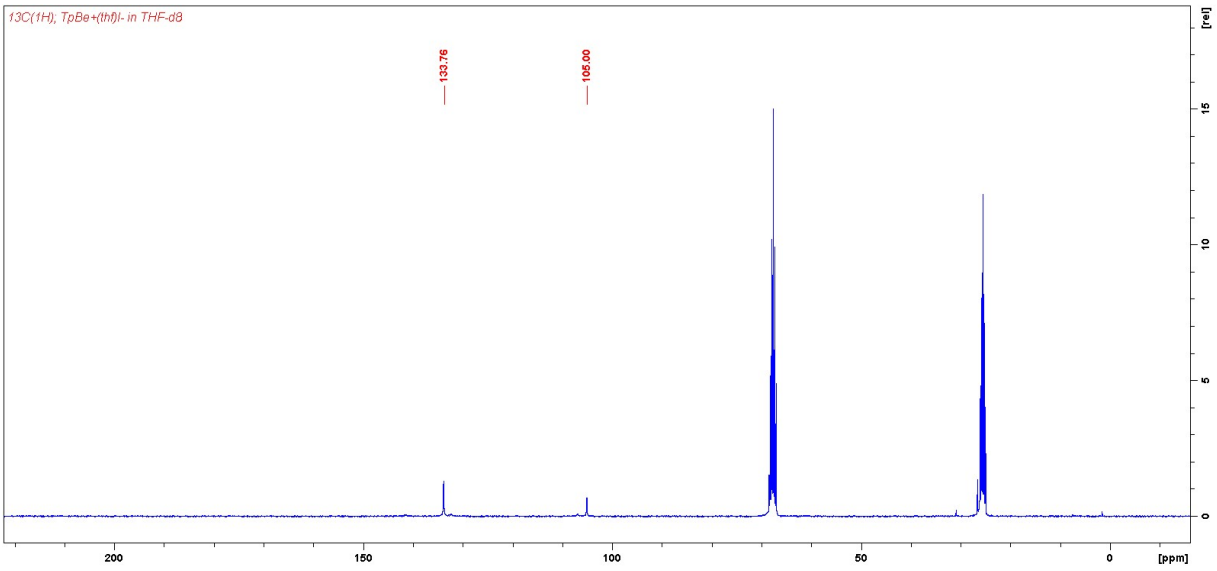


Fig. S4. ^{9}Be NMR spectrum of **3** in thf-d_8

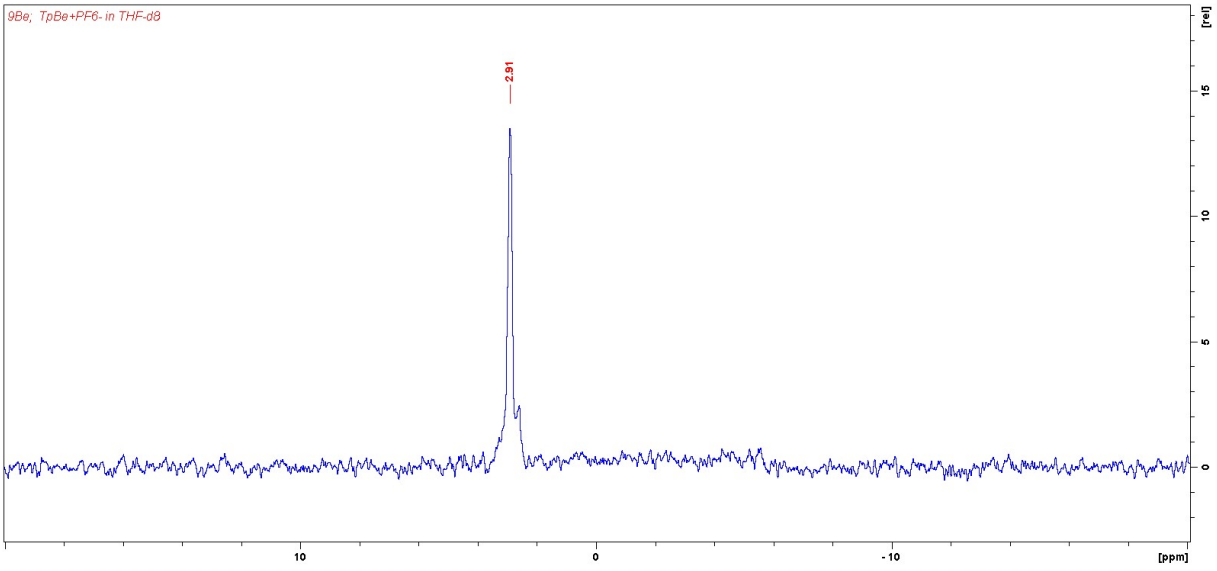


Fig. S5. ^{9}Be NMR spectrum of **4** in thf-d_8

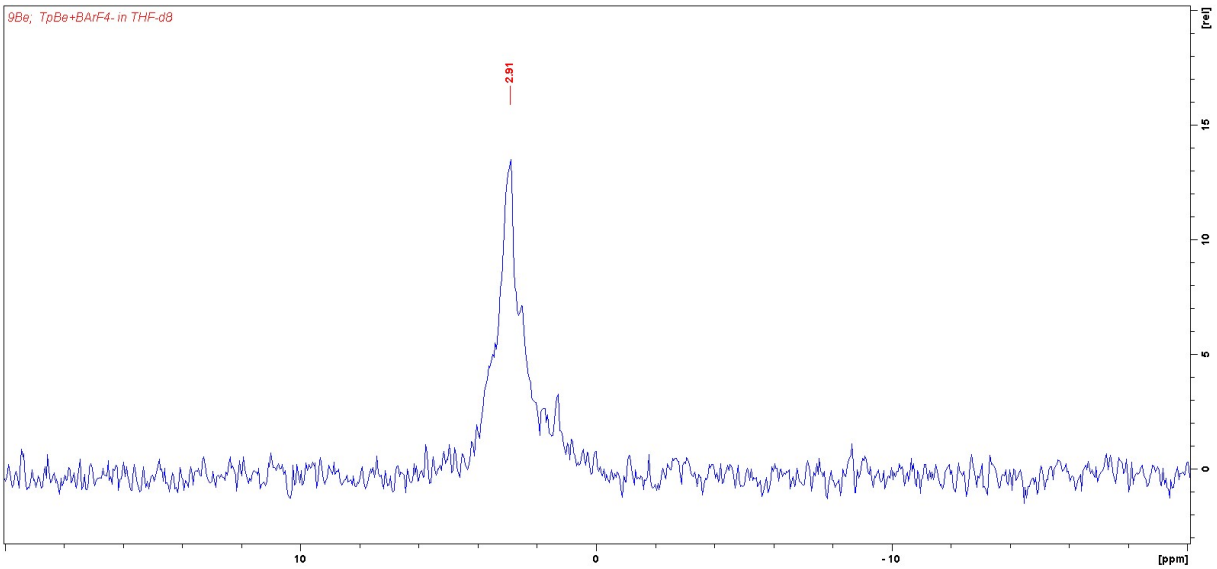


Fig. S6. ^{9}Be NMR spectrum of **5** in thf-d_8

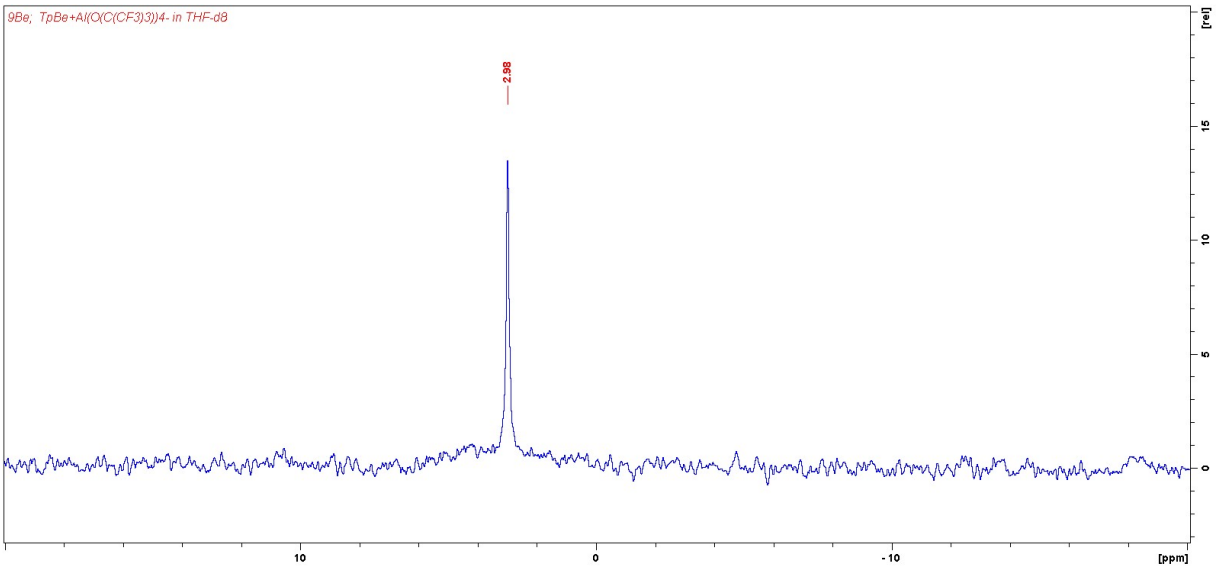


Table S1. Crystallographic details of **2**.

	2
Empirical formula	$C_{17}H_{26}BBeIN_6O_2$
M	493.16
Crystal size [mm]	0.280 × 0.170 × 0.120
T [K]	100(1)
Crystal system	orthorhombic
Space group	*P n m a*
a [Å]	14.4590(6)
b [Å]	9.8300(4)
c [Å]	15.3574(6)
$\alpha = \beta = \gamma$ [°]	90
V [Å^3]	2182.78(15)
Z	4
D_{calc} [g·cm^{-1}]	1.501
μ(MoK_α [mm^{-1}])	1.491
Transmissions	0.75/0.43
F(000)	992
Index ranges	$-20 \le h \le 11$
	$-11 \le k \le 14$
	$-21 \le l \le 21$
θ_{max} [°]	30.506
Reflections collected	14005
Independent reflections	3429
R_{int}	0.0331
Refined parameters	160
R_1 [$I > 2\sigma(I)$]	0.0343
wR_2 [all data]	0.0743
GooF	1.190
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	0.597/-1.150

[a] *R1* = $\Sigma(||F_o| - |F_c||)/\Sigma|F_o|$ (for I > 2σ(I)). - [b]*wR2* = $\{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. - [c] Goodness of fit = $\{\Sigma[w(|F_o^2| - |F_c^2|)^2]/(N_{observns} - N_{params})\}^{1/2}$. $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$ with $P = [F_o^2 + 2F_c^2]/3$, *a* and *b* are constants chosen by the programme.

Table S2: Bond lengths [Å] and bond angles [°] for **2**.

