

## Supporting Information

### Combining covalent bonding and electrostatic attraction to achieve more viable species possessing ultrashort beryllium-beryllium distances: a computational design

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## Contents

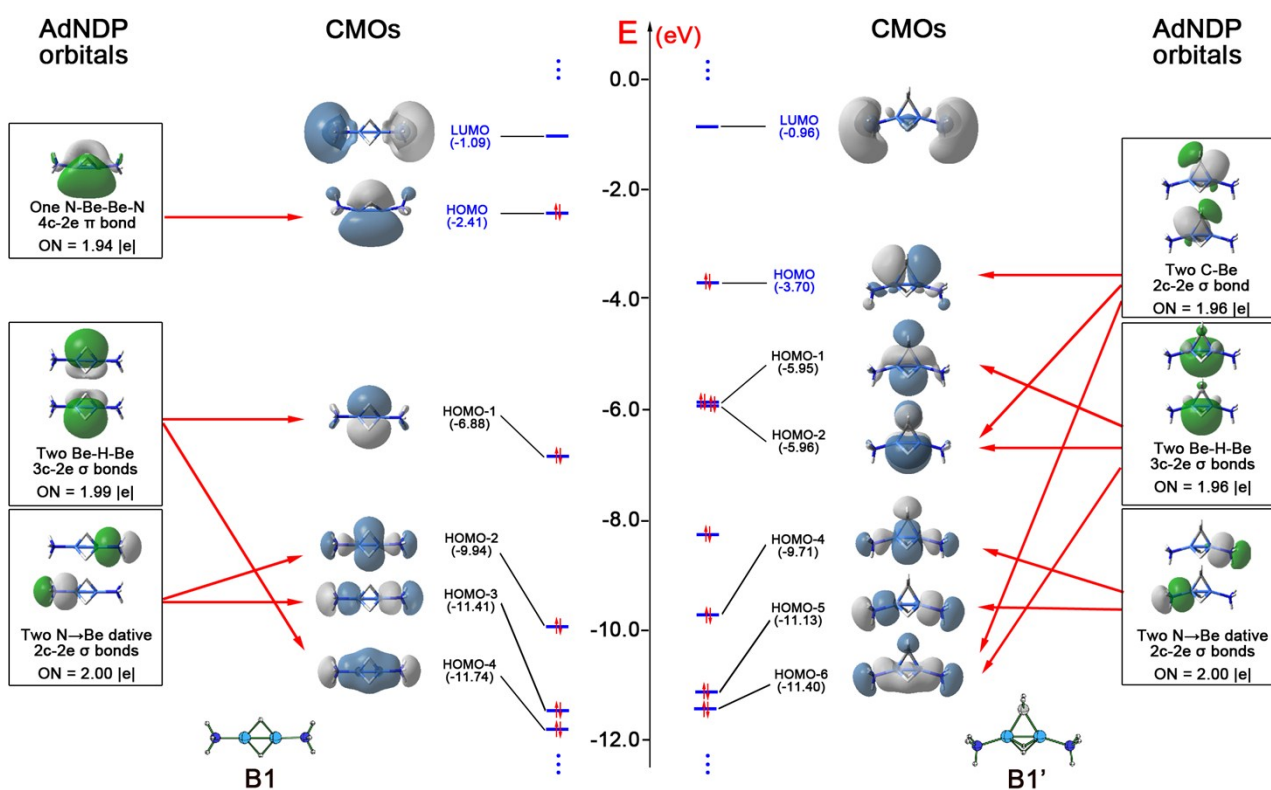
**Fig. S1.** The comparative AdNDP and CMO analyses of **B1** versus **B1'**. Two phases of AdNDP and CMO orbitals are shown in green/white and blue/white, respectively.

**Fig. S2.** The comparative AdNDP and CMO analyses of **C1** versus **C1'**. Two phases of AdNDP and CMO orbitals are shown in green/white and blue/white, respectively.

