# Supplementary Materials

## *First Examples of s-Metal Complexes with Subporphyrazine and Its Phenylene-Annulated Derivatives: DFT Calculations*

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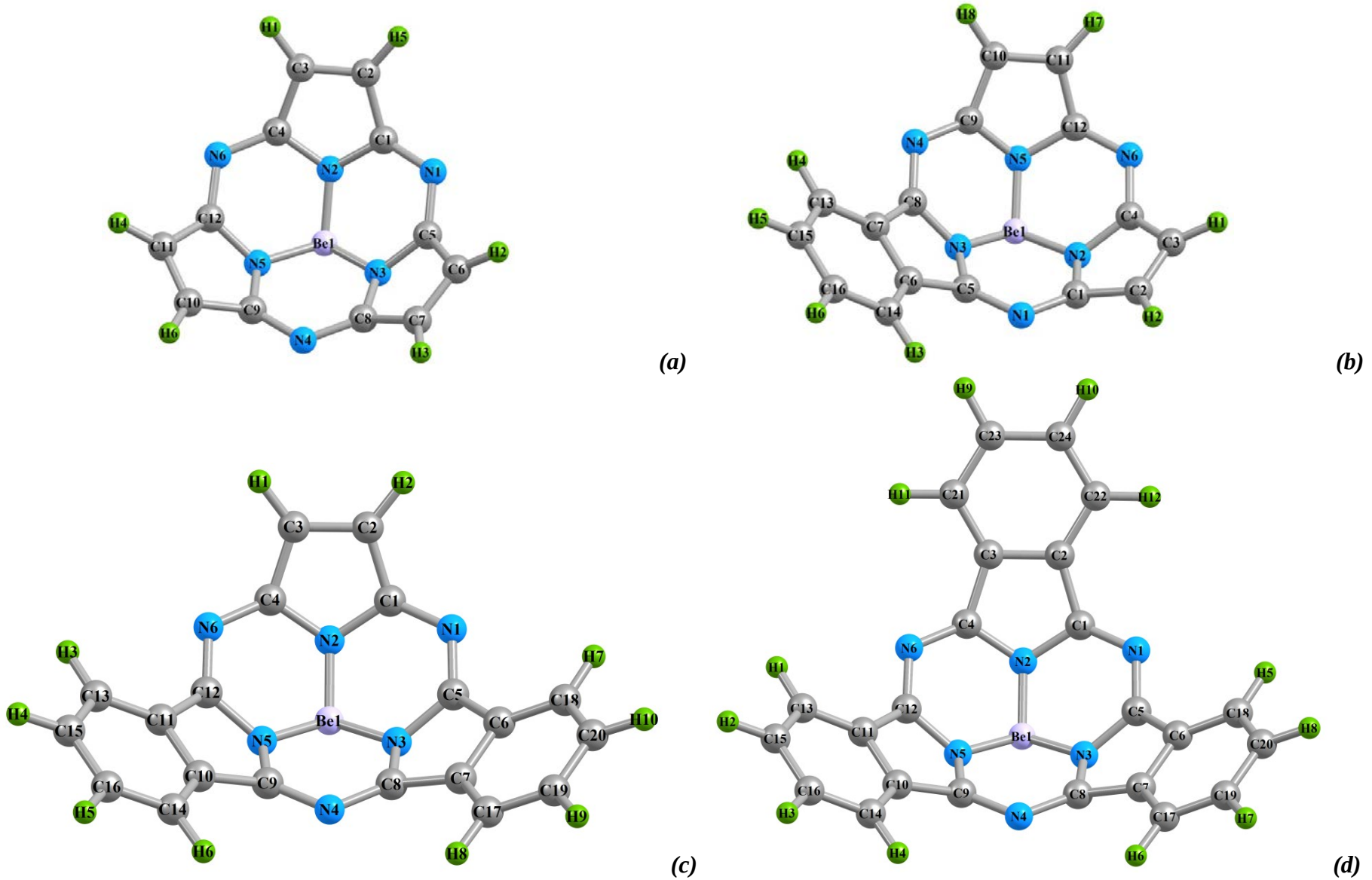



Figure S1. Molecular structures of the beryllium complexes with subporphyrazine and its mono-, di- and tri[benzo]-annelated derivatives obtained by using quantum-chemical calculation by DFT M062X/def2TZVP method: *a*: [Be**SP**], *b*: [Be**MBSP**], *c*: [Be**DBSP**], *d*: [Be**TBSP**].