B(1)-N(4)	1.525(5)	N(3)-N(4)	1.370(4)
B(1)-N(2)	1.551(4)	N(4)-C(6)	1.341(5)
B(1)-N(2)#1	1.551(4)	C(1)-C(2)	1.395(4)
Be(1)-O(1)	1.595(6)	C(2)-C(3)	1.372(5)
Be(1)-N(3)	1.707(6)	C(4)-C(5)	1.388(5)
Be(1)-N(1)#1	1.721(4)	C(5)-C(6)	1.402(5)
Be(1)-N(1)	1.721(4)	C(7)-C(8)	1.426(7)
O(1)-C(7')	1.403(6)	C(8)-C(8)#1	1.515(9)
O(1)-C(7')#1	1.403(6)	C(8)-C(7')	1.562(7)
O(1)-C(7)#1	1.531(6)	O(2)-C(10)	1.380(6)
O(1)-C(7)	1.531(6)	O(2)-C(11)	1.410(9)
N(1)-C(1)	1.338(4)	O(2)-O(2)#1	1.780(11)
N(1)-N(2)	1.375(3)	C(9)-C(10)#1	1.512(5)
N(2)-C(3)	1.342(4)	C(9)-C(10)	1.512(5)
N(3)-C(4)	1.334(5)	C(11)-C(10)#1	1.583(9)
N(4)-B(1)-N(2)	107.4(2)	C(4)-N(3)-Be(1)	141.0(3)
N(4)-B(1)-N(2)#1	107.4(2)	N(4)-N(3)-Be(1)	111.5(3)
N(2)-B(1)-N(2)#1	104.8(3)	C(6)-N(4)-N(3)	109.4(3)
O(1)-Be(1)-N(3)	116.6(3)	C(6)-N(4)-B(1)	133.2(3)
O(1)-Be(1)-N(1)#1	115.9(2)	N(3)-N(4)-B(1)	117.5(3)
N(3)-Be(1)-N(1)#1	102.3(2)	N(1)-C(1)-C(2)	110.2(3)
O(1)-Be(1)-N(1)	115.9(2)	C(3)-C(2)-C(1)	105.1(3)
N(3)-Be(1)-N(1)	102.3(2)	N(2)-C(3)-C(2)	109.0(3)
N(1)#1-Be(1)-N(1)	101.4(3)	N(3)-C(4)-C(5)	109.9(3)
C(7')-O(1)-C(7')#1	109.9(6)	C(4)-C(5)-C(6)	105.2(3)
C(7)#1-O(1)-C(7)	96.0(5)	N(4)-C(6)-C(5)	108.0(3)
C(7')-O(1)-Be(1)	124.5(3)	C(8)-C(7)-O(1)	104.7(5)
C(7')#1-O(1)-Be(1)	124.5(3)	C(7)-C(8)-C(8)#1	105.5(3)
C(7)#1-O(1)-Be(1)	120.7(3)	C(8)#1-C(8)-C(7')	104.5(3)
C(7)-O(1)-Be(1)	120.7(3)	O(1)-C(7')-C(8)	104.2(5)
C(1)-N(1)-N(2)	106.4(2)	C(10)-O(2)-C(11)	99.7(6)

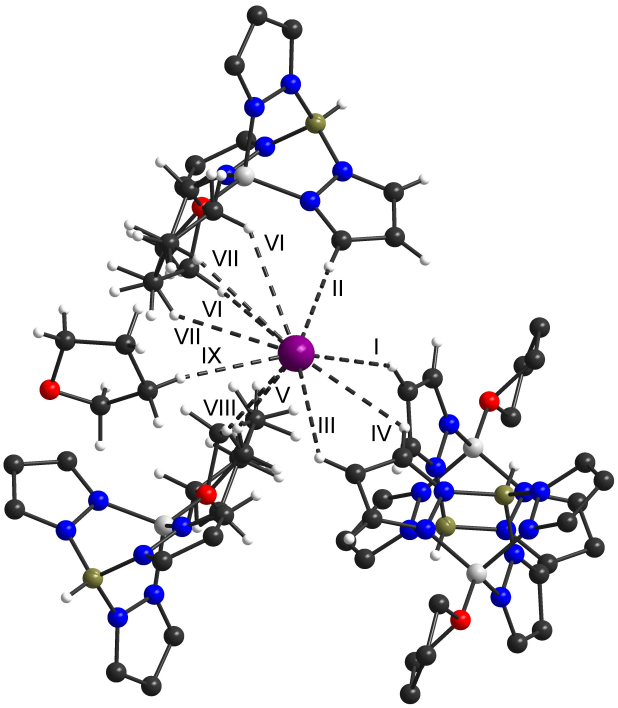
C(1)-N(1)-Be(1)	141.6(3)	C(10)-O(2)-O(2)#1	102.9(3)
N(2)-N(1)-Be(1)	111.4(2)	C(11)-O(2)-O(2)#1	20.9(4)
C(3)-N(2)-N(1)	109.3(2)	C(10)#1-C(9)-C(10)	104.7(4)
C(3)-N(2)-B(1)	133.6(3)	O(2)-C(10)-C(9)	112.3(4)
N(1)-N(2)-B(1)	116.7(2)	O(2)-C(11)-C(10)#1	112.0(7)
C(4)-N(3)-N(4)	107.5(3)		

#1 x,-y+1/2,z

Table S3: Hydrogen bonding interactions in TpBe(THF)I **2**.

#	D-H···A	d (D-H)	d (H···A)	< DHA	D (D···A)	symmetry operation
I	C2-H2···I1	0.950	3.200	143.16	4.001	I1 [−*x*+2, −*y*+1, −*z*+1]
II	C4-H4···I1	0.951	3.011	177.20	3.961	I1 [*x*−1/2, *y*, −*z*+3/2]
III	C5-H5···I1	0.049	3.220	120.17	3.786	—
IV	C6-H6···I1	0.050	3.240	120.10	3.806	—
V	C7-H7A···I1	0.960	3.038	150.66	3.904	I1 [−*x*+3/2, −*y*, *z*−1/2]
VI	C7-H7B···I1	0.991	3.277	137.38	4.062	I1 [*x*-1/2, *y*, -*z*+3/2]
VII	C8-H8C···I1	0.960	3.324	136.80	4.077	I1 [*x*−1/2, *y*, −*z*+3/2]
VIII	C7'-H7'A···I1	0.960	3.173	123.26	3.786	I1 [-*x*+3/2, -*y*, *z*-1/2]
IX	C9-H9···I1	0.990	3.220	170.75	4.200	I1 [*x*, *y*, *z*−1]

Figure S7: Hydrogen bonding interactions in TpBe(THF)I **2**. Hydrogen atom an disordered parts omitted for clarity were suitable. For labeling see Table S2.



Quantum Chemical Calculations

All geometries were optimized with TURBOMOLE using RI-DFT (resolution of identity density functional theory) methods, employing the B3-LYP functional, including a third generation Becke-Johnson dispersion-correction at TZVPP basis set levels, using effective core potential (ECP) for I.

Additionally, single-point counterpoise corrections were performed to calculate the bond dissociation energies using the same methods.

Atomic coordinates, energies and LOL plots are presented below.

Fig. S8. LOL plot of TpBeF through the N-Be-F plane.

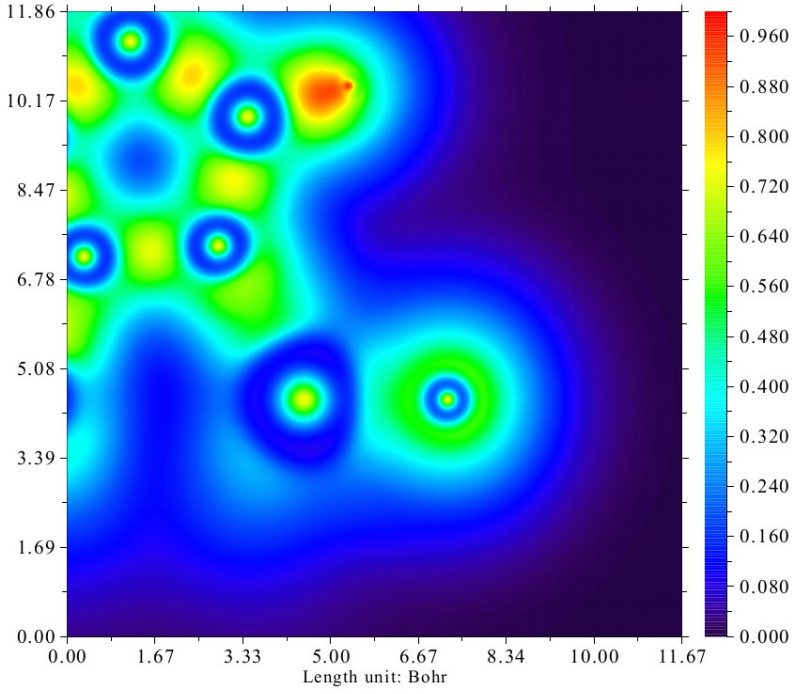


Fig. S9. LOL plot of TpBeCl through the N-Be-Cl plane.

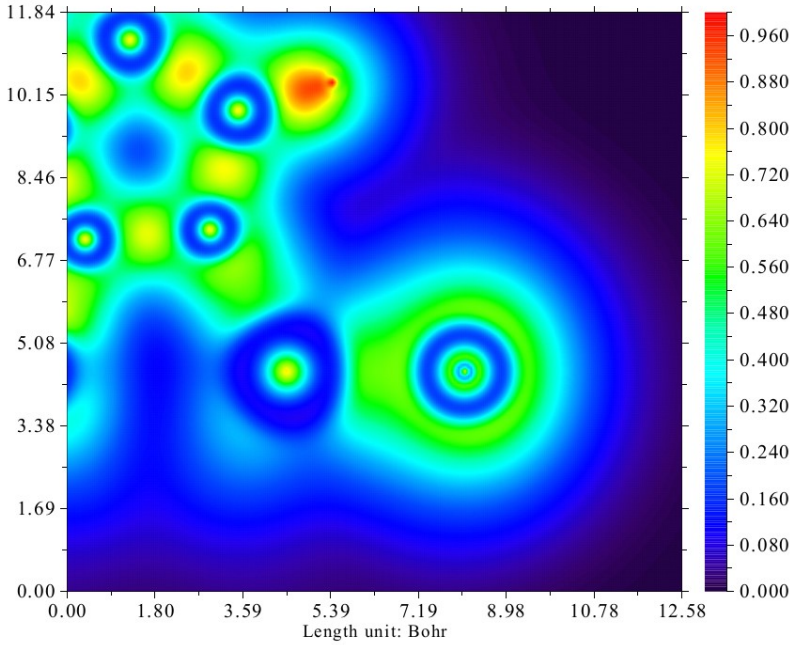


Fig. S10. LOL plot of TpBeBr through the N-Be-Br plane.