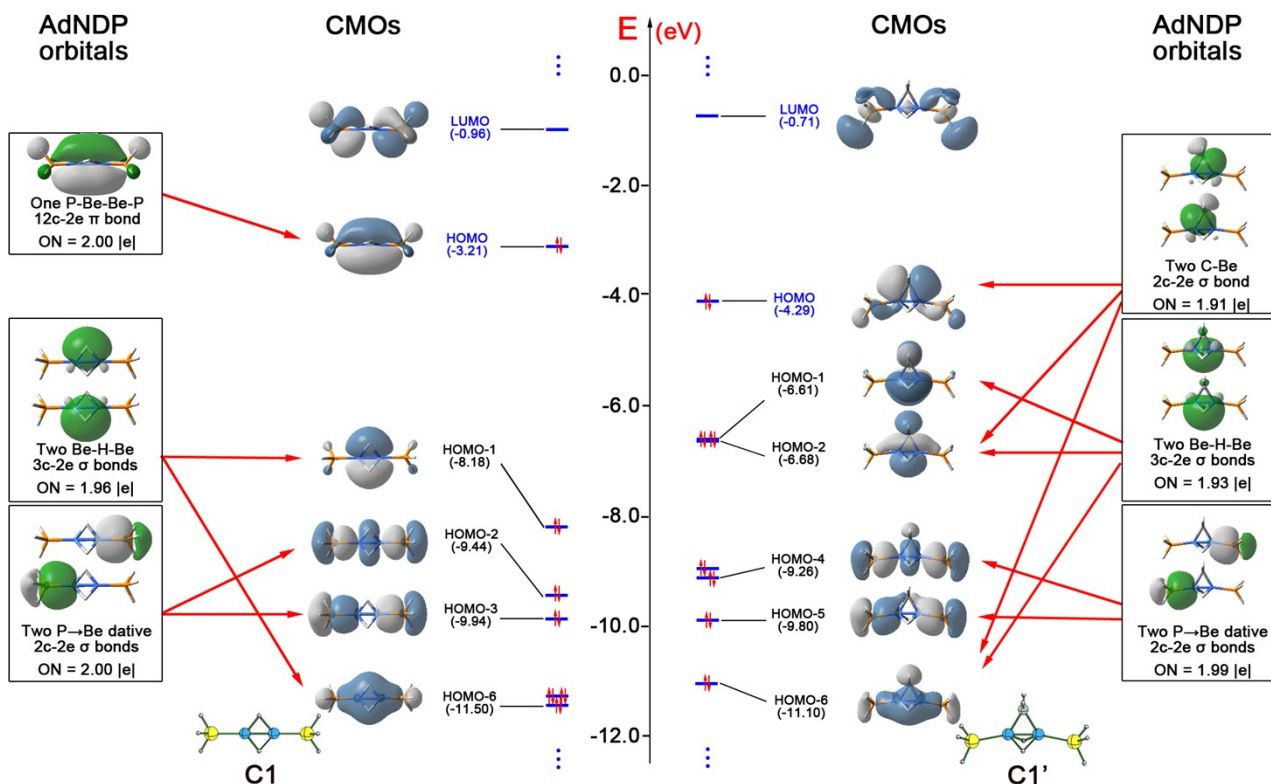
**Table S1.** The lowest vibrational frequencies ( $\nu_{\min}$ , in  $\text{cm}^{-1}$ ), the CMO energy levels ( $E$ ) of LUMOs, HOMOs, and HOMO-1s (in eV), as well as the HOMO-LUMO gaps (Gap, in eV) of the species studied in this work.

**Table S2.** The NBO results at the B3LYP/BS1 level, including the natural charges ( $Q$ , in  $|e|$ ) and total Wiberg bond indices (WBI) of Be, H, X ( $X = \text{C}, \text{N}, \text{and P}$ ), and C of  $-\text{CH}_2-$  moiety and the WBI for Be-Be, Be-H, Be-X, and Be-C bonding.

The Cartesian coordinates of **A1–C1**, **A1'–C1'**, **A2–C2**, **A2'–C2'**, **A1''**, and **A2''** structures.



**Fig. S1.** The comparative AdNDP and CMO analyses of B1 versus B1'. Two phases of AdNDP and CMO orbitals are shown in green/white and blue/white, respectively.



**Fig. S2.** The comparative AdNDP and CMO analyses of C1 versus C1'. Two phases of AdNDP and CMO orbitals are shown in green/white and blue/white, respectively.

**Table S1.** The lowest vibrational frequencies ( $\nu_{\min}$ , in  $\text{cm}^{-1}$ ), the CMO energy levels (E) of LUMOs, HOMOs, and HOMO-1s (in eV), as well as the HOMO-LUMO gaps (Gap, in eV) of the species studied in this work.