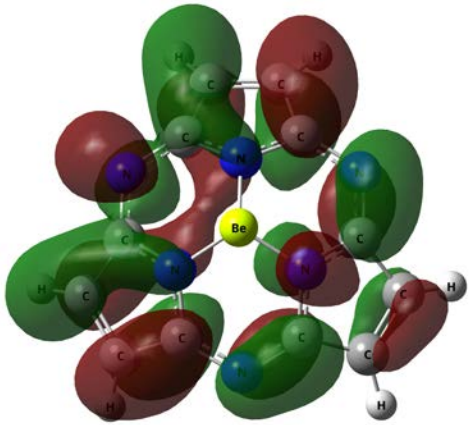
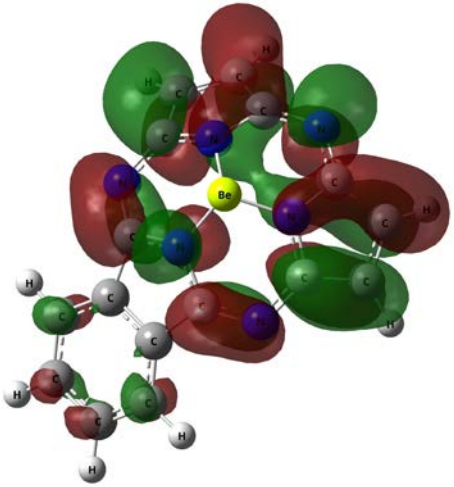
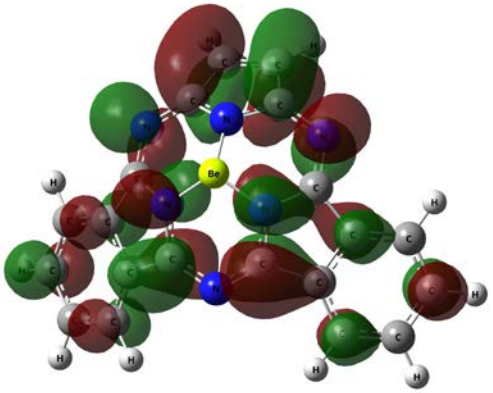
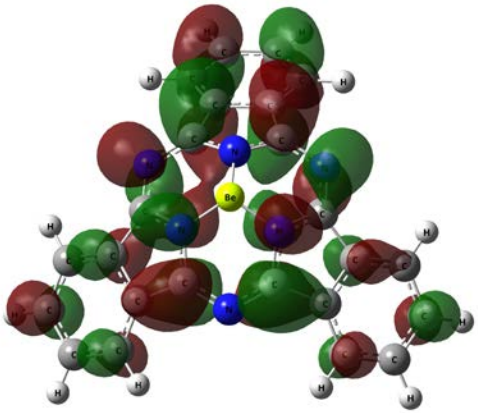
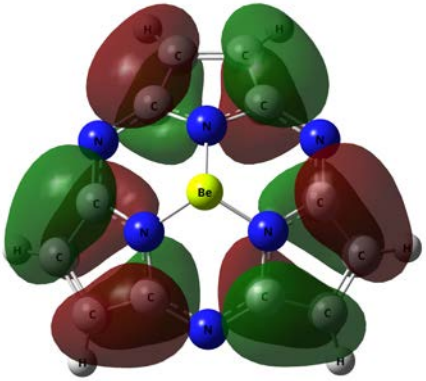
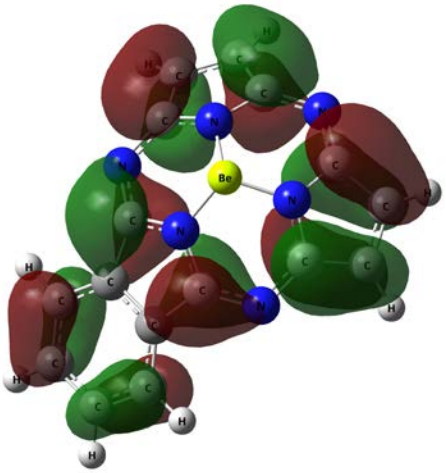
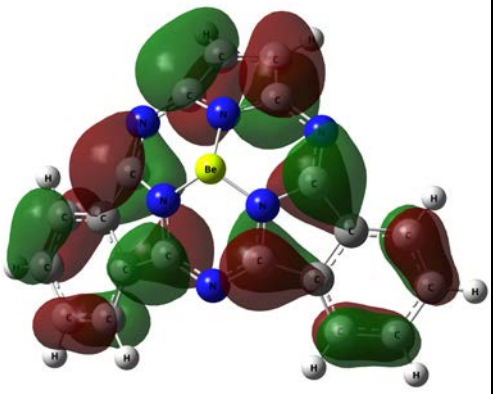
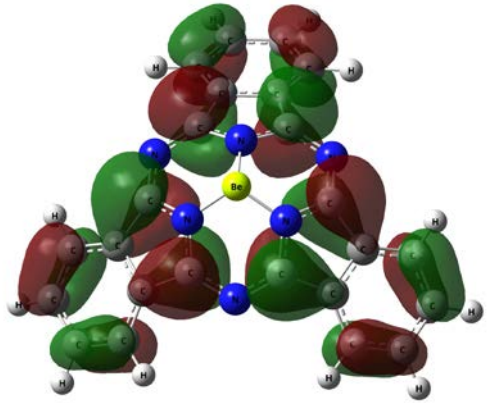
| | | | |
|---|---|---|---|
|  |  |  |  |
| LUMO (**-1.973**) | LUMO (**-2.050**) | LUMO (**-1.986**) | LUMO (**-1.814**) |
|  |  |  |  |
| HOMO (**-6.832**) | HOMO (**-6.592**) | HOMO (**-6.351**) | HOMO (**-6.037**) |
| [Be**SP**] | [Be**MBSP**] | [Be**DBSP**] | [Be**TBSP**] |

Figure S2. The pictures of HOMO and LUMO in the [Be**SP**], [Be**MBSP**], [Be**DBSP**] and [Be**TBSP**] complexes (ground state – spin singlet, $M_S$ = 1) according to the DFT M062X/def2TZVP method. The energies values of the given MOs (in brackets) are expressed in eV.