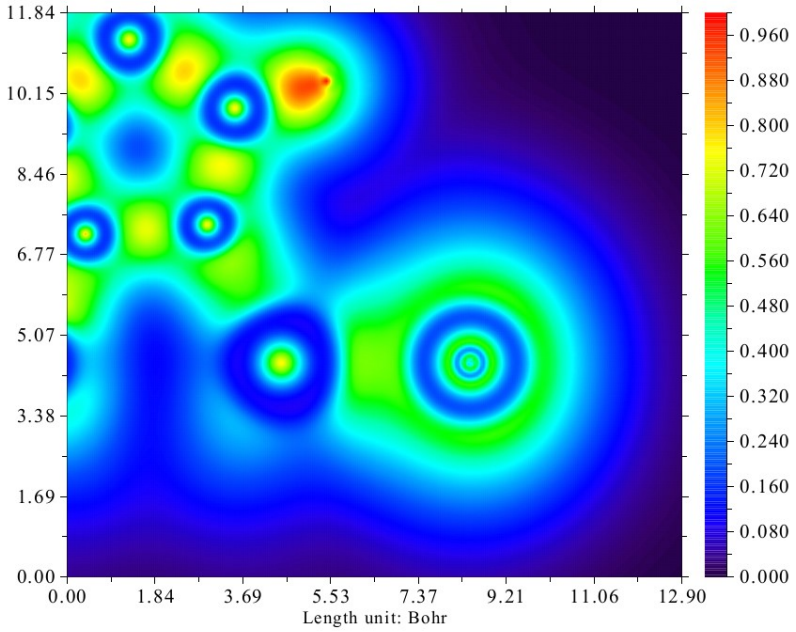


Fig. S11. LOL plot of TpBeI through the N-Be-I plane.

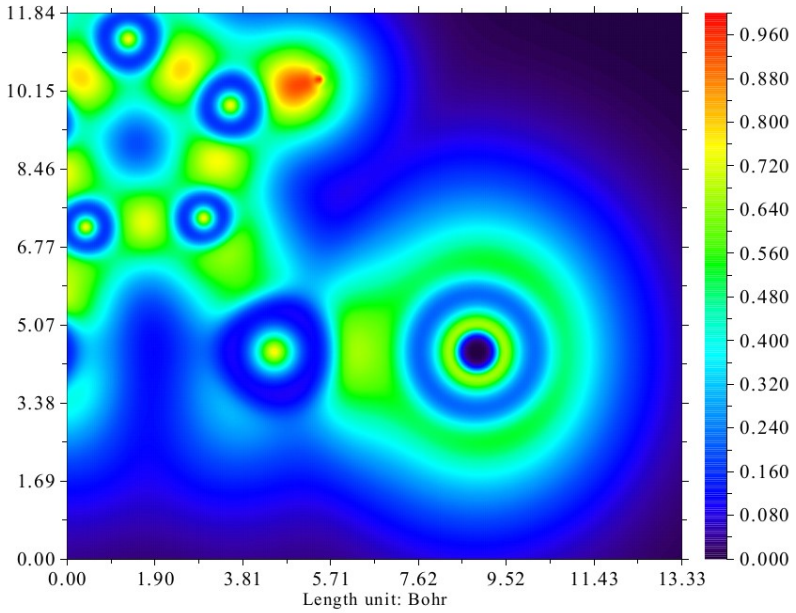


Fig. S12. LOL plot of TpBe(THF)$^{+}$ through the N-Be-O plane.

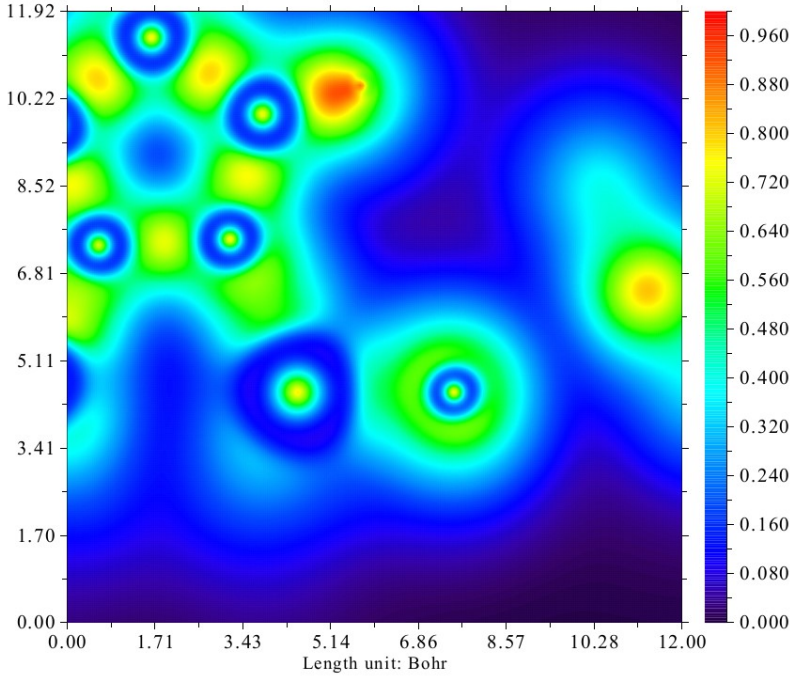


Table S4. Data of the BDE calculations.

def2-TZVPP, B3LYP, m4, ri, marij, d3					
Hartree	TpBeF	TpBeCl	TpBeBr	TpBeI	TpBe_THF_plus
Dimer	−817,0601023	−1177,366195	−3291,246384	−1014,903641	−949,3861793
Ghost1	−716,8691255	−716,8733593	−716,8749298	−716,8763128	−716,8844304
Ghost2	−99,8603627	−460,1025559	−2574,002163	−297,6843972	−232,4055817
Monomer1	−716,8687894	−716,8730429	−716,8745849	−716,8760156	−716,8836103
Monomer2	−99,8387826	−460,1017852	−2574,001565	−297,6842208	−232,4045841
Counterpoise correction	0,021915951	0,001086956	0,000942475	0,000473609	0,001817792
Corrected Dimer	−817,0381863	−1177,365108	−3291,245442	−1014,903168	−949,3843615
TpBe_plus energy	−716,8925608270	−716,8925608270	−716,8925608270	−716,8925608270	−716,8925608
THF energy					−232,3997677
Hartree					
Interaction energy	−0,330613932 6	−0,3902793974	−0,3692919744	−0,3429311627	−0,096167199
BDE	−0,306842544 3	−0,3707615085	−0,3513160907	−0,3263859730	−0,087216656
kJ/mol	TpBeF	TpBeCl	TpBeBr	TpBeI	TpBe_THF_plus
Interaction energy	−868,0264982147	−1024,6781070154	−969,5756521747	−900,3653715082	−252,4868691
BDE	−805,6147456943	−973,4339122558	−922,3799902864	−856,9259950644	−228,9872298

xyz-data of the calculated structures.

TpBeF_d3_opt.xyz

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28
Energy = -817.0381863340
C    -1.7543777    1.0189170    2.9735123
C    -2.3705942    0.5279998    1.8167444
N    -1.4508959    0.2441672    0.8999897
N    -0.2401838    0.5397600    1.4333056
C    -0.3995993    1.0078069    2.6819187
B     1.0075042    0.2878426    0.5456696
N     0.7866047    1.1011562   -0.7574515
N    -0.3432263    0.8482749   -1.4625151
C    -0.3327798    1.6398724   -2.5302468
C     0.8241190    2.4275344   -2.5278302
C     1.5045791    2.0493127   -1.3813002
N     0.9557206   -1.2088321    0.1382194
N    -0.1613089   -1.6417565   -0.4963867
C     0.0012446   -2.9363508   -0.7507248
C     1.2465835   -3.3627316   -0.2751519
C     1.8168917   -2.2292313    0.2820203
Be   -1.3877709   -0.3899854   -0.7510382
F    -2.6211076   -0.7349830   -1.4173839
H    -0.7753808   -3.4856515   -1.2553828
H    -1.1467172    1.6017136   -3.2342079
H    -3.4127163    0.3663160    1.5990525
H     2.0263319    0.5761222    1.0970997
H     2.7670619   -2.0822121    0.7657733
H     1.6699314   -4.3496105   -0.3284401
H     2.4409048    2.3876650   -0.9723924
H     1.1218816    3.1634957   -3.2528521
H     0.4518649    1.2982888    3.2727477
H    -2.2245655    1.3350991    3.8872512
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TpBeCl_d3_opt.xyz

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Energy = -1177.365107571
Cl   -0.2208611    1.3728532    3.2091895
Be   -0.0982424    0.6171731    1.4405990
N    -0.7677640   -0.9731610    1.1682928
N    -0.8557738    1.4700738    0.1179411
N     1.4865978    0.3758715    0.7473493
N    -0.6339423   -1.4184901   -0.1059741
C    -1.3967885   -1.9174716    1.8605865
N    -0.7156518    0.8600510   -1.0855634
C    -1.5591496    2.5814387   -0.0736544
N     1.4691285   -0.1608206   -0.4983847
C     2.7577804    0.5643696    1.0865858
B     0.0778754   -0.4745052   -1.1128598
C    -1.1786274   -2.6410390   -0.2125016
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C    -1.6821951   -3.0042232    1.0269268
H    -1.6056810   -1.7634707    2.9055928
C    -1.3308822    1.5884165   -2.0308763
C    -1.8881309    2.7053601   -1.4278584
H    -1.7857838    3.2204380    0.7628440
C     2.7284995   -0.3087485   -0.9396621
H     2.9966132    0.9861033    2.0481026
C     3.5924096    0.1441863    0.0453176
H     0.1533882   -0.9425509   -2.2078103
H    -1.1716978   -3.1654183   -1.1524697
H    -2.1815389   -3.9200943    1.2871153
H    -1.3312916    1.2672134   -3.0581833
H    -2.4491346    3.4918373   -1.8996449
H     2.9240443   -0.7217954   -1.9141840
H     4.6667997    0.1664030    0.0131841
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TpBeBr_d3_opt.xyz