|            | $\nu_{\min}$ | $E_{\text{LUMO}}$ | $E_{\text{HOMO}}$ | $E_{\text{HOMO-1}}$ | Gap  |
|------------|--------------|-------------------|-------------------|---------------------|------|
| <b>A1</b>  | 30           | −0.39             | −2.17             | −6.78               | 1.78 |
| <b>B1</b>  | 91           | −1.09             | −2.41             | −6.88               | 1.32 |
| <b>C1</b>  | 39           | −0.94             | −3.20             | −8.17               | 2.27 |
| <b>A1'</b> | 31           | −0.43             | −3.23             | −5.42               | 2.80 |
| <b>B1'</b> | 96           | −0.97             | −3.70             | −5.95               | 2.74 |
| <b>C1'</b> | 48           | −0.71             | −4.29             | −6.60               | 3.58 |
| <b>A2</b>  | 11           | −0.67             | −2.27             | −6.43               | 1.61 |
| <b>B2</b>  | 10           | −0.91             | −2.39             | −6.27               | 1.49 |
| <b>C2</b>  | 5            | −1.05             | −2.69             | −6.66               | 1.63 |
| <b>A2'</b> | 4            | −0.37             | −3.16             | −5.37               | 2.79 |
| <b>B2'</b> | 13           | −0.88             | −3.70             | −5.91               | 2.82 |
| <b>C2'</b> | 6            | −1.02             | −3.71             | −5.99               | 2.69 |

**Table S2.** The NBO results at the B3LYP/BS1 level, including the natural charges (Q, in  $|e|$ ) and total Wiberg bond indices (WBI) of Be, H, X (X = C, N, and P), and C of  $-\text{CH}_2-$  moiety and the WBI for Be-Be, Be-H, Be-X, and Be-C bonding.

|            | Q     |       |       | WBI   |      |      |      |      |       |           |      |      |
|------------|-------|-------|-------|-------|------|------|------|------|-------|-----------|------|------|
|            | Be    | H     | X     | C     | Be   | H    | X    | C    | Be-Be | Be-H      | Be-X | Be-C |
| <b>A1</b>  | 0.06  | −0.17 | 0.04  | N/A   | 2.88 | 0.98 | 3.60 | N/A  | 0.78  | 0.47      | 0.86 | N/A  |
| <b>B1</b>  | −0.02 | −0.19 | −1.09 | N/A   | 2.73 | 0.97 | 2.84 | N/A  | 1.26  | 0.48      | 0.44 | N/A  |
| <b>C1</b>  | −0.15 | −0.14 | 0.16  | N/A   | 3.04 | 0.99 | 3.74 | N/A  | 1.03  | 0.48      | 0.83 | N/A  |
| <b>A1'</b> | 0.25  | −0.15 | 0.19  | −1.32 | 2.74 | 0.98 | 3.55 | 3.44 | 0.40  | 0.46      | 0.65 | 0.69 |
| <b>B1'</b> | 0.43  | −0.20 | −1.07 | −1.29 | 2.53 | 0.97 | 2.84 | 3.48 | 0.40  | 0.46      | 0.41 | 0.75 |
| <b>C1'</b> | 0.14  | −0.13 | 0.21  | −1.17 | 2.85 | 0.99 | 3.68 | 3.61 | 0.42  | 0.47      | 0.69 | 0.75 |
| <b>A2</b>  | 0.15  | −0.22 | 0.02  | N/A   | 2.80 | 0.97 | 3.59 | N/A  | 0.68  | 0.46      | 0.82 | N/A  |
| <b>B2</b>  | 0.20  | −0.22 | −0.63 | N/A   | 2.62 | 0.96 | 3.29 | N/A  | 0.91  | 0.45/0.46 | 0.31 | N/A  |
| <b>C2</b>  | −0.12 | −0.17 | 1.00  | N/A   | 3.02 | 0.98 | 3.84 | N/A  | 0.95  | 0.47      | 0.79 | N/A  |
| <b>A2'</b> | 0.27  | −0.18 | 0.18  | −1.20 | 2.73 | 0.99 | 3.56 | 3.57 | 0.37  | 0.45/0.46 | 0.64 | 0.67 |
| <b>B2'</b> | 0.53  | −0.21 | −0.61 | −1.38 | 2.40 | 0.97 | 3.31 | 3.39 | 0.36  | 0.45      | 0.27 | 0.69 |
| <b>C2'</b> | 0.16  | −0.15 | 1.05  | −1.24 | 2.83 | 0.98 | 3.77 | 3.54 | 0.38  | 0.46      | 0.68 | 0.74 |