# NBO Analysis Data (Complex [BeSP])

**B3PW91/TZVP**

ΔE(multipl.=1) = 0.0 кДж/моль
ΔE(multipl.=3) = 159.0 кДж/моль
Alpha occupied eigenvalues (highest) = -6.1010262 eV
Alpha virtual eigenvalues (lowest)  = -2.8390914 eV

<S**2>= 0.0000

Summary of Natural Population Analysis:

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.40051 | 1.99932 | 5.38573 | 0.01545 | 7.40051 |
| C | 2 | 0.33186 | 1.99922 | 3.64473 | 0.02418 | 5.66814 |
| C | 3 | -0.22714 | 1.99910 | 4.21491 | 0.01313 | 6.22714 |
| N | 4 | -0.82790 | 1.99937 | 5.80616 | 0.02237 | 7.82790 |
| C | 5 | -0.22715 | 1.99910 | 4.21492 | 0.01313 | 6.22715 |
| C | 6 | 0.33183 | 1.99922 | 3.64476 | 0.02418 | 5.66817 |
| H | 7 | 0.23584 | 0.00000 | 0.76284 | 0.00132 | 0.76416 |
| C | 8 | 0.33186 | 1.99922 | 3.64473 | 0.02418 | 5.66814 |
| C | 9 | -0.22714 | 1.99910 | 4.21491 | 0.01313 | 6.22714 |
| N | 10 | -0.82790 | 1.99937 | 5.80616 | 0.02237 | 7.82790 |
| C | 11 | -0.22714 | 1.99910 | 4.21492 | 0.01313 | 6.22714 |
| H | 12 | 0.23584 | 0.00000 | 0.76284 | 0.00132 | 0.76416 |
| C | 13 | 0.33183 | 1.99922 | 3.64476 | 0.02418 | 5.66817 |
| H | 14 | 0.23584 | 0.00000 | 0.76284 | 0.00132 | 0.76416 |
| N | 15 | -0.40052 | 1.99932 | 5.38574 | 0.01545 | 7.40052 |
| C | 16 | 0.33186 | 1.99922 | 3.64473 | 0.02419 | 5.66814 |
| C | 17 | -0.22714 | 1.99910 | 4.21492 | 0.01313 | 6.22714 |
| N | 18 | -0.82788 | 1.99937 | 5.80613 | 0.02238 | 7.82788 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C | 19 | -0.22714 | 1.99910 | 4.21492 | 0.01313 | 6.22714 |
| C | 20 | 0.33186 | 1.99922 | 3.64473 | 0.02419 | 5.66814 |
| H | 21 | 0.23584 | 0.00000 | 0.76284 | 0.00132 | 0.76416 |
| H | 22 | 0.23584 | 0.00000 | 0.76284 | 0.00132 | 0.76416 |
| H | 23 | 0.23584 | 0.00000 | 0.76284 | 0.00132 | 0.76416 |
| N | 24 | -0.40052 | 1.99932 | 5.38574 | 0.01545 | 7.40052 |
| Be | 25 | 1.64193 | 1.99829 | 0.27451 | 0.08526 | 2.35807 |
| * Total * | | 0.00000 | 37.98429 | 85.58516 | 0.43055 | 124.00000 |

# NBO Analysis Data (Complex [BeSP])

**M062X/def2TZVP**

ΔE(multipl.=1) = 0.0 кДж/моль
ΔE(multipl.=3) = 157.3 кДж/моль
Alpha occupied eigenvalues (highest) = -6.832431 eV
Alpha virtual eigenvalues (lowest)  = -1.9729971 eV

<S**2>= 0.0000

Summary of Natural Population Analysis:

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.41569 | 1.99933 | 5.38657 | 0.02978 | 7.41569 |
| C | 2 | 0.34411 | 1.99924 | 3.63140 | 0.02525 | 5.65589 |
| C | 3 | -0.22676 | 1.99910 | 4.20912 | 0.01854 | 6.22676 |
| N | 4 | -0.84936 | 1.99935 | 5.81529 | 0.03471 | 7.84936 |
| C | 5 | -0.22676 | 1.99910 | 4.20912 | 0.01854 | 6.22676 |
| C | 6 | 0.34412 | 1.99924 | 3.63139 | 0.02525 | 5.65588 |
| H | 7 | 0.23553 | 0.00000 | 0.76340 | 0.00106 | 0.76447 |
| C | 8 | 0.34412 | 1.99924 | 3.63138 | 0.02525 | 5.65588 |
| C | 9 | -0.22673 | 1.99910 | 4.20908 | 0.01854 | 6.22673 |
| N | 10 | -0.84934 | 1.99935 | 5.81528 | 0.03471 | 7.84934 |
| C | 11 | -0.22677 | 1.99910 | 4.20912 | 0.01854 | 6.22677 |
| H | 12 | 0.23553 | 0.00000 | 0.76341 | 0.00106 | 0.76447 |
| C | 13 | 0.34412 | 1.99924 | 3.63138 | 0.02525 | 5.65588 |
| H | 14 | 0.23555 | 0.00000 | 0.76339 | 0.00106 | 0.76445 |
| N | 15 | -0.41567 | 1.99933 | 5.38655 | 0.02979 | 7.41567 |
| C | 16 | 0.34408 | 1.99924 | 3.63143 | 0.02525 | 5.65592 |
| C | 17 | -0.22676 | 1.99910 | 4.20911 | 0.01854 | 6.22676 |
| N | 18 | -0.84933 | 1.99935 | 5.81527 | 0.03471 | 7.84933 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C | 19 | -0.22677 | 1.99910 | 4.20912 | 0.01855 | 6.22677 |
| C | 20 | 0.34413 | 1.99924 | 3.63138 | 0.02525 | 5.65587 |
| H | 21 | 0.23553 | 0.00000 | 0.76341 | 0.00106 | 0.76447 |
| H | 22 | 0.23554 | 0.00000 | 0.76339 | 0.00106 | 0.76446 |
| H | 23 | 0.23554 | 0.00000 | 0.76340 | 0.00106 | 0.76446 |
| N | 24 | -0.41569 | 1.99933 | 5.38658 | 0.02978 | 7.41569 |
| Be | 25 | 1.67771 | 1.99831 | 0.25159 | 0.07239 | 2.32229 |
| * Total * | | 0.00000 | 37.98443 | 85.48055 | 0.53502 | 124.00000 |