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Energy = -3291.245441902
Br   -0.2701168    1.5367623    3.2988937
Be   -0.1124441    0.6531554    1.4031161
N     1.4781638    0.3997006    0.7447164
N    -0.8588197    1.4652478    0.0577237
N    -0.7754002   -0.9406520    1.1844789
N     1.4761849   -0.1761094   -0.4841500
C     2.7447770    0.6059622    1.0912522
N    -0.7047492    0.8191565   -1.1256483
C    -1.5642619    2.5678724   -0.1735936
N    -0.6274109   -1.4270119   -0.0736835
C    -1.4111319   -1.8623701    1.9009039
B     0.0924430   -0.5136303   -1.1032557
C     2.7408521   -0.3301843   -0.9072024
H     2.9707136    1.0589010    2.0416772
C     3.5919094    0.1582258    0.0721237
C    -1.3135429    1.5166790   -2.0977826
H    -1.8007646    3.2304603    0.6416269
C    -1.8803377    2.6492459   -1.5338243
C    -1.1702529   -2.6527464   -0.1454462
H    -1.6309699   -1.6738023    2.9380208
C    -1.6866105   -2.9756599    1.0999481
H     0.1804148   -1.0157153   -2.1818441
H     2.9490199   -0.7722241   -1.8662851
H     4.6664241    0.1855418    0.0503632
H    -1.3033230    1.1648657   -3.1149762
H    -2.4394618    3.4191002   -2.0343405
H    -1.1532943   -3.2077499   -1.0675565
H    -2.1880104   -3.8830211    1.3847443
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Energy = -1014.903167560
I   -1.6685092   -2.9521844   -1.8484283
Be   -0.6637361   -1.1715051   -0.7331665
N   -0.4992885   -1.2845677   0.9899601
N   0.9659710   -0.7645472   -1.1652584
N   -1.4098400   0.3885876   -0.8638642
N   0.0977100   -0.2005171   1.5484863
C   -0.7857892   -2.1366167   1.9696595
N   1.4658468   0.2848654   -0.4635923
C   1.9135882   -1.1792250   -2.0006470
N   -0.7520524   1.3614520   -0.1823950
C   -2.4647938   0.9483021   -1.4482937
B   0.5295002   0.9410209   0.5876865
C   0.1849109   -0.3742123   2.8765766
H   -1.2682586   -3.0713350   1.7391380
C   -0.3700541   -1.6043404   3.1942404
C   2.7253741   0.5265900   -0.8595959
H   1.7196229   -2.0115896   -2.6557598
C   3.0570811   -0.3891350   -1.8462925
C   -1.3949380   2.5291011   -0.3404072
H   -3.1269544   0.3436703   -2.0446123
C   -2.5021719   2.3133139   -1.1463847
H   1.0446245   1.8532314   1.1579128
H   0.6312216   0.3806339   3.5008053
H   -0.4599301   -2.0490703   4.1688554
H   3.2959893   1.3253260   -0.4179551
H   3.9894126   -0.4715648   -2.3751678
H   -1.0260783   3.4263366   0.1259804
H   -3.2284585   3.0379795   -1.4674805

TpBe_THF_plus_d3_opt.xyz
40
Energy = -949.3861792369
C   -3.5103490   1.4722214   -0.1959277
C   -2.1587392   1.5138453   -0.8845348
O   -1.6214972   0.1495068   -0.7228412
C   -2.6867274   -0.7695648   -0.2820274
C   -3.9697637   0.0290406   -0.4404155
Be   -0.0854340   -0.0770880   -0.2681612
N   0.2219792   0.3397746   1.3781726
N   1.5301589   0.1533445   1.6958218
C   1.7334719   0.4889888   2.9774380
C   0.5270559   0.9079128   3.5192851
C   -0.3895605   0.7953279   2.4752353
B   2.4630812   -0.3761234   0.5725542
N   1.8273925   -1.7056778   0.0759090
N   0.5417213   -1.6705724   -0.3739123
C   0.2337932   -2.9058151   -0.7796715
C   1.3218593   -3.7555689   -0.5917979

```
C     2.3106357   -2.9495272   -0.0484259
N     2.3303275    0.6279550   -0.6073104
N     1.0851293    0.8506475   -1.1105930
C     1.2176553    1.7054298   -2.1287031
C     2.5587552    2.0476896   -2.2913348
C     3.2276494    1.3383111   -1.3050404
H     3.5873923   -0.5133694    0.9335706
H     4.2745871    1.2936112   -1.0590653
H     3.3178802   -3.1795671    0.2534136
H     2.7121135    0.4095907    3.4184495
H     0.3578558    2.0269328   -2.6918055
H     2.9834831    2.7129782   -3.0209855
H    -0.7379625   -3.1266901   -1.1868625
H     1.3834060   -4.8043529   -0.8189549
H    -1.4435214    1.0175917    2.4651604
H     0.3426838    1.2441621    4.5234721
H    -2.6290628   -1.6525998   -0.9116901
H    -2.4778197   -1.0386765    0.7530788
H    -1.4430950    2.2024623   -0.4420540
H    -2.2389616    1.6976013   -1.9548988
H    -4.3653599   -0.0811459   -1.4503286
H    -4.7344283   -0.2972643    0.2610952
H    -3.4020214    1.6684026    0.8716336
H    -4.1957642    2.2102750   -0.6069472
```

THF_d3_opt.xyz

```
13
Energy = -232.3997677059
C    -0.5534910    0.8954435   -0.2113198
C     0.9386940    0.8084714   -0.5431993
O     1.4371609   -0.3623632    0.1170888
C     0.3559517   -1.0992965    0.6957267
C    -0.9155912   -0.5746405    0.0324821
H     0.5311121   -2.1616300    0.5193310
H     0.3339602   -0.9302086    1.7792230
H     1.5023279    1.6768345   -0.1958316
H     1.1033295    0.7031252   -1.6207853
H    -1.0895981   -1.0875300   -0.9156499
H    -1.8003553   -0.7035112    0.6553895
H    -0.7103856    1.4789276    0.6980327
H    -1.1331151    1.3563778   -1.0104878
```

```
TpBe_plus_d3_opt.xyz
27
Energy = -716.8925608270
Be   -0.6251186   -1.1062058   -0.6916519
N    -0.5750636   -1.4281217    0.9310311
N     0.9149687   -0.8997039   -1.2613355
N    -1.5011293    0.2730706   -0.9548334
N     0.0295162   -0.3252648    1.4791105
C    -0.8571085   -2.2701204    1.9300511
N     1.4045223    0.1621824   -0.5437300
C     1.8799106   -1.3008801   -2.0946933
N    -0.8248193    1.2442145   -0.2606903
C    -2.5569033    0.8537995   -1.5333093
B     0.4649783    0.8242193    0.5145899
C     0.1160483   -0.4932723    2.8052083
H    -1.3395396   -3.2134604    1.7363522
C    -0.4375793   -1.7211169    3.1379115
C     2.6612532    0.4077050   -0.9369709
H     1.7209754   -2.1298055   -2.7638932
C     3.0066956   -0.5020620   -1.9258319
C    -1.4643056    2.4111015   -0.4147663
H    -3.2400360    0.2796756   -2.1365210
C    -2.5760661    2.2094268   -1.2197965
H     0.9773945    1.7314632    1.0813697
H     0.5628344    0.2654985    3.4247161
H    -0.5237105   -2.1546566    4.1176959
H     3.2270843    1.2083885   -0.4921229
H     3.9430884   -0.5740542   -2.4486909
H    -1.0911710    3.3053925    0.0543976
H    -3.2967195    2.9425868   -1.5335967
```

SEN data of the calculated structures.

```
y TpBeF:
*****************************************************************
*                        shared electron numbers

 TWO center shared electron numbers ge 0.1000E-01 :

  shared electron number for the pair       1 c  -   2 c   =     1.8053

  shared electron number for the pair       1 c  -   3 n   =     0.0178

  shared electron number for the pair       1 c  -   4 n   =     0.0200

  shared electron number for the pair       1 c  -   5 c   =     1.8624

  shared electron number for the pair       1 c  -  21 h   =     0.0134

  shared electron number for the pair       1 c  -  27 h   =     0.0106

  shared electron number for the pair       1 c  -  28 h   =     1.3899

  shared electron number for the pair       2 c  -   3 n   =     1.6774
```

```
shared electron number for the pair      2 c  -   4 n   =     0.0156
shared electron number for the pair      2 c  -   5 c   =     0.0835
shared electron number for the pair      2 c  -  21 h   =     1.3830
shared electron number for the pair      2 c  -  28 h   =     0.0110
shared electron number for the pair      3 n  -   4 n   =     1.3356
shared electron number for the pair      3 n  -   6 b   =     0.0339
shared electron number for the pair      3 n  -  17 be  =     0.2890
shared electron number for the pair      3 n  -  21 h   =     0.0125
shared electron number for the pair      4 n  -   5 c   =     1.6446
shared electron number for the pair      4 n  -   6 b   =     1.2450
shared electron number for the pair      4 n  -   7 n   =     0.0125
shared electron number for the pair      4 n  -  12 n   =     0.0126
shared electron number for the pair      4 n  -  17 be  =     0.0398
shared electron number for the pair      4 n  -  22 h   =     0.0124
shared electron number for the pair      5 c  -   6 b   =     0.0316
shared electron number for the pair      5 c  -  27 h   =     1.3813
shared electron number for the pair      5 c  -  28 h   =     0.0124
shared electron number for the pair      6 b  -   7 n   =     1.2451
shared electron number for the pair      6 b  -   8 n   =     0.0338
shared electron number for the pair      6 b  -  11 c   =     0.0315
shared electron number for the pair      6 b  -  12 n   =     1.2445
shared electron number for the pair      6 b  -  13 n   =     0.0338
shared electron number for the pair      6 b  -  16 c   =     0.0316
shared electron number for the pair      6 b  -  17 be  =     0.0585
shared electron number for the pair      6 b  -  22 h   =     1.4210
shared electron number for the pair      7 n  -   8 n   =     1.3356
shared electron number for the pair      7 n  -   9 c   =     0.0156
shared electron number for the pair      7 n  -  10 c   =     0.0200
shared electron number for the pair      7 n  -  11 c   =     1.6445
shared electron number for the pair      7 n  -  12 n   =     0.0126
shared electron number for the pair      7 n  -  17 be  =     0.0395
shared electron number for the pair      7 n  -  22 h   =     0.0125
```

```
shared electron number for the pair      8 n  -   9 c   =     1.6771
shared electron number for the pair      8 n  -  10 c   =     0.0178
shared electron number for the pair      8 n  -  17 be  =     0.2818
shared electron number for the pair      8 n  -  20 h   =     0.0124
shared electron number for the pair      9 c  -  10 c   =     1.8048
shared electron number for the pair      9 c  -  11 c   =     0.0835
shared electron number for the pair      9 c  -  20 h   =     1.3828
shared electron number for the pair      9 c  -  26 h   =     0.0109
shared electron number for the pair     10 c  -  11 c   =     1.8621
shared electron number for the pair     10 c  -  20 h   =     0.0134
shared electron number for the pair     10 c  -  25 h   =     0.0107
shared electron number for the pair     10 c  -  26 h   =     1.3898
shared electron number for the pair     11 c  -  25 h   =     1.3811
shared electron number for the pair     11 c  -  26 h   =     0.0124
shared electron number for the pair     12 n  -  13 n   =     1.3352
shared electron number for the pair     12 n  -  14 c   =     0.0157
shared electron number for the pair     12 n  -  15 c   =     0.0200
shared electron number for the pair     12 n  -  16 c   =     1.6446
shared electron number for the pair     12 n  -  17 be  =     0.0390
shared electron number for the pair     12 n  -  22 h   =     0.0124
shared electron number for the pair     13 n  -  14 c   =     1.6771
shared electron number for the pair     13 n  -  15 c   =     0.0179
shared electron number for the pair     13 n  -  17 be  =     0.2563
shared electron number for the pair     13 n  -  19 h   =     0.0124
shared electron number for the pair     14 c  -  15 c   =     1.8053
shared electron number for the pair     14 c  -  16 c   =     0.0837
shared electron number for the pair     14 c  -  19 h   =     1.3830
shared electron number for the pair     14 c  -  24 h   =     0.0109
shared electron number for the pair     15 c  -  16 c   =     1.8627
shared electron number for the pair     15 c  -  19 h   =     0.0135
shared electron number for the pair     15 c  -  23 h   =     0.0107
shared electron number for the pair     15 c  -  24 h   =     1.3899
```

```
  shared electron number for the pair      16 c  -  23 h   =     1.3813

  shared electron number for the pair      16 c  -  24 h   =     0.0124

  shared electron number for the pair      17 be -  18 f   =     0.9884

*************************************************************************
*                                                                       *
*              atomic charges with multicenter corrections              *
*              AS RESULTING FROM 2-CENTER SEN CONTRIBUTIONS             *
*                                                                       *
*************************************************************************
```