# The Cartesian coordinates of **A1–C1**, **A1'–C1'**, **A2–C2**, and **A2'–C2'** structures

## A1

CCSD(T)/BS1

|    |              |               |               |
|----|--------------|---------------|---------------|
| C  | 0.0000000000 | 0.0000000000  | 2.6041948611  |
| C  | 0.0000000000 | 0.6863139415  | 4.7988337010  |
| C  | 0.0000000000 | -0.6863139415 | 4.7988337010  |
| H  | 0.0000000000 | -1.4008090985 | 5.6214054521  |
| N  | 0.0000000000 | -1.0719364758 | 3.4578867476  |
| C  | 0.0000000000 | 0.0000000000  | -2.6041948611 |
| C  | 0.0000000000 | -0.6863139415 | -4.7988337010 |
| H  | 0.0000000000 | -1.4008090985 | -5.6214054521 |
| N  | 0.0000000000 | -1.0719364758 | -3.4578867476 |
| N  | 0.0000000000 | 1.0719364758  | 3.4578867476  |
| H  | 0.0000000000 | 1.4008090985  | 5.6214054521  |
| N  | 0.0000000000 | 1.0719364758  | -3.4578867476 |
| C  | 0.0000000000 | 0.6863139415  | -4.7988337010 |
| H  | 0.0000000000 | 1.4008090985  | -5.6214054521 |
| Be | 0.0000000000 | 0.0000000000  | 0.9136478501  |
| Be | 0.0000000000 | 0.0000000000  | -0.9136478501 |
| H  | 0.0000000000 | -2.0267623886 | -3.1188815229 |
| H  | 0.0000000000 | -2.0267623886 | 3.1188815229  |
| H  | 0.0000000000 | 2.0267623886  | 3.1188815229  |
| H  | 0.0000000000 | 2.0267623886  | -3.1188815229 |
| H  | 0.0000000000 | -1.1173230089 | 0.0000000000  |
| H  | 0.0000000000 | 1.1173230089  | 0.0000000000  |

## B1

CCSD(T)/BS1

|    |               |               |               |
|----|---------------|---------------|---------------|
| Be | 0.0000000000  | 0.8814032029  | -0.3724082116 |
| Be | 0.0000000000  | -0.8814032029 | -0.3724082116 |
| H  | -1.0255894597 | 0.0000000000  | 0.2628354694  |
| H  | 1.0255894597  | 0.0000000000  | 0.2628354694  |
| N  | 0.0000000000  | -2.5485341611 | 0.0815861527  |
| H  | -0.8197244743 | -3.0111758346 | -0.3154462989 |
| H  | 0.8197244743  | -3.0111758346 | -0.3154462989 |
| N  | 0.0000000000  | 2.5485341611  | 0.0815861527  |
| H  | 0.8197244743  | 3.0111758346  | -0.3154462989 |
| H  | -0.8197244743 | 3.0111758346  | -0.3154462989 |
| H  | 0.0000000000  | -2.7164140492 | 1.0905591873  |
| H  | 0.0000000000  | 2.7164140492  | 1.0905591873  |

## C1

CCSD(T)/BS1

|    |               |               |               |
|----|---------------|---------------|---------------|
| Be | 0.0000000000  | 0.8923494738  | -0.2874999093 |
| Be | 0.0000000000  | -0.8923494738 | -0.2874999093 |
| P  | 0.0000000000  | 2.9307477935  | 0.0400320485  |
| H  | 1.0836741230  | 3.6329891187  | -0.5359725096 |
| H  | -1.0836741230 | 3.6329891187  | -0.5359725096 |
| H  | 0.0000000000  | 3.5760421116  | 1.3137833288  |
| P  | 0.0000000000  | -2.9307477935 | 0.0400320485  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | 0.0000000000  | -3.5760421116 | 1.3137833288  |
| H | -1.0836741230 | -3.6329891187 | -0.5359725096 |
| H | 1.0836741230  | -3.6329891187 | -0.5359725096 |
| H | -1.0796702312 | 0.0000000000  | 0.0930225512  |
| H | 1.0796702312  | 0.0000000000  | 0.0930225512  |