# NBO Analysis Data (Complex [BeMBSP])

**B3PW91/TZVP**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 140.6 кДж/моль**
**Alpha occupied eigenvalues (highest) = -5.8360008 eV**
**Alpha virtual eigenvalues (lowest)  = -2.8627641 eV**

**<S**2>= 0.0000**

**Summary of Natural Population Analysis:**

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.41868 | 1.99932 | 5.40364 | 0.01571 | 7.41868 |
| C | 2 | 0.33633 | 1.99921 | 3.64022 | 0.02424 | 5.66367 |
| C | 3 | -0.24131 | 1.99910 | 4.22894 | 0.01327 | 6.24131 |
| N | 4 | -0.82837 | 1.99937 | 5.80597 | 0.02302 | 7.82837 |
| C | 5 | -0.22278 | 1.99911 | 4.21023 | 0.01344 | 6.22278 |
| C | 6 | 0.31369 | 1.99921 | 3.66265 | 0.02445 | 5.68631 |
| H | 7 | 0.23456 | 0.00000 | 0.76396 | 0.00147 | 0.76544 |
| C | 8 | 0.37509 | 1.99918 | 3.60137 | 0.02435 | 5.62491 |
| C | 9 | -0.07896 | 1.99904 | 4.06272 | 0.01721 | 6.07896 |
| N | 10 | -0.81001 | 1.99940 | 5.78594 | 0.02468 | 7.81001 |
| C | 11 | -0.07893 | 1.99904 | 4.06268 | 0.01720 | 6.07893 |
| C | 12 | 0.37501 | 1.99918 | 3.60145 | 0.02435 | 5.62499 |
| N | 13 | -0.41859 | 1.99932 | 5.40355 | 0.01571 | 7.41859 |
| C | 14 | 0.33616 | 1.99921 | 3.64039 | 0.02424 | 5.66384 |
| C | 15 | -0.24130 | 1.99910 | 4.22892 | 0.01327 | 6.24130 |
| N | 16 | -0.82830 | 1.99937 | 5.80590 | 0.02303 | 7.82830 |
| C | 17 | -0.22284 | 1.99911 | 4.21030 | 0.01344 | 6.22284 |
| C | 18 | 0.31364 | 1.99921 | 3.66271 | 0.02445 | 5.68636 |
| H | 19 | 0.23474 | 0.00000 | 0.76400 | 0.00126 | 0.76526 |

| | | | | | | |
|---|---|---|---|---|---|---|
| N | 20 | -0.38852 | 1.99933 | 5.37286 | 0.01633 | 7.38852 |
| Be | 21 | 1.64368 | 1.99828 | 0.27407 | 0.08397 | 2.35632 |
| C | 22 | -0.17479 | 1.99912 | 4.16181 | 0.01387 | 6.17479 |
| C | 23 | -0.17478 | 1.99912 | 4.16180 | 0.01387 | 6.17478 |
| C | 24 | -0.20118 | 1.99924 | 4.18786 | 0.01408 | 6.20118 |
| C | 25 | -0.20120 | 1.99924 | 4.18787 | 0.01408 | 6.20120 |
| H | 26 | 0.23124 | 0.00000 | 0.76717 | 0.00159 | 0.76876 |
| H | 27 | 0.23124 | 0.00000 | 0.76717 | 0.00159 | 0.76876 |
| H | 28 | 0.21793 | 0.00000 | 0.78095 | 0.00112 | 0.78207 |
| H | 29 | 0.21793 | 0.00000 | 0.78095 | 0.00112 | 0.78207 |
| H | 30 | 0.23455 | 0.00000 | 0.76398 | 0.00147 | 0.76545 |
| H | 31 | 0.23473 | 0.00000 | 0.76401 | 0.00126 | 0.76527 |
| * Total * | | -0.00000 | 45.98080 | 103.51605 | 0.50316 | 150.00000 |

# NBO Analysis Data (Complex [BeMBSP])

**M062X/Def2TZVP**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 138.9 кДж/моль**
**Alpha occupied eigenvalues (highest) = -6.5916225 eV**
**Alpha virtual eigenvalues (lowest)  = -2.0502735 eV**