atom	charge
1 c	-0.1387
2 c	-0.0533
3 n	-0.1023
4 n	0.2289
5 c	-0.0280
6 b	-0.3381
7 n	0.2281
8 n	-0.1060
9 c	-0.0540
10 c	-0.1389
11 c	-0.0286
12 n	0.2287
13 n	-0.1185
14 c	-0.0537
15 c	-0.1389
16 c	-0.0284
17 be	0.2509
18 f	-0.3133
19 h	0.0859
20 h	0.0863
21 h	0.0860
22 h	-0.0002
23 h	0.0770
24 h	0.0717
25 h	0.0775
26 h	0.0717
27 h	0.0768
28 h	0.0714

```
THREE and FOUR center SEN greater than 0.010:

n(  1  2  3)     =    -0.0460
n(  1  2  3  4) =     0.0397
n(  1  2  4)     =     0.0118
n(  1  2  4  5) =     0.0327
n(  1  2  5)     =     0.0765
n(  1  2  5 27) =    -0.0139
n(  1  3  4)     =     0.0109
n(  1  3  4  5) =     0.0362
n(  1  3 28)     =    -0.0112
n(  1  4  5)     =    -0.0168
n(  1  4 28)     =    -0.0118
n(  2  3  4)     =     0.0351
n(  2  3  4  5) =     0.0658
n(  2  3  5)     =    -0.0112
```

```
n(  2  4  5)     =     0.0161
n(  2  5 27)     =    -0.0165
n(  3  4  6)     =     0.0289
n(  3  4  6 17) =     0.0220
n(  3  4  6 22) =    -0.0131
n(  3  4  8 17) =    -0.0116
n(  3  4 13 17) =    -0.0105
n(  3  4 17)     =     0.0268
n(  3  4 17 18) =    -0.0110
n(  3  6 17)     =     0.0111
n(  3  6 22)     =    -0.0132
n(  3  7  8 17) =    -0.0118
n(  3  7 13 17) =     0.0105
n(  3  7 17)     =    -0.0135
n(  3  8 12 17) =     0.0111
n(  3  8 13 17) =     0.1149
n(  3  8 17)     =    -0.1410
n(  3 12 13 17) =    -0.0110
n(  3 12 17)     =    -0.0127
n(  3 13 17)     =    -0.1259
n(  3 17 18)     =    -0.0138
n(  4  5  6)     =     0.0239
n(  4  5 17 18) =    -0.0105
n(  4  6  7)     =    -0.0437
n(  4  6 12)     =    -0.0442
n(  4  6 17)     =     0.0271
n(  4  6 17 18) =    -0.0376
n(  4  8 13 17) =     0.0103
n(  4  8 17)     =    -0.0133
n(  4 13 17)     =    -0.0121
n(  4 17 18)     =    -0.0452
n(  5 17 18)     =    -0.0127
n(  6  7  8)     =     0.0287
n(  6  7  8 17) =     0.0219
n(  6  7  8 22) =    -0.0131
n(  6  7 11)     =     0.0236
n(  6  7 12)     =    -0.0439
n(  6  7 17)     =     0.0271
n(  6  7 17 18) =    -0.0376
n(  6  8 17)     =     0.0113
n(  6  8 22)     =    -0.0131
n(  6 12 13)     =     0.0287
n(  6 12 13 17) =     0.0215
n(  6 12 13 22) =    -0.0131
n(  6 12 16)     =     0.0239
n(  6 12 17)     =     0.0267
n(  6 12 17 18) =    -0.0387
n(  6 13 17)     =     0.0119
n(  6 13 22)     =    -0.0132
n(  6 17 18)     =    -0.1234
n(  6 17 22)     =    -0.0278
n(  7  8  9)     =     0.0352
n(  7  8  9 10) =     0.0397
n(  7  8  9 11) =     0.0657
n(  7  8 10)     =     0.0109
n(  7  8 10 11) =     0.0363
n(  7  8 13 17) =    -0.0104
n(  7  8 17)     =     0.0265
n(  7  8 17 18) =    -0.0109
n(  7  9 10)     =     0.0118
n(  7  9 10 11) =     0.0330
n(  7  9 11)     =     0.0164
n(  7 10 11)     =    -0.0164
n(  7 10 26)     =    -0.0118
```

```
 n(  7 11 17 18) =    -0.0105
 n(  7 13 17)    =    -0.0119
 n(  7 17 18)    =    -0.0451
 n(  8  9 10)    =    -0.0462
 n(  8  9 11)    =    -0.0114
 n(  8 10 26)    =    -0.0113
 n(  8 12 13 17) =    -0.0107
 n(  8 12 17)    =    -0.0122
 n(  8 13 17)    =    -0.1221
 n(  8 17 18)    =    -0.0139
 n(  9 10 11)    =     0.0762
 n(  9 10 11 25) =    -0.0137
 n(  9 11 25)    =    -0.0163
 n( 11 17 18)    =    -0.0126
 n( 12 13 14)    =     0.0353
 n( 12 13 14 15) =     0.0397
 n( 12 13 14 16) =     0.0659
 n( 12 13 15)    =     0.0110
 n( 12 13 15 16) =     0.0364
 n( 12 13 17)    =     0.0257
 n( 12 13 17 18) =    -0.0126
 n( 12 14 15)    =     0.0118
 n( 12 14 15 16) =     0.0326
 n( 12 14 16)    =     0.0161
 n( 12 15 16)    =    -0.0169
 n( 12 15 24)    =    -0.0117
 n( 12 16 17 18) =    -0.0111
 n( 12 17 18)    =    -0.0472
 n( 13 14 15)    =    -0.0463
 n( 13 14 16)    =    -0.0115
 n( 13 15 24)    =    -0.0112
 n( 13 17 18)    =    -0.0144
 n( 14 15 16)    =     0.0765
 n( 14 15 16 23) =    -0.0137
 n( 14 16 23)    =    -0.0165
 n( 16 17 18)    =    -0.0134

 multicenter rest contribution =  0.145829 (correct sign for five center
terms)

**************************************************************************
*                                                                        *
*              atomic charges with multicenter corrections               *
*                                                                        *
**************************************************************************

                        -------------------------
                           atom   |     charge
                        -------------------------
                            1 c   |    -0.1547
                            2 c   |    -0.0746
                            3 n   |     0.0081
                            4 n   |     0.2266
                            5 c   |    -0.0538
                            6 b   |    -0.4054
                            7 n   |     0.2259
                            8 n   |     0.0037
                            9 c   |    -0.0750
                           10 c   |    -0.1549
                           11 c   |    -0.0544
                           12 n   |     0.2266
                           13 n   |    -0.0132
```

```
   14 c   |   -0.0746
   15 c   |   -0.1550
   16 c   |   -0.0545
   17 be  |    0.3713
   18 f   |   -0.2848
   19 h   |    0.0616
   20 h   |    0.0618
   21 h   |    0.0616
   22 h   |   -0.0193
   23 h   |    0.0574
   24 h   |    0.0515
   25 h   |    0.0579
   26 h   |    0.0515
   27 h   |    0.0573
   28 h   |    0.0512
 ------------------------

 moments (from total density versus population analysis)
 <charge> =          -0.000000          -0.000000
 <x   >   =           1.456194           0.250839
 <y   >   =           0.407549           0.128616
 <z   >   =           0.787739           0.163453


================================================================================
=

TpBeCl:
************************************************************************
*                                                                      *
*                        shared electron numbers                       *
*                                                                      *
************************************************************************


 TWO center shared electron numbers ge 0.1000E-01 :

  shared electron number for the pair       1 cl -   2 be  =     0.0603

  shared electron number for the pair       2 be -   3 n   =     0.3779

  shared electron number for the pair       2 be -   4 n   =     1.0267

  shared electron number for the pair       2 be -   5 n   =     0.5003

  shared electron number for the pair       2 be -   6 n   =     0.0424

  shared electron number for the pair       2 be -   7 c   =     0.0158

  shared electron number for the pair       2 be -   8 n   =     0.0512

  shared electron number for the pair       2 be -   9 c   =     0.0481

  shared electron number for the pair       2 be -  10 n   =     0.0445

  shared electron number for the pair       2 be -  11 c   =     0.0235

  shared electron number for the pair       2 be -  12 b   =     0.0512

  shared electron number for the pair       2 be -  16 c   =     0.0123
```

```
shared electron number for the pair      2 be -  17 c   =     0.0111
shared electron number for the pair      3 n  -   6 n   =     1.3237
shared electron number for the pair      3 n  -   7 c   =     1.6635
shared electron number for the pair      3 n  -  12 b   =     0.0362
shared electron number for the pair      3 n  -  14 c   =     0.0154
shared electron number for the pair      3 n  -  15 h   =     0.0138
shared electron number for the pair      4 n  -   8 n   =     1.3235
shared electron number for the pair      4 n  -   9 c   =     1.6638
shared electron number for the pair      4 n  -  12 b   =     0.0363
shared electron number for the pair      4 n  -  17 c   =     0.0154
shared electron number for the pair      4 n  -  18 h   =     0.0138
shared electron number for the pair      5 n  -  10 n   =     1.3234
shared electron number for the pair      5 n  -  11 c   =     1.6637
shared electron number for the pair      5 n  -  12 b   =     0.0362
shared electron number for the pair      5 n  -  20 h   =     0.0137
shared electron number for the pair      5 n  -  21 c   =     0.0154
shared electron number for the pair      6 n  -   7 c   =     0.0158
shared electron number for the pair      6 n  -   8 n   =     0.0122
shared electron number for the pair      6 n  -  10 n   =     0.0122
shared electron number for the pair      6 n  -  12 b   =     1.2336
shared electron number for the pair      6 n  -  13 c   =     1.6387
shared electron number for the pair      6 n  -  14 c   =     0.0171
shared electron number for the pair      6 n  -  22 h   =     0.0120
shared electron number for the pair      7 c  -  13 c   =     0.0836
shared electron number for the pair      7 c  -  14 c   =     1.7991
shared electron number for the pair      7 c  -  15 h   =     1.3800
shared electron number for the pair      8 n  -   9 c   =     0.0158
shared electron number for the pair      8 n  -  10 n   =     0.0122
shared electron number for the pair      8 n  -  12 b   =     1.2341
shared electron number for the pair      8 n  -  16 c   =     1.6387
shared electron number for the pair      8 n  -  17 c   =     0.0170
shared electron number for the pair      8 n  -  22 h   =     0.0120
```

```
  shared electron number for the pair      9 c  -  16 c   =     0.0837
  shared electron number for the pair      9 c  -  17 c   =     1.7991
  shared electron number for the pair      9 c  -  18 h   =     1.3801
  shared electron number for the pair     10 n  -  11 c   =     0.0158
  shared electron number for the pair     10 n  -  12 b   =     1.2339
  shared electron number for the pair     10 n  -  19 c   =     1.6387
  shared electron number for the pair     10 n  -  21 c   =     0.0170
  shared electron number for the pair     10 n  -  22 h   =     0.0120
  shared electron number for the pair     11 c  -  19 c   =     0.0836
  shared electron number for the pair     11 c  -  20 h   =     1.3800
  shared electron number for the pair     11 c  -  21 c   =     1.7991
  shared electron number for the pair     12 b  -  13 c   =     0.0293
  shared electron number for the pair     12 b  -  16 c   =     0.0295
  shared electron number for the pair     12 b  -  19 c   =     0.0294
  shared electron number for the pair     12 b  -  22 h   =     1.4296
  shared electron number for the pair     13 c  -  14 c   =     1.8558
  shared electron number for the pair     13 c  -  23 h   =     1.3794
  shared electron number for the pair     13 c  -  24 h   =     0.0126
  shared electron number for the pair     14 c  -  15 h   =     0.0124
  shared electron number for the pair     14 c  -  24 h   =     1.3869
  shared electron number for the pair     16 c  -  17 c   =     1.8558
  shared electron number for the pair     16 c  -  25 h   =     1.3791
  shared electron number for the pair     16 c  -  26 h   =     0.0126
  shared electron number for the pair     17 c  -  18 h   =     0.0124
  shared electron number for the pair     17 c  -  26 h   =     1.3869
  shared electron number for the pair     19 c  -  21 c   =     1.8558
  shared electron number for the pair     19 c  -  27 h   =     1.3793
  shared electron number for the pair     19 c  -  28 h   =     0.0126
  shared electron number for the pair     20 h  -  21 c   =     0.0123
  shared electron number for the pair     21 c  -  28 h   =     1.3869

*************************************************************************
*                                                                       *
*             atomic charges with multicenter corrections               *
```

```
*              AS RESULTING FROM 2-CENTER SEN CONTRIBUTIONS             *
*                                                                       *
*************************************************************************
```