## A1'

### CCSD(T)/BS1

|    |               |               |               |
|----|---------------|---------------|---------------|
| C  | -0.0000069079 | 2.6609397259  | -0.4158064756 |
| C  | -0.0003468971 | 4.9375512993  | -0.4683453316 |
| C  | -0.0003890456 | 4.5476702616  | 0.8538204070  |
| H  | -0.0005941899 | 5.1378459375  | 1.7697602217  |
| N  | -0.0001674100 | 3.1585108887  | 0.8371770159  |
| C  | 0.0000069079  | -2.6609397259 | -0.4158064756 |
| C  | 0.0003468971  | -4.9375512993 | -0.4683453316 |
| H  | 0.0003380796  | -5.9274529170 | -0.9248806385 |
| N  | 0.0000187192  | -3.7563699511 | -1.2112222171 |
| N  | -0.0000187192 | 3.7563699511  | -1.2112222171 |
| H  | -0.0003380796 | 5.9274529170  | -0.9248806385 |
| N  | 0.0001674100  | -3.1585108887 | 0.8371770159  |
| C  | 0.0003890456  | -4.5476702616 | 0.8538204070  |
| H  | 0.0005941899  | -5.1378459375 | 1.7697602217  |
| Be | 0.0000921226  | 0.8945461741  | -0.3987905918 |
| Be | -0.0000921226 | -0.8945461741 | -0.3987905918 |
| H  | 0.0002289583  | -3.6962488405 | -2.2233827538 |
| H  | -0.0001791473 | 2.4587339800  | 1.5952251037  |
| H  | -0.0002289583 | 3.6962488405  | -2.2233827538 |
| H  | 0.0001791473  | -2.4587339800 | 1.5952251037  |
| H  | -1.0367670322 | 0.0000333090  | -1.0886223967 |
| H  | 1.0367670322  | -0.0000333090 | -1.0886223967 |
| C  | 0.0000000000  | 0.0000000000  | 1.1423373031  |
| H  | 0.8996860999  | -0.0000608887 | 1.7754970051  |
| H  | -0.8996860999 | 0.0000608887  | 1.7754970051  |

## B1'

### CCSD(T)/BS1

|    |               |               |               |
|----|---------------|---------------|---------------|
| Be | 0.0000000000  | 0.8971855836  | -0.0249193668 |
| Be | 0.0000000000  | -0.8971855836 | -0.0249193668 |
| H  | 1.0397702606  | 0.0000000000  | -0.7408711216 |
| H  | -1.0397702606 | 0.0000000000  | -0.7408711216 |
| N  | 0.0000000000  | -2.5566682032 | -0.5387311815 |
| H  | 0.8207860268  | -3.0306519189 | -0.1563840842 |
| H  | -0.8207860268 | -3.0306519189 | -0.1563840842 |
| N  | 0.0000000000  | 2.5566682032  | -0.5387311815 |
| H  | -0.8207860268 | 3.0306519189  | -0.1563840842 |
| H  | 0.8207860268  | 3.0306519189  | -0.1563840842 |
| H  | 0.0000000000  | -2.6883916678 | -1.5524331939 |
| H  | 0.0000000000  | 2.6883916678  | -1.5524331939 |
| C  | 0.0000000000  | 0.0000000000  | 1.4742831972  |
| H  | -0.8963249308 | 0.0000000000  | 2.1071739337  |
| H  | 0.8963249308  | 0.0000000000  | 2.1071739337  |

**C1'****CCSD(T)/BS1**

|    |               |               |               |
|----|---------------|---------------|---------------|
| Be | 0.0000000000  | 0.8851844897  | 0.0799341820  |
| Be | 0.0000000000  | -0.8851844897 | 0.0799341820  |
| P  | 0.0000000000  | 2.9829759021  | -0.3627323861 |
| H  | -1.0764393234 | 3.6938151891  | 0.2147670024  |
| H  | 1.0764393234  | 3.6938151891  | 0.2147670024  |
| H  | 0.0000000000  | 3.5816807988  | -1.6495923135 |
| P  | 0.0000000000  | -2.9829759021 | -0.3627323861 |
| H  | 0.0000000000  | -3.5816807988 | -1.6495923135 |
| H  | 1.0764393234  | -3.6938151891 | 0.2147670024  |
| H  | -1.0764393234 | -3.6938151891 | 0.2147670024  |
| H  | 1.0264329177  | 0.0000000000  | -0.6291772264 |
| H  | -1.0264329177 | 0.0000000000  | -0.6291772264 |
| C  | 0.0000000000  | 0.0000000000  | 1.5841307819  |
| H  | 0.8976282060  | 0.0000000000  | 2.2109943483  |
| H  | -0.8976282060 | 0.0000000000  | 2.2109943483  |