**<S**2>= 0.0000**

**Summary of Natural Population Analysis:**

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.43831 | 1.99932 | 5.40905 | 0.02994 | 7.43831 |
| C | 2 | 0.35173 | 1.99922 | 3.62406 | 0.02499 | 5.64827 |
| C | 3 | -0.24691 | 1.99911 | 4.22945 | 0.01836 | 6.24691 |
| N | 4 | -0.84725 | 1.99935 | 5.81295 | 0.03494 | 7.84725 |
| C | 5 | -0.21750 | 1.99911 | 4.20008 | 0.01831 | 6.21750 |
| C | 6 | 0.31286 | 1.99922 | 3.66298 | 0.02493 | 5.68714 |
| H | 7 | 0.23411 | 0.00000 | 0.76483 | 0.00105 | 0.76589 |
| C | 8 | 0.39807 | 1.99921 | 3.57872 | 0.02399 | 5.60193 |
| C | 9 | -0.08215 | 1.99903 | 4.06278 | 0.02033 | 6.08215 |
| N | 10 | -0.83754 | 1.99938 | 5.80335 | 0.03480 | 7.83754 |
| C | 11 | -0.08221 | 1.99903 | 4.06284 | 0.02033 | 6.08221 |
| C | 12 | 0.39818 | 1.99921 | 3.57861 | 0.02400 | 5.60182 |
| N | 13 | -0.43838 | 1.99933 | 5.40913 | 0.02993 | 7.43838 |
| C | 14 | 0.35200 | 1.99922 | 3.62380 | 0.02498 | 5.64800 |
| C | 15 | -0.24691 | 1.99911 | 4.22944 | 0.01836 | 6.24691 |
| N | 16 | -0.84727 | 1.99935 | 5.81297 | 0.03495 | 7.84727 |
| C | 17 | -0.21733 | 1.99911 | 4.19991 | 0.01831 | 6.21733 |
| C | 18 | 0.31301 | 1.99922 | 3.66284 | 0.02493 | 5.68699 |

| | | | | | | |
|---|---|---|---|---|---|---|
| H | 19 | 0.23465 | 0.00000 | 0.76435 | 0.00100 | 0.76535 |
| N | 20 | -0.39211 | 1.99933 | 5.36274 | 0.03005 | 7.39211 |
| Be | 21 | 1.67885 | 1.99829 | 0.25108 | 0.07179 | 2.32115 |
| C | 22 | -0.17360 | 1.99913 | 4.15677 | 0.01770 | 6.17360 |
| C | 23 | -0.17362 | 1.99913 | 4.15679 | 0.01770 | 6.17362 |
| C | 24 | -0.19923 | 1.99926 | 4.18210 | 0.01788 | 6.19923 |
| C | 25 | -0.19920 | 1.99926 | 4.18207 | 0.01788 | 6.19920 |
| H | 26 | 0.23121 | 0.00000 | 0.76760 | 0.00119 | 0.76879 |
| H | 27 | 0.23122 | 0.00000 | 0.76760 | 0.00119 | 0.76878 |
| H | 28 | 0.21743 | 0.00000 | 0.78164 | 0.00094 | 0.78257 |
| H | 29 | 0.21743 | 0.00000 | 0.78164 | 0.00094 | 0.78257 |
| H | 30 | 0.23412 | 0.00000 | 0.76483 | 0.00105 | 0.76588 |
| H | 31 | 0.23467 | 0.00000 | 0.76433 | 0.00100 | 0.76533 |
| * Total * | | 0.00000 | 45.98094 | 103.41131 | 0.60775 | 150.00000 |

# NBO Analysis Data (Complex [BeDBSP])

**B3PW91/TZVP**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 131.1 кДж/моль**
**Alpha occupied eigenvalues (highest) = -5.5853967 eV**
**Alpha virtual eigenvalues (lowest)  = -2.7688896 eV**

**<S**2>= 0.0000**

**Summary of Natural Population Analysis:**

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.40452 | 1.99932 | 5.38929 | 0.01590 | 7.40452 |
| C | 2 | 0.31302 | 1.99918 | 3.66326 | 0.02454 | 5.68698 |
| C | 3 | -0.23894 | 1.99911 | 4.22624 | 0.01359 | 6.23894 |
| N | 4 | -0.82996 | 1.99938 | 5.80707 | 0.02351 | 7.82996 |
| C | 5 | -0.23894 | 1.99911 | 4.22624 | 0.01359 | 6.23894 |
| C | 6 | 0.31302 | 1.99918 | 3.66326 | 0.02454 | 5.68698 |
| H | 7 | 0.23303 | 0.00000 | 0.76552 | 0.00145 | 0.76697 |
| C | 8 | 0.35535 | 1.99918 | 3.62140 | 0.02407 | 5.64465 |
| C | 9 | -0.07355 | 1.99904 | 4.05748 | 0.01702 | 6.07355 |
| N | 10 | -0.80784 | 1.99940 | 5.78405 | 0.02439 | 7.80784 |
| C | 11 | -0.08622 | 1.99904 | 4.07010 | 0.01708 | 6.08622 |
| C | 12 | 0.38163 | 1.99917 | 3.59510 | 0.02410 | 5.61837 |
| N | 13 | -0.43648 | 1.99933 | 5.42130 | 0.01585 | 7.43648 |
| C | 14 | 0.38163 | 1.99917 | 3.59510 | 0.02410 | 5.61837 |
| C | 15 | -0.08622 | 1.99904 | 4.07010 | 0.01708 | 6.08622 |
| N | 16 | -0.80784 | 1.99940 | 5.78405 | 0.02439 | 7.80784 |
| C | 17 | -0.07355 | 1.99904 | 4.05748 | 0.01702 | 6.07355 |
| C | 18 | 0.35535 | 1.99918 | 3.62140 | 0.02407 | 5.64465 |