atom	charge
1 cl	-0.8625
2 be	0.3669
3 n	-0.0541
4 n	0.2700
5 n	0.0066
6 n	0.2216
7 c	-0.0597
8 n	0.2267
9 c	-0.0435
10 n	0.2227
11 c	-0.0561
12 b	-0.3638
13 c	-0.0348
14 c	-0.1497
15 h	0.0847
16 c	-0.0314
17 c	-0.1466
18 h	0.0866
19 c	-0.0340
20 h	0.0853
21 c	-0.1489
22 h	-0.0006
23 h	0.0713
24 h	0.0669
25 h	0.0713
26 h	0.0670
27 h	0.0711
28 h	0.0670

THREE and FOUR center SEN greater than 0.010:

```
n(  1  2  3)     =    -0.0147
n(  1  2  3  5) =     0.0324
n(  1  2  4)     =    -0.0655
n(  1  2  5)     =    -0.0235
n(  2  3  4)     =    -0.0529
n(  2  3  5)     =    -0.3403
n(  2  3  5  6) =    -0.0269
n(  2  3  5  7) =    -0.0303
n(  2  3  5 10) =    -0.0230
n(  2  3  5 11) =    -0.0264
n(  2  3  6)     =     0.0430
n(  2  3  6 12) =     0.0292
n(  2  3  7)     =     0.0151
n(  2  3 10)     =    -0.0298
n(  2  3 10 12) =    -0.0121
n(  2  3 11)     =    -0.0248
n(  2  3 12)     =     0.0125
n(  2  4  5)     =    -0.0282
n(  2  4  5 11) =    -0.0101
n(  2  4  6)     =    -0.0136
n(  2  4  8)     =     0.0486
n(  2  4  8  9) =     0.0109
n(  2  4  8 12) =     0.0244
n(  2  4  9)     =     0.0501
n(  2  4 12)     =     0.0142
```

```
n(  2  4 16)     =     0.0119
n(  2  4 17)     =     0.0102
n(  2  5  6)     =    -0.0339
n(  2  5  6 12) =    -0.0127
n(  2  5  7)     =    -0.0285
n(  2  5 10)     =     0.0447
n(  2  5 10 12) =     0.0283
n(  2  5 11)     =     0.0236
n(  2  5 12)     =     0.0127
n(  2  6 12)     =     0.0185
n(  2  8  9)     =     0.0116
n(  2  8 12)     =     0.0182
n(  2 10 12)     =     0.0184
n(  2 12 22)     =    -0.0268
n(  3  6  7)     =     0.0299
n(  3  6  7 13) =     0.0599
n(  3  6  7 14) =     0.0340
n(  3  6 12)     =     0.0313
n(  3  6 12 22) =    -0.0114
n(  3  6 13 14) =     0.0336
n(  3  6 13 23) =    -0.0103
n(  3  7 13)     =    -0.0193
n(  3  7 14)     =    -0.0573
n(  3 12 22)     =    -0.0112
n(  3 13 23)     =    -0.0106
n(  3 14 24)     =    -0.0124
n(  4  8  9)     =     0.0299
n(  4  8  9 16) =     0.0600
n(  4  8  9 17) =     0.0340
n(  4  8 12)     =     0.0314
n(  4  8 12 22) =    -0.0114
n(  4  8 16 17) =     0.0335
n(  4  8 16 25) =    -0.0103
n(  4  9 16)     =    -0.0190
n(  4  9 17)     =    -0.0571
n(  4 12 22)     =    -0.0113
n(  4 16 25)     =    -0.0106
n(  4 17 26)     =    -0.0125
n(  5 10 11)     =     0.0300
n(  5 10 11 19) =     0.0600
n(  5 10 11 21) =     0.0340
n(  5 10 12)     =     0.0313
n(  5 10 12 22) =    -0.0114
n(  5 10 19 21) =     0.0335
n(  5 10 19 27) =    -0.0103
n(  5 11 19)     =    -0.0191
n(  5 11 21)     =    -0.0573
n(  5 12 22)     =    -0.0113
n(  5 19 27)     =    -0.0106
n(  5 21 28)     =    -0.0124
n(  6  7 13)     =     0.0201
n(  6  7 13 14) =     0.0349
n(  6  7 14)     =     0.0101
n(  6  8 12)     =    -0.0480
n(  6 10 12)     =    -0.0481
n(  6 12 13)     =     0.0234
n(  6 13 14)     =    -0.0161
n(  6 14 24)     =    -0.0128
n(  7 13 14)     =     0.0761
n(  7 13 14 23) =    -0.0151
n(  7 13 23)     =    -0.0179
n(  8  9 16)     =     0.0198
n(  8  9 16 17) =     0.0346
n(  8  9 17)     =     0.0101
```

```
 n(  8 10 12)     =    -0.0477
 n(  8 12 16)     =     0.0236
 n(  8 16 17)     =    -0.0165
 n(  8 17 26)     =    -0.0128
 n(  9 16 17)     =     0.0763
 n(  9 16 17 25) =    -0.0150
 n(  9 16 25)     =    -0.0180
 n( 10 11 19)     =     0.0200
 n( 10 11 19 21) =     0.0349
 n( 10 11 21)     =     0.0101
 n( 10 12 19)     =     0.0234
 n( 10 19 21)     =    -0.0163
 n( 10 21 28)     =    -0.0128
 n( 11 19 21)     =     0.0763
 n( 11 19 21 27) =    -0.0151
 n( 11 19 27)     =    -0.0180

 multicenter rest contribution =  0.199548 (correct sign for five center
terms)

*************************************************************************
*                                                                       *
*              atomic charges with multicenter corrections              *
*                                                                       *
*************************************************************************
```