**A2****B3LYP/BS1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.00000000  | 0.00000000  | 2.60307300  |
| C  | -0.15028900 | 0.66259300  | 4.79020500  |
| C  | 0.15028900  | -0.66259300 | 4.79020500  |
| C  | 0.00000000  | 0.00000000  | -2.60307300 |
| C  | -0.15028900 | -0.66259300 | -4.79020500 |
| C  | 0.15028900  | 0.66259300  | -4.79020500 |
| N  | 0.24005300  | -1.05923400 | 3.45991400  |
| N  | -0.24005300 | -1.05923400 | -3.45991400 |
| N  | -0.24005300 | 1.05923400  | 3.45991400  |
| N  | 0.24005300  | 1.05923400  | -3.45991400 |
| H  | 0.31152500  | -1.35610700 | 5.60766300  |
| H  | -0.31152500 | -1.35610700 | -5.60766300 |
| H  | -0.31152500 | 1.35610700  | 5.60766300  |
| H  | 0.31152500  | 1.35610700  | -5.60766300 |
| Be | 0.00000000  | 0.00000000  | 0.92001000  |
| Be | 0.00000000  | 0.00000000  | -0.92001000 |
| C  | 0.60038100  | -2.38721100 | 3.04141400  |
| C  | 1.96840100  | -2.70076800 | 2.88451300  |
| C  | 2.29603700  | -4.01468400 | 2.51906200  |
| C  | 1.30495800  | -4.97349100 | 2.31367400  |
| C  | -0.03884200 | -4.63549800 | 2.46586100  |
| C  | -0.42235000 | -3.33588600 | 2.82867100  |
| C  | 3.07617400  | -1.68004900 | 3.12891100  |
| C  | -1.89811000 | -2.99705900 | 3.01446400  |
| C  | -2.45803500 | -3.64959000 | 4.29308400  |
| C  | -2.73906000 | -3.37447300 | 1.78325000  |
| C  | -0.60038100 | -2.38721100 | -3.04141400 |
| C  | -1.96840100 | -2.70076800 | -2.88451300 |
| C  | -2.29603700 | -4.01468400 | -2.51906200 |
| C  | -1.30495800 | -4.97349100 | -2.31367400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.03884200  | -4.63549800 | -2.46586100 |
| C | 0.42235000  | -3.33588600 | -2.82867100 |
| C | -3.07617400 | -1.68004900 | -3.12891100 |
| C | -3.96777600 | -1.49039800 | -1.88921700 |
| C | -3.91247600 | -2.05257200 | -4.36796900 |
| C | 1.89811000  | -2.99705900 | -3.01446400 |
| C | 2.45803500  | -3.64959000 | -4.29308400 |
| C | 2.73906000  | -3.37447300 | -1.78325000 |
| C | 3.96777600  | -1.49039800 | 1.88921700  |
| C | 3.91247600  | -2.05257200 | 4.36796900  |
| C | -0.60038100 | 2.38721100  | 3.04141400  |
| C | 0.60038100  | 2.38721100  | -3.04141400 |
| C | -1.96840100 | 2.70076800  | 2.88451300  |
| C | 0.42235000  | 3.33588600  | 2.82867100  |
| C | 0.03884200  | 4.63549800  | 2.46586100  |
| C | 1.89811000  | 2.99705900  | 3.01446400  |
| C | 2.45803500  | 3.64959000  | 4.29308400  |
| C | 2.73906000  | 3.37447300  | 1.78325000  |
| C | -1.30495800 | 4.97349100  | 2.31367400  |
| C | -2.29603700 | 4.01468400  | 2.51906200  |
| C | -3.07617400 | 1.68004900  | 3.12891100  |
| C | -3.96777600 | 1.49039800  | 1.88921700  |
| C | -3.91247600 | 2.05257200  | 4.36796900  |
| C | 1.96840100  | 2.70076800  | -2.88451300 |
| C | -0.42235000 | 3.33588600  | -2.82867100 |
| C | 2.29603700  | 4.01468400  | -2.51906200 |
| C | 3.07617400  | 1.68004900  | -3.12891100 |
| C | -0.03884200 | 4.63549800  | -2.46586100 |
| C | -1.89811000 | 2.99705900  | -3.01446400 |
| C | 1.30495800  | 4.97349100  | -2.31367400 |
| C | 3.96777600  | 1.49039800  | -1.88921700 |
| C | 3.91247600  | 2.05257200  | -4.36796900 |
| C | -2.45803500 | 3.64959000  | -4.29308400 |
| C | -2.73906000 | 3.37447300  | -1.78325000 |
| H | 1.58217900  | -5.99235300 | 2.03232700  |