| | | | | | | |
|---|---|---|---|---|---|---|
| H | 19 | 0.23303 | 0.00000 | 0.76552 | 0.00145 | 0.76697 |
| N | 20 | -0.40452 | 1.99932 | 5.38929 | 0.01590 | 7.40452 |
| Be | 21 | 1.64514 | 1.99827 | 0.27351 | 0.08308 | 2.35486 |
| C | 22 | -0.17720 | 1.99912 | 4.16420 | 0.01388 | 6.17720 |
| C | 23 | -0.17355 | 1.99912 | 4.16061 | 0.01383 | 6.17355 |
| C | 24 | -0.19998 | 1.99924 | 4.18664 | 0.01410 | 6.19998 |
| C | 25 | -0.20570 | 1.99924 | 4.19229 | 0.01417 | 6.20570 |
| H | 26 | 0.23074 | 0.00000 | 0.76767 | 0.00159 | 0.76926 |
| H | 27 | 0.21727 | 0.00000 | 0.78161 | 0.00112 | 0.78273 |
| H | 28 | 0.21732 | 0.00000 | 0.78155 | 0.00113 | 0.78268 |
| H | 29 | 0.22979 | 0.00000 | 0.76860 | 0.00161 | 0.77021 |
| C | 30 | -0.17355 | 1.99912 | 4.16061 | 0.01383 | 6.17355 |
| C | 31 | -0.17720 | 1.99912 | 4.16420 | 0.01388 | 6.17720 |
| C | 32 | -0.20570 | 1.99924 | 4.19229 | 0.01417 | 6.20570 |
| C | 33 | -0.19998 | 1.99924 | 4.18664 | 0.01410 | 6.19998 |
| H | 34 | 0.23074 | 0.00000 | 0.76767 | 0.00159 | 0.76926 |
| H | 35 | 0.22979 | 0.00000 | 0.76860 | 0.00161 | 0.77021 |
| H | 36 | 0.21732 | 0.00000 | 0.78155 | 0.00113 | 0.78268 |
| H | 37 | 0.21727 | 0.00000 | 0.78161 | 0.00112 | 0.78273 |
| * Total * | | 0.00000 | 53.97730 | 121.45313 | 0.56957 | 176.00000 |

# NBO Analysis Data (Complex [BeDBSP])

**M062X/Def2TZVP**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 132.2 кДж/моль**
**Alpha occupied eigenvalues (highest) = -6.3508140 eV**
**Alpha virtual eigenvalues (lowest)  = -1.9860579 eV**

**<S**2>= 0.0000**

**Summary of Natural Population Analysis:**

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.41092 | 1.99932 | 5.38202 | 0.02959 | 7.41092 |
| C | 2 | 0.30806 | 1.99918 | 3.66775 | 0.02501 | 5.69194 |
| C | 3 | -0.24285 | 1.99911 | 4.22566 | 0.01807 | 6.24285 |
| N | 4 | -0.84751 | 1.99936 | 5.81317 | 0.03499 | 7.84751 |
| C | 5 | -0.24285 | 1.99911 | 4.22566 | 0.01807 | 6.24285 |
| C | 6 | 0.30806 | 1.99918 | 3.66775 | 0.02501 | 5.69194 |
| H | 7 | 0.23219 | 0.00000 | 0.76681 | 0.00100 | 0.76781 |
| C | 8 | 0.36745 | 1.99921 | 3.60961 | 0.02374 | 5.63255 |
| C | 9 | -0.07176 | 1.99904 | 4.05275 | 0.01997 | 6.07176 |
| N | 10 | -0.83274 | 1.99938 | 5.79891 | 0.03445 | 7.83274 |
| C | 11 | -0.09379 | 1.99904 | 4.07477 | 0.01999 | 6.09379 |
| C | 12 | 0.41520 | 1.99920 | 3.56177 | 0.02383 | 5.58480 |
| N | 13 | -0.46594 | 1.99933 | 5.43659 | 0.03002 | 7.46594 |
| C | 14 | 0.41520 | 1.99920 | 3.56177 | 0.02383 | 5.58480 |
| C | 15 | -0.09380 | 1.99904 | 4.07477 | 0.01999 | 6.09380 |
| N | 16 | -0.83274 | 1.99938 | 5.79891 | 0.03445 | 7.83274 |
| C | 17 | -0.07176 | 1.99904 | 4.05275 | 0.01997 | 6.07176 |
| C | 18 | 0.36745 | 1.99921 | 3.60961 | 0.02374 | 5.63255 |

| | | | | | | |
|---|---|---|---|---|---|---|
| H | 19 | 0.23219 | 0.00000 | 0.76681 | 0.00100 | 0.76781 |
| N | 20 | -0.41092 | 1.99932 | 5.38202 | 0.02959 | 7.41092 |
| Be | 21 | 1.67966 | 1.99828 | 0.25050 | 0.07156 | 2.32034 |
| C | 22 | -0.17718 | 1.99913 | 4.16033 | 0.01772 | 6.17718 |
| C | 23 | -0.17063 | 1.99913 | 4.15387 | 0.01763 | 6.17063 |
| C | 24 | -0.19562 | 1.99926 | 4.17851 | 0.01785 | 6.19562 |
| C | 25 | -0.20535 | 1.99925 | 4.18810 | 0.01799 | 6.20535 |
| H | 26 | 0.23095 | 0.00000 | 0.76787 | 0.00118 | 0.76905 |
| H | 27 | 0.21688 | 0.00000 | 0.78218 | 0.00094 | 0.78312 |
| H | 28 | 0.21706 | 0.00000 | 0.78199 | 0.00094 | 0.78294 |
| H | 29 | 0.22994 | 0.00000 | 0.76887 | 0.00120 | 0.77006 |
| C | 30 | -0.17063 | 1.99913 | 4.15387 | 0.01763 | 6.17063 |
| C | 31 | -0.17718 | 1.99913 | 4.16033 | 0.01772 | 6.17718 |
| C | 32 | -0.20535 | 1.99925 | 4.18810 | 0.01799 | 6.20535 |
| C | 33 | -0.19562 | 1.99926 | 4.17851 | 0.01785 | 6.19562 |
| H | 34 | 0.23095 | 0.00000 | 0.76787 | 0.00118 | 0.76905 |
| H | 35 | 0.22994 | 0.00000 | 0.76887 | 0.00120 | 0.77006 |
| H | 36 | 0.21706 | 0.00000 | 0.78199 | 0.00094 | 0.78294 |
| H | 37 | 0.21688 | 0.00000 | 0.78218 | 0.00094 | 0.78312 |
| * Total * | | 0.00000 | 53.97744 | 121.34383 | 0.67873 | 176.00000 |