atom	charge
1 cl	-0.8289
2 be	0.4249
3 n	0.0687
4 n	0.3056
5 n	0.1230
6 n	0.2247
7 c	-0.0802
8 n	0.2297
9 c	-0.0707
10 n	0.2263
11 c	-0.0793
12 b	-0.4073
13 c	-0.0544
14 c	-0.1593
15 h	0.0631
16 c	-0.0494
17 c	-0.1546
18 h	0.0643
19 c	-0.0532
20 h	0.0630
21 c	-0.1582
22 h	-0.0159
23 h	0.0556
24 h	0.0507
25 h	0.0554
26 h	0.0505
27 h	0.0554
28 h	0.0508

```
 moments (from total density versus population analysis)
 <charge> =            -0.000000           -0.000000
```

```
 <x   >   =             0.133784          -0.038683
 <y   >   =            -0.836323          -0.666662
 <z   >   =            -1.954221          -3.333141


================================================================================
=

TpBeBr:
************************************************************************
*                                                                      *
*                        shared electron numbers                       *
*                                                                      *
************************************************************************


 TWO center shared electron numbers ge 0.1000E-01 :
  shared electron number for the pair       1 br -   2 be  =     0.0473
  shared electron number for the pair       2 be -   3 n   =     0.3380
  shared electron number for the pair       2 be -   4 n   =     1.0115
  shared electron number for the pair       2 be -   5 n   =     0.5864
  shared electron number for the pair       2 be -   6 n   =     0.0379
  shared electron number for the pair       2 be -   7 c   =     0.0130
  shared electron number for the pair       2 be -   8 n   =     0.0482
  shared electron number for the pair       2 be -   9 c   =     0.0448
  shared electron number for the pair       2 be -  10 n   =     0.0427
  shared electron number for the pair       2 be -  11 c   =     0.0267
  shared electron number for the pair       2 be -  12 b   =     0.0469
  shared electron number for the pair       2 be -  16 c   =     0.0113
  shared electron number for the pair       2 be -  18 c   =     0.0100
  shared electron number for the pair       3 n  -   6 n   =     1.3199
  shared electron number for the pair       3 n  -   7 c   =     1.6577
  shared electron number for the pair       3 n  -  12 b   =     0.0351
  shared electron number for the pair       3 n  -  14 h   =     0.0136
  shared electron number for the pair       3 n  -  15 c   =     0.0151
  shared electron number for the pair       4 n  -   8 n   =     1.3200
  shared electron number for the pair       4 n  -   9 c   =     1.6580
  shared electron number for the pair       4 n  -  12 b   =     0.0351
  shared electron number for the pair       4 n  -  17 h   =     0.0137
```

```
shared electron number for the pair      4 n  -  18 c   =    0.0152
shared electron number for the pair      5 n  -  10 n   =    1.3201
shared electron number for the pair      5 n  -  11 c   =    1.6576
shared electron number for the pair      5 n  -  12 b   =    0.0350
shared electron number for the pair      5 n  -  20 h   =    0.0137
shared electron number for the pair      5 n  -  21 c   =    0.0152
shared electron number for the pair      6 n  -   7 c   =    0.0161
shared electron number for the pair      6 n  -   8 n   =    0.0119
shared electron number for the pair      6 n  -  10 n   =    0.0119
shared electron number for the pair      6 n  -  12 b   =    1.2345
shared electron number for the pair      6 n  -  13 c   =    1.6413
shared electron number for the pair      6 n  -  15 c   =    0.0173
shared electron number for the pair      6 n  -  22 h   =    0.0121
shared electron number for the pair      7 c  -  13 c   =    0.0844
shared electron number for the pair      7 c  -  14 h   =    1.3794
shared electron number for the pair      7 c  -  15 c   =    1.7990
shared electron number for the pair      8 n  -   9 c   =    0.0160
shared electron number for the pair      8 n  -  10 n   =    0.0119
shared electron number for the pair      8 n  -  12 b   =    1.2343
shared electron number for the pair      8 n  -  16 c   =    1.6412
shared electron number for the pair      8 n  -  18 c   =    0.0173
shared electron number for the pair      8 n  -  22 h   =    0.0121
shared electron number for the pair      9 c  -  16 c   =    0.0844
shared electron number for the pair      9 c  -  17 h   =    1.3794
shared electron number for the pair      9 c  -  18 c   =    1.7990
shared electron number for the pair     10 n  -  11 c   =    0.0162
shared electron number for the pair     10 n  -  12 b   =    1.2341
shared electron number for the pair     10 n  -  19 c   =    1.6412
shared electron number for the pair     10 n  -  21 c   =    0.0174
shared electron number for the pair     10 n  -  22 h   =    0.0121
shared electron number for the pair     11 c  -  19 c   =    0.0843
shared electron number for the pair     11 c  -  20 h   =    1.3792
```

```
  shared electron number for the pair      11 c  -  21 c   =     1.7990
  shared electron number for the pair      12 b  -  13 c   =     0.0294
  shared electron number for the pair      12 b  -  16 c   =     0.0294
  shared electron number for the pair      12 b  -  19 c   =     0.0293
  shared electron number for the pair      12 b  -  22 h   =     1.4274
  shared electron number for the pair      13 c  -  15 c   =     1.8549
  shared electron number for the pair      13 c  -  23 h   =     1.3792
  shared electron number for the pair      13 c  -  24 h   =     0.0125
  shared electron number for the pair      14 h  -  15 c   =     0.0120
  shared electron number for the pair      15 c  -  24 h   =     1.3867
  shared electron number for the pair      16 c  -  18 c   =     1.8550
  shared electron number for the pair      16 c  -  25 h   =     1.3791
  shared electron number for the pair      16 c  -  26 h   =     0.0125
  shared electron number for the pair      17 h  -  18 c   =     0.0121
  shared electron number for the pair      18 c  -  26 h   =     1.3867
  shared electron number for the pair      19 c  -  21 c   =     1.8550
  shared electron number for the pair      19 c  -  27 h   =     1.3793
  shared electron number for the pair      19 c  -  28 h   =     0.0125
  shared electron number for the pair      20 h  -  21 c   =     0.0121
  shared electron number for the pair      21 c  -  28 h   =     1.3868

**************************************************************************
*                                                                        *
*              atomic charges with multicenter corrections               *
*              AS RESULTING FROM 2-CENTER SEN CONTRIBUTIONS              *
*                                                                        *
**************************************************************************

                        -------------------------
                          atom   |     charge
                        -------------------------
                           1 br  |   -0.8584
                           2 be  |    0.3552
                           3 n   |   -0.0717
                           4 n   |    0.2651
                           5 n   |    0.0534
                           6 n   |    0.2194
                           7 c   |   -0.0622
                           8 n   |    0.2247
                           9 c   |   -0.0458
                          10 n   |    0.2212
                          11 c   |   -0.0554
                          12 b   |   -0.3660
                          13 c   |   -0.0347
```

```
                          14 h   |    0.0837
                          15 c   |   -0.1502
                          16 c   |   -0.0308
                          17 h   |    0.0854
                          18 c   |   -0.1473
                          19 c   |   -0.0325
                          20 h   |    0.0848
                          21 c   |   -0.1488
                          22 h   |   -0.0014
                          23 h   |    0.0708
                          24 h   |    0.0667
                          25 h   |    0.0708
                          26 h   |    0.0667
                          27 h   |    0.0708
                          28 h   |    0.0665
                        -------------------------

THREE and FOUR center SEN greater than 0.010:

n(  1  2  3  5) =     0.0253
n(  1  2  4)    =    -0.0500
n(  1  2  5)    =    -0.0230
n(  2  3  4)    =    -0.0811
n(  2  3  4  6) =    -0.0114
n(  2  3  5)    =    -0.3221
n(  2  3  5  6) =    -0.0263
n(  2  3  5  7) =    -0.0274
n(  2  3  5 10) =    -0.0188
n(  2  3  5 11) =    -0.0206
n(  2  3  6)    =     0.0392
n(  2  3  6 12) =     0.0273
n(  2  3  7)    =     0.0114
n(  2  3 10)    =    -0.0240
n(  2  3 11)    =    -0.0201
n(  2  3 12)    =     0.0133
n(  2  4  5)    =    -0.0348
n(  2  4  5 11) =    -0.0130
n(  2  4  6)    =    -0.0149
n(  2  4  8)    =     0.0472
n(  2  4  8  9) =     0.0109
n(  2  4  8 12) =     0.0232
n(  2  4  9)    =     0.0447
n(  2  4 11)    =    -0.0120
n(  2  4 12)    =     0.0157
n(  2  4 16)    =     0.0106
n(  2  5  6)    =    -0.0317
n(  2  5  6 12) =    -0.0106
n(  2  5  7)    =    -0.0263
n(  2  5 10)    =     0.0435
n(  2  5 10 12) =     0.0260
n(  2  5 11)    =     0.0260
n(  2  5 12)    =     0.0133
n(  2  6 12)    =     0.0167
n(  2  8  9)    =     0.0115
n(  2  8 12)    =     0.0165
n(  2 10 12)    =     0.0168
n(  2 12 22)    =    -0.0270
n(  3  6  7)    =     0.0307
n(  3  6  7 13) =     0.0602
n(  3  6  7 15) =     0.0337
n(  3  6 12)    =     0.0301
n(  3  6 12 22) =    -0.0121
n(  3  6 13 15) =     0.0331
n(  3  6 13 23) =    -0.0100
```

```
 n(  3  7 13)     =    -0.0201
 n(  3  7 15)     =    -0.0590
 n(  3 12 22)     =    -0.0117
 n(  3 13 23)     =    -0.0105
 n(  3 15 24)     =    -0.0125
 n(  4  8  9)     =     0.0306
 n(  4  8  9 16) =     0.0602
 n(  4  8  9 18) =     0.0337
 n(  4  8 12)     =     0.0302
 n(  4  8 12 22) =    -0.0122
 n(  4  8 16 18) =     0.0332
 n(  4  9 16)     =    -0.0200
 n(  4  9 18)     =    -0.0587
 n(  4 12 22)     =    -0.0118
 n(  4 16 25)     =    -0.0105
 n(  4 18 26)     =    -0.0126
 n(  5 10 11)     =     0.0307
 n(  5 10 11 19) =     0.0601
 n(  5 10 11 21) =     0.0337
 n(  5 10 12)     =     0.0301
 n(  5 10 12 22) =    -0.0121
 n(  5 10 19 21) =     0.0332
 n(  5 10 19 27) =    -0.0100
 n(  5 11 19)     =    -0.0203
 n(  5 11 21)     =    -0.0590
 n(  5 12 22)     =    -0.0117
 n(  5 19 27)     =    -0.0105
 n(  5 21 28)     =    -0.0125
 n(  6  7 13)     =     0.0201
 n(  6  7 13 15) =     0.0352
 n(  6  7 15)     =     0.0104
 n(  6  8 12)     =    -0.0472
 n(  6 10 12)     =    -0.0474
 n(  6 12 13)     =     0.0233
 n(  6 13 15)     =    -0.0163
 n(  6 15 24)     =    -0.0128
 n(  7 13 15)     =     0.0779
 n(  7 13 15 23) =    -0.0151
 n(  7 13 23)     =    -0.0179
 n(  8  9 16)     =     0.0200
 n(  8  9 16 18) =     0.0351
 n(  8  9 18)     =     0.0104
 n(  8 10 12)     =    -0.0473
 n(  8 12 16)     =     0.0234
 n(  8 16 18)     =    -0.0163
 n(  8 18 26)     =    -0.0128
 n(  9 16 18)     =     0.0778
 n(  9 16 18 25) =    -0.0150
 n(  9 16 25)     =    -0.0178
 n( 10 11 19)     =     0.0202
 n( 10 11 19 21) =     0.0353
 n( 10 11 21)     =     0.0104
 n( 10 12 19)     =     0.0232
 n( 10 19 21)     =    -0.0160
 n( 10 21 28)     =    -0.0128
 n( 11 19 21)     =     0.0777
 n( 11 19 21 27) =    -0.0150
 n( 11 19 27)     =    -0.0178

 multicenter rest contribution =  0.199097 (correct sign for five center
terms)
```

```
**********************************************************************
*                                                                    *
*              atomic charges with multicenter corrections           *
*                                                                    *
**********************************************************************
```