| H | -0.80574400 | -5.39457400 | 2.30055800  |
| H | 2.60094600  | -0.70995400 | 3.33078200  |
| H | -1.97782700 | -1.90727800 | 3.13405200  |
| H | -2.41449900 | -4.75001500 | 4.23345000  |
| H | -3.51204700 | -3.36296000 | 4.44404500  |
| H | -1.89138400 | -3.34147600 | 5.18655000  |
| H | -2.33858500 | -2.90189400 | 0.87390800  |
| H | -2.76712800 | -4.46485000 | 1.62136100  |
| H | 0.80574400  | -5.39457400 | -2.30055800 |
| H | -2.60094600 | -0.70995400 | -3.33078200 |
| H | -3.36581500 | -1.17670800 | -1.02220100 |
| H | -3.28265100 | -2.14702100 | -5.26734400 |
| H | 1.97782700  | -1.90727800 | -3.13405200 |
| H | 2.41449900  | -4.75001500 | -4.23345000 |
| H | 3.51204700  | -3.36296000 | -4.44404500 |
| H | 1.89138400  | -3.34147600 | -5.18655000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.33858500  | -2.90189400 | -0.87390800 |
| H | 3.77925300  | -3.03438100 | -1.91741500 |
| H | 2.76712800  | -4.46485000 | -1.62136100 |
| H | 3.34511400  | -4.29105900 | 2.39549200  |
| H | -3.77925300 | -3.03438100 | 1.91741500  |
| H | -3.34511400 | -4.29105900 | -2.39549200 |
| H | -1.58217900 | -5.99235300 | -2.03232700 |
| H | -4.50562100 | -2.41588000 | -1.62386300 |
| H | -4.72360800 | -0.71069000 | -2.08130800 |
| H | -4.67364400 | -1.27978500 | -4.56570200 |
| H | -4.43855100 | -3.01140200 | -4.22706800 |
| H | 4.50562100  | -2.41588000 | 1.62386300  |
| H | 4.72360800  | -0.71069000 | 2.08130800  |
| H | 3.36581500  | -1.17670800 | 1.02220100  |
| H | 3.28265100  | -2.14702100 | 5.26734400  |
| H | 4.67364400  | -1.27978500 | 4.56570200  |
| H | 4.43855100  | -3.01140200 | 4.22706800  |
| H | 1.97782700  | 1.90727800  | 3.13405200  |
| H | 2.33858500  | 2.90189400  | 0.87390800  |
| H | 3.77925300  | 3.03438100  | 1.91741500  |
| H | 2.76712800  | 4.46485000  | 1.62136100  |
| H | 0.80574400  | 5.39457400  | 2.30055800  |
| H | -1.58217900 | 5.99235300  | 2.03232700  |
| H | -2.60094600 | 0.70995400  | 3.33078200  |
| H | -4.50562100 | 2.41588000  | 1.62386300  |
| H | -4.72360800 | 0.71069000  | 2.08130800  |
| H | -3.36581500 | 1.17670800  | 1.02220100  |
| H | -3.28265100 | 2.14702100  | 5.26734400  |
| H | -4.67364400 | 1.27978500  | 4.56570200  |
| H | -4.43855100 | 3.01140200  | 4.22706800  |
| H | 2.41449900  | 4.75001500  | 4.23345000  |
| H | 3.51204700  | 3.36296000  | 4.44404500  |
| H | 1.89138400  | 3.34147600  | 5.18655000  |
| H | -3.34511400 | 4.29105900  | 2.39549200  |
| H | 3.34511400  | 4.29105900  | -2.39549200 |
| H | 2.60094600  | 0.70995400  | -3.33078200 |
| H | -0.80574400 | 5.39457400  | -2.30055800 |
| H | -1.97782700 | 1.90727800  | -3.13405200 |
| H | 1.58217900  | 5.99235300  | -2.03232700 |
| H | 4.50562100  | 2.41588000  | -1.62386300 |
| H | 4.72360800  | 0.71069000  | -2.08130800 |
| H | 3.36581500  | 1.17670800  | -1.02220100 |
| H | 3.28265100  | 2.14702100  | -5.26734400 |
| H | 4.67364400  | 1.27978500  | -4.56570200 |
| H | 4.43855100  | 3.01140200  | -4.22706800 |
| H | -2.41449900 | 4.75001500  | -4.23345000 |
| H | -3.51204700 | 3.36296000  | -4.44404500 |
| H | -1.89138400 | 3.34147600  | -5.18655000 |
| H | -2.33858500 | 2.90189400  | -0.87390800 |
| H | -3.77925300 | 3.03438100  | -1.91741500 |
| H | -2.76712800 | 4.46485000  | -1.62136100 |