# NBO Analysis Data (Complex [BeTBSP])

**B3PW91/TZVP**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 126.8 кДж/моль**
**Alpha occupied eigenvalues (highest) = -5.3307111 eV**
**Alpha virtual eigenvalues (lowest)  = -2.5936572 eV**

**<S**2>= 0.0000**

**Summary of Natural Population Analysis:**

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.42037 | 1.99932 | 5.40539 | 0.01566 | 7.42037 |
| C | 2 | 0.35652 | 1.99916 | 3.62035 | 0.02398 | 5.64348 |
| C | 3 | -0.08137 | 1.99904 | 4.06533 | 0.01700 | 6.08137 |
| N | 4 | -0.80603 | 1.99940 | 5.78250 | 0.02413 | 7.80603 |
| C | 5 | -0.08137 | 1.99904 | 4.06533 | 0.01700 | 6.08137 |
| C | 6 | 0.35653 | 1.99916 | 3.62033 | 0.02398 | 5.64347 |
| C | 7 | 0.35656 | 1.99916 | 3.62030 | 0.02398 | 5.64344 |
| C | 8 | -0.08135 | 1.99904 | 4.06531 | 0.01700 | 6.08135 |
| N | 9 | -0.80608 | 1.99940 | 5.78255 | 0.02413 | 7.80608 |
| C | 10 | -0.08138 | 1.99904 | 4.06534 | 0.01700 | 6.08138 |
| C | 11 | 0.35663 | 1.99916 | 3.62022 | 0.02398 | 5.64337 |
| N | 12 | -0.42043 | 1.99932 | 5.40545 | 0.01566 | 7.42043 |
| C | 13 | 0.35664 | 1.99916 | 3.62022 | 0.02398 | 5.64336 |
| C | 14 | -0.08138 | 1.99904 | 4.06533 | 0.01700 | 6.08138 |
| N | 15 | -0.80610 | 1.99940 | 5.78256 | 0.02413 | 7.80610 |
| C | 16 | -0.08135 | 1.99904 | 4.06531 | 0.01700 | 6.08135 |
| C | 17 | 0.35656 | 1.99916 | 3.62030 | 0.02398 | 5.64344 |
| N | 18 | -0.42037 | 1.99932 | 5.40540 | 0.01566 | 7.42037 |
| Be | 19 | 1.64686 | 1.99827 | 0.27268 | 0.08219 | 2.35314 |
| C | 20 | -0.17652 | 1.99912 | 4.16353 | 0.01387 | 6.17652 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C | 21 | -0.17651 | 1.99912 | 4.16352 | 0.01387 | 6.17651 |
| C | 22 | -0.20530 | 1.99924 | 4.19183 | 0.01422 | 6.20530 |
| C | 23 | -0.20531 | 1.99924 | 4.19184 | 0.01422 | 6.20531 |
| H | 24 | 0.22895 | 0.00000 | 0.76944 | 0.00161 | 0.77105 |
| H | 25 | 0.21642 | 0.00000 | 0.78245 | 0.00113 | 0.78358 |
| H | 26 | 0.21642 | 0.00000 | 0.78245 | 0.00113 | 0.78358 |
| H | 27 | 0.22895 | 0.00000 | 0.76944 | 0.00161 | 0.77105 |
| C | 28 | -0.17651 | 1.99912 | 4.16352 | 0.01387 | 6.17651 |
| C | 29 | -0.17652 | 1.99912 | 4.16354 | 0.01387 | 6.17652 |
| C | 30 | -0.20531 | 1.99924 | 4.19185 | 0.01422 | 6.20531 |
| C | 31 | -0.20530 | 1.99924 | 4.19183 | 0.01422 | 6.20530 |
| H | 32 | 0.22895 | 0.00000 | 0.76944 | 0.00161 | 0.77105 |
| H | 33 | 0.22895 | 0.00000 | 0.76943 | 0.00161 | 0.77105 |
| H | 34 | 0.21642 | 0.00000 | 0.78245 | 0.00113 | 0.78358 |
| H | 35 | 0.21642 | 0.00000 | 0.78245 | 0.00113 | 0.78358 |
| C | 36 | -0.17652 | 1.99912 | 4.16353 | 0.01387 | 6.17652 |
| C | 37 | -0.17652 | 1.99912 | 4.16353 | 0.01387 | 6.17652 |
| C | 38 | -0.20532 | 1.99924 | 4.19185 | 0.01422 | 6.20532 |
| H | 39 | 0.21642 | 0.00000 | 0.78245 | 0.00113 | 0.78358 |
| C | 40 | -0.20532 | 1.99924 | 4.19185 | 0.01422 | 6.20532 |
| H | 41 | 0.21642 | 0.00000 | 0.78245 | 0.00113 | 0.78358 |
| H | 42 | 0.22895 | 0.00000 | 0.76944 | 0.00161 | 0.77105 |
| H | 43 | 0.22895 | 0.00000 | 0.76944 | 0.00161 | 0.77105 |
| * Total * | | -0.00000 | 61.97385 | 139.39376 | 0.63239 | 202.00000 |