atom	charge
1 br	-0.8345
2 be	0.4139
3 n	0.0510
4 n	0.3053
5 n	0.1634
6 n	0.2237
7 c	-0.0810
8 n	0.2276
9 c	-0.0715
10 n	0.2250
11 c	-0.0788
12 b	-0.4079
13 c	-0.0537
14 h	0.0628
15 c	-0.1589
16 c	-0.0490
17 h	0.0638
18 c	-0.1552
19 c	-0.0515
20 h	0.0628
21 c	-0.1575
22 h	-0.0162
23 h	0.0552
24 h	0.0508
25 h	0.0549
26 h	0.0504
27 h	0.0551
28 h	0.0503

```
 moments (from total density versus population analysis)
 <charge> =            -0.000000           -0.000000
 <x   >   =             0.171637           -0.341487
 <y   >   =            -0.984463           -1.174769
 <z   >   =            -2.114978           -3.479775


======================================================================
=

TpBeI:
**********************************************************************
*                                                                    *
*                        shared electron numbers                     *
*                                                                    *
**********************************************************************


 TWO center shared electron numbers ge 0.1000E-01 :

  shared electron number for the pair       1 i  -   2 be  =     0.0439
```

```
shared electron number for the pair      2 be -   3 n   =     0.8117
shared electron number for the pair      2 be -   4 n   =     0.2899
shared electron number for the pair      2 be -   5 n   =     0.8113
shared electron number for the pair      2 be -   6 n   =     0.0498
shared electron number for the pair      2 be -   7 c   =     0.0361
shared electron number for the pair      2 be -   8 n   =     0.0408
shared electron number for the pair      2 be -  10 n   =     0.0498
shared electron number for the pair      2 be -  11 c   =     0.0362
shared electron number for the pair      2 be -  12 b   =     0.0526
shared electron number for the pair      3 n  -   6 n   =     1.3136
shared electron number for the pair      3 n  -   7 c   =     1.6527
shared electron number for the pair      3 n  -  12 b   =     0.0354
shared electron number for the pair      3 n  -  14 h   =     0.0135
shared electron number for the pair      3 n  -  15 c   =     0.0148
shared electron number for the pair      4 n  -   8 n   =     1.3134
shared electron number for the pair      4 n  -   9 c   =     1.6530
shared electron number for the pair      4 n  -  12 b   =     0.0356
shared electron number for the pair      4 n  -  17 h   =     0.0135
shared electron number for the pair      4 n  -  18 c   =     0.0148
shared electron number for the pair      5 n  -  10 n   =     1.3134
shared electron number for the pair      5 n  -  11 c   =     1.6533
shared electron number for the pair      5 n  -  12 b   =     0.0355
shared electron number for the pair      5 n  -  20 h   =     0.0135
shared electron number for the pair      5 n  -  21 c   =     0.0148
shared electron number for the pair      6 n  -   7 c   =     0.0163
shared electron number for the pair      6 n  -   8 n   =     0.0117
shared electron number for the pair      6 n  -  10 n   =     0.0117
shared electron number for the pair      6 n  -  12 b   =     1.2319
shared electron number for the pair      6 n  -  13 c   =     1.6417
shared electron number for the pair      6 n  -  15 c   =     0.0174
shared electron number for the pair      6 n  -  22 h   =     0.0121
shared electron number for the pair      7 c  -  13 c   =     0.0849
```

```
shared electron number for the pair      7 c  -  14 h   =    1.3787
shared electron number for the pair      7 c  -  15 c   =    1.7993
shared electron number for the pair      8 n  -   9 c   =    0.0163
shared electron number for the pair      8 n  -  10 n   =    0.0117
shared electron number for the pair      8 n  -  12 b   =    1.2315
shared electron number for the pair      8 n  -  16 c   =    1.6416
shared electron number for the pair      8 n  -  18 c   =    0.0173
shared electron number for the pair      8 n  -  22 h   =    0.0121
shared electron number for the pair      9 c  -  16 c   =    0.0852
shared electron number for the pair      9 c  -  17 h   =    1.3790
shared electron number for the pair      9 c  -  18 c   =    1.7998
shared electron number for the pair     10 n  -  11 c   =    0.0163
shared electron number for the pair     10 n  -  12 b   =    1.2325
shared electron number for the pair     10 n  -  19 c   =    1.6417
shared electron number for the pair     10 n  -  21 c   =    0.0173
shared electron number for the pair     10 n  -  22 h   =    0.0121
shared electron number for the pair     11 c  -  19 c   =    0.0851
shared electron number for the pair     11 c  -  20 h   =    1.3789
shared electron number for the pair     11 c  -  21 c   =    1.7994
shared electron number for the pair     12 b  -  13 c   =    0.0294
shared electron number for the pair     12 b  -  16 c   =    0.0295
shared electron number for the pair     12 b  -  19 c   =    0.0295
shared electron number for the pair     12 b  -  22 h   =    1.4251
shared electron number for the pair     13 c  -  15 c   =    1.8542
shared electron number for the pair     13 c  -  23 h   =    1.3788
shared electron number for the pair     13 c  -  24 h   =    0.0125
shared electron number for the pair     14 h  -  15 c   =    0.0118
shared electron number for the pair     15 c  -  24 h   =    1.3866
shared electron number for the pair     16 c  -  18 c   =    1.8544
shared electron number for the pair     16 c  -  25 h   =    1.3789
shared electron number for the pair     16 c  -  26 h   =    0.0124
shared electron number for the pair     17 h  -  18 c   =    0.0118
```

```
  shared electron number for the pair      18 c  -  26 h   =     1.3866

  shared electron number for the pair      19 c  -  21 c   =     1.8543

  shared electron number for the pair      19 c  -  27 h   =     1.3788

  shared electron number for the pair      19 c  -  28 h   =     0.0124

  shared electron number for the pair      20 h  -  21 c   =     0.0118

  shared electron number for the pair      21 c  -  28 h   =     1.3864

*************************************************************************
*                                                                       *
*              atomic charges with multicenter corrections              *
*              AS RESULTING FROM 2-CENTER SEN CONTRIBUTIONS             *
*                                                                       *
*************************************************************************
```

atom	charge
1 i	-0.8408
2 be	0.3421
3 n	0.1636
4 n	-0.0975
5 n	0.1641
6 n	0.2235
7 c	-0.0489
8 n	0.2194
9 c	-0.0620
10 n	0.2239
11 c	-0.0485
12 b	-0.3672
13 c	-0.0299
14 h	0.0843
15 c	-0.1466
16 c	-0.0334
17 h	0.0824
18 c	-0.1491
19 c	-0.0301
20 h	0.0837
21 c	-0.1466
22 h	-0.0013
23 h	0.0713
24 h	0.0668
25 h	0.0709
26 h	0.0672
27 h	0.0712
28 h	0.0673

```
 THREE and FOUR center SEN greater than 0.010:

 n(  1  2  3)     =    -0.0391
 n(  1  2  3  4) =     0.0212
 n(  1  2  4  5) =     0.0204
 n(  1  2  5)     =    -0.0370
 n(  2  3  4)     =    -0.2024
 n(  2  3  4  5) =    -0.0254
 n(  2  3  4  6) =    -0.0114
 n(  2  3  4  8) =    -0.0229
 n(  2  3  4  9) =    -0.0178
```

```
n(  2  3  5)     =    -0.0605
n(  2  3  5  7) =    -0.0158
n(  2  3  5 11) =    -0.0159
n(  2  3  6)     =     0.0483
n(  2  3  6 12) =     0.0260
n(  2  3  7)     =     0.0354
n(  2  3  8)     =    -0.0287
n(  2  3  8 12) =    -0.0117
n(  2  3  9)     =    -0.0166
n(  2  3 11)     =    -0.0156
n(  2  3 12)     =     0.0143
n(  2  4  5)     =    -0.2053
n(  2  4  5  8) =    -0.0232
n(  2  4  5  9) =    -0.0180
n(  2  4  5 10) =    -0.0115
n(  2  4  6)     =    -0.0164
n(  2  4  8)     =     0.0410
n(  2  4  8 12) =     0.0293
n(  2  4 10)     =    -0.0165
n(  2  4 12)     =     0.0137
n(  2  5  7)     =    -0.0155
n(  2  5  8)     =    -0.0290
n(  2  5  8 12) =    -0.0119
n(  2  5  9)     =    -0.0168
n(  2  5 10)     =     0.0483
n(  2  5 10 12) =     0.0260
n(  2  5 11)     =     0.0355
n(  2  5 12)     =     0.0141
n(  2  6  7)     =     0.0103
n(  2  6 12)     =     0.0186
n(  2  8 12)     =     0.0183
n(  2 10 11)     =     0.0102
n(  2 10 12)     =     0.0186
n(  2 12 22)     =    -0.0283
n(  3  6  7)     =     0.0309
n(  3  6  7 13) =     0.0601
n(  3  6  7 15) =     0.0332
n(  3  6 12)     =     0.0299
n(  3  6 12 22) =    -0.0123
n(  3  6 13 15) =     0.0329
n(  3  7 13)     =    -0.0218
n(  3  7 15)     =    -0.0606
n(  3 12 22)     =    -0.0119
n(  3 13 23)     =    -0.0106
n(  3 15 24)     =    -0.0127
n(  4  8  9)     =     0.0309
n(  4  8  9 16) =     0.0602
n(  4  8  9 18) =     0.0332
n(  4  8 12)     =     0.0300
n(  4  8 12 22) =    -0.0123
n(  4  8 16 18) =     0.0328
n(  4  9 16)     =    -0.0216
n(  4  9 18)     =    -0.0605
n(  4 12 22)     =    -0.0120
n(  4 16 25)     =    -0.0106
n(  4 18 26)     =    -0.0127
n(  5 10 11)     =     0.0310
n(  5 10 11 19) =     0.0602
n(  5 10 11 21) =     0.0332
n(  5 10 12)     =     0.0299
n(  5 10 12 22) =    -0.0124
n(  5 10 19 21) =     0.0328
n(  5 11 19)     =    -0.0214
n(  5 11 21)     =    -0.0603
```

```
 n(  5 12 22)     =    -0.0120
 n(  5 19 27)     =    -0.0105
 n(  5 21 28)     =    -0.0127
 n(  6  7 13)     =     0.0201
 n(  6  7 13 15) =     0.0351
 n(  6  7 15)     =     0.0105
 n(  6  8 12)     =    -0.0481
 n(  6 10 12)     =    -0.0474
 n(  6 12 13)     =     0.0232
 n(  6 13 15)     =    -0.0165
 n(  6 15 24)     =    -0.0129
 n(  7 13 15)     =     0.0792
 n(  7 13 15 23) =    -0.0151
 n(  7 13 23)     =    -0.0179
 n(  8  9 16)     =     0.0198
 n(  8  9 16 18) =     0.0348
 n(  8  9 18)     =     0.0105
 n(  8 10 12)     =    -0.0480
 n(  8 12 16)     =     0.0233
 n(  8 16 18)     =    -0.0170
 n(  8 18 26)     =    -0.0129
 n(  9 16 18)     =     0.0796
 n(  9 16 18 25) =    -0.0150
 n(  9 16 25)     =    -0.0179
 n( 10 11 19)     =     0.0199
 n( 10 11 19 21) =     0.0348
 n( 10 11 21)     =     0.0105
 n( 10 12 19)     =     0.0233
 n( 10 19 21)     =    -0.0169
 n( 10 21 28)     =    -0.0129
 n( 11 19 21)     =     0.0795
 n( 11 19 21 27) =    -0.0150
 n( 11 19 27)     =    -0.0178

 multicenter rest contribution =  0.166862 (correct sign for five center
terms)

**************************************************************************
*                                                                        *
*              atomic charges with multicenter corrections               *
*                                                                        *
**************************************************************************

                        -------------------------
                           atom   |     charge
                        -------------------------
                            1 i   |   -0.8119
                            2 be  |    0.4026
                            3 n   |    0.2407
                            4 n   |    0.0222
                            5 n   |    0.2410
                            6 n   |    0.2256
                            7 c   |   -0.0743
                            8 n   |    0.2219
                            9 c   |   -0.0806
                           10 n   |    0.2261
                           11 c   |   -0.0741
                           12 b   |   -0.4105
                           13 c   |   -0.0489
                           14 h   |    0.0628
                           15 c   |   -0.1551
                           16 c   |   -0.0536
```

```
                          17 h   |    0.0624
                          18 c   |   -0.1585
                          19 c   |   -0.0492
                          20 h   |    0.0623
                          21 c   |   -0.1552
                          22 h   |   -0.0156
                          23 h   |    0.0557
                          24 h   |    0.0507
                          25 h   |    0.0556
                          26 h   |    0.0514
                          27 h   |    0.0556
                          28 h   |    0.0512
                        -------------------------

 moments (from total density versus population analysis)
 <charge> =             -0.000000            -0.000000
 <x   >   =              1.113576             1.067450
 <y   >   =              1.968224             3.061109
 <z   >   =              1.232492             2.237522


 ================================================================================
 =
```