# NBO Analysis Data (Complex [BeDBSP])

**M062X/Def2TZVP**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 128.3 кДж/моль**
**Alpha occupied eigenvalues (highest) = -6.0368106 eV**
**Alpha virtual eigenvalues (lowest)  = -1.8135465 eV**

**<S**2>= 0.0000**

**Summary of Natural Population Analysis:**

| | | | Natural Population | | | |
|---|---|---|---|---|---|---|
| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
| N | 1 | -0.43376 | 1.99932 | 5.40508 | 0.02936 | 7.43376 |
| C | 2 | 0.36947 | 1.99919 | 3.60755 | 0.02379 | 5.63053 |
| C | 3 | -0.08463 | 1.99905 | 4.06567 | 0.01992 | 6.08463 |
| N | 4 | -0.82682 | 1.99938 | 5.79343 | 0.03401 | 7.82682 |
| C | 5 | -0.08458 | 1.99905 | 4.06562 | 0.01992 | 6.08458 |
| C | 6 | 0.36944 | 1.99919 | 3.60758 | 0.02379 | 5.63056 |
| C | 7 | 0.36946 | 1.99919 | 3.60756 | 0.02379 | 5.63054 |
| C | 8 | -0.08462 | 1.99905 | 4.06566 | 0.01992 | 6.08462 |
| N | 9 | -0.82674 | 1.99938 | 5.79334 | 0.03402 | 7.82674 |
| C | 10 | -0.08459 | 1.99905 | 4.06563 | 0.01992 | 6.08459 |
| C | 11 | 0.36946 | 1.99919 | 3.60756 | 0.02379 | 5.63054 |
| N | 12 | -0.43376 | 1.99932 | 5.40508 | 0.02936 | 7.43376 |
| C | 13 | 0.36942 | 1.99919 | 3.60760 | 0.02379 | 5.63058 |
| C | 14 | -0.08461 | 1.99905 | 4.06565 | 0.01992 | 6.08461 |
| N | 15 | -0.82678 | 1.99938 | 5.79339 | 0.03401 | 7.82678 |
| C | 16 | -0.08461 | 1.99905 | 4.06565 | 0.01992 | 6.08461 |
| C | 17 | 0.36943 | 1.99919 | 3.60759 | 0.02379 | 5.63057 |
| N | 18 | -0.43375 | 1.99932 | 5.40507 | 0.02936 | 7.43375 |
| Be | 19 | 1.68089 | 1.99828 | 0.24946 | 0.07137 | 2.31911 |
| C | 20 | -0.17535 | 1.99913 | 4.15853 | 0.01769 | 6.17535 |
| C | 21 | -0.17534 | 1.99913 | 4.15852 | 0.01769 | 6.17534 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C | 22 | -0.20395 | 1.99926 | 4.18663 | 0.01806 | 6.20395 |
| C | 23 | -0.20395 | 1.99926 | 4.18664 | 0.01806 | 6.20395 |
| H | 24 | 0.22872 | 0.00000 | 0.77009 | 0.00119 | 0.77128 |
| H | 25 | 0.21585 | 0.00000 | 0.78321 | 0.00094 | 0.78415 |
| H | 26 | 0.21585 | 0.00000 | 0.78321 | 0.00094 | 0.78415 |
| H | 27 | 0.22872 | 0.00000 | 0.77008 | 0.00119 | 0.77128 |
| C | 28 | -0.17535 | 1.99913 | 4.15853 | 0.01769 | 6.17535 |
| C | 29 | -0.17535 | 1.99913 | 4.15853 | 0.01769 | 6.17535 |
| C | 30 | -0.20394 | 1.99926 | 4.18663 | 0.01806 | 6.20394 |
| C | 31 | -0.20394 | 1.99926 | 4.18663 | 0.01806 | 6.20394 |
| H | 32 | 0.22872 | 0.00000 | 0.77008 | 0.00119 | 0.77128 |
| H | 33 | 0.22872 | 0.00000 | 0.77008 | 0.00119 | 0.77128 |
| H | 34 | 0.21585 | 0.00000 | 0.78321 | 0.00094 | 0.78415 |
| H | 35 | 0.21585 | 0.00000 | 0.78320 | 0.00094 | 0.78415 |
| C | 36 | -0.17534 | 1.99913 | 4.15852 | 0.01769 | 6.17534 |
| C | 37 | -0.17534 | 1.99913 | 4.15852 | 0.01769 | 6.17534 |
| C | 38 | -0.20395 | 1.99926 | 4.18664 | 0.01806 | 6.20395 |
| H | 39 | 0.21585 | 0.00000 | 0.78321 | 0.00094 | 0.78415 |
| C | 40 | -0.20393 | 1.99926 | 4.18662 | 0.01806 | 6.20393 |
| H | 41 | 0.21585 | 0.00000 | 0.78321 | 0.00094 | 0.78415 |
| H | 42 | 0.22872 | 0.00000 | 0.77009 | 0.00119 | 0.77128 |
| H | 43 | 0.22872 | 0.00000 | 0.77009 | 0.00119 | 0.77128 |
| * Total * | | -0.00000 | 61.97409 | 139.27487 | 0.75104 | 202.00000 |