|   |            |             |            |
|---|------------|-------------|------------|
| H | 0.00000000 | -1.09501900 | 0.00000000 |
| H | 0.00000000 | 1.09501900  | 0.00000000 |

## B2

### B3LYP/BS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Be | -0.11713800 | -0.87892900 | -0.24963100 |
| Be | 0.11713800  | 0.87892900  | -0.24963100 |
| H  | 1.04679700  | -0.12277600 | 0.22450200  |
| H  | -1.04679700 | 0.12277600  | 0.22450200  |
| C  | 0.47852800  | 2.98301000  | 1.40415600  |
| C  | -0.40123800 | 2.41605800  | 2.33070200  |
| C  | 1.41480800  | 3.93794400  | 1.81540900  |
| C  | -0.33757400 | 2.79465000  | 3.67196800  |
| H  | -1.12158300 | 1.66901500  | 1.99428600  |
| C  | 1.48939500  | 4.29305300  | 3.16955100  |
| H  | 2.08960000  | 4.39734100  | 1.09486700  |
| C  | 0.61965600  | 3.72493500  | 4.10015200  |
| H  | -1.03370300 | 2.35126400  | 4.38687800  |
| H  | 2.23390400  | 5.02602100  | 3.48813700  |
| H  | 0.68204200  | 4.00502400  | 5.15386400  |
| C  | -0.47852800 | -2.98301000 | 1.40415600  |
| C  | 0.40123800  | -2.41605800 | 2.33070200  |
| C  | -1.41480800 | -3.93794400 | 1.81540900  |
| C  | 0.33757400  | -2.79465000 | 3.67196800  |
| H  | 1.12158300  | -1.66901500 | 1.99428600  |
| C  | -1.48939500 | -4.29305300 | 3.16955100  |
| H  | -2.08960000 | -4.39734100 | 1.09486700  |
| C  | -0.61965600 | -3.72493500 | 4.10015200  |
| H  | 1.03370300  | -2.35126400 | 4.38687800  |
| H  | -2.23390400 | -5.02602100 | 3.48813700  |
| H  | -0.68204200 | -4.00502400 | 5.15386400  |
| C  | 1.59958400  | 2.67134700  | -0.81622000 |
| C  | 1.63198000  | 3.23276300  | -2.09871000 |
| C  | 2.77816600  | 2.16372600  | -0.24365000 |
| C  | 2.83004200  | 3.25897900  | -2.81405300 |
| H  | 0.72416200  | 3.62757700  | -2.54991600 |
| C  | 3.96743300  | 2.18715200  | -0.97539600 |
| H  | 2.75647800  | 1.72751000  | 0.75308600  |
| C  | 4.00369400  | 2.73100100  | -2.26179000 |
| H  | 2.83851800  | 3.68782700  | -3.81816500 |
| H  | 4.87451400  | 1.77685500  | -0.52596300 |
| H  | 4.93788400  | 2.75210700  | -2.82642600 |
| C  | -0.78964400 | 3.35711400  | -0.62157100 |
| C  | -1.82180200 | 2.67119100  | -1.26333300 |
| C  | -0.80855400 | 4.75315200  | -0.53790100 |
| C  | -2.87325900 | 3.39580200  | -1.84170400 |
| H  | -1.78046900 | 1.58102600  | -1.33790400 |
| C  | -1.86042400 | 5.46705600  | -1.11538500 |
| H  | -0.00798700 | 5.28462300  | -0.02484200 |
| C  | -2.89517400 | 4.78883800  | -1.77173000 |
| H  | -3.67819900 | 2.85588500  | -2.34470700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.86984000 | 6.55701100  | -1.05082600 |
| H | -3.71892900 | 5.34908000  | -2.21977800 |
| C | -1.59958400 | -2.67134700 | -0.81622000 |
| C | -1.63198000 | -3.23276300 | -2.09871000 |
| C | -2.77816600 | -2.16372600 | -0.24365000 |
| C | -2.83004200 | -3.25897900 | -2.81405300 |
| H | -0.72416200 | -3.62757700 | -2.54991600 |
| C | -3.96743300 | -2.18715200 | -0.97539600 |
| H | -2.75647800 | -1.72751000 | 0.75308600  |
| C | -4.00369400 | -2.73100100 | -2.26179000 |
| H | -2.83851800 | -3.68782700 | -3.81816500 |
| H | -4.87451400 | -1.77685500 | -0.52596300 |
| H | -4.93788400 | -2.75210700 | -2.82642600 |
| C | 0.78964400  | -3.35711400 | -0.62157100 |
| C | 0.80855400  | -4.75315200 | -0.53790100 |
| C | 1.82180200  | -2.67119100 | -1.26333300 |
| C | 1.86042400  | -5.46705600 | -1.11538500 |
| H | 0.00798700  | -5.28462300 | -0.02484200 |
| C | 2.87325900  | -3.39580200 | -1.84170400 |
| H | 1.78046900  | -1.58102600 | -1.33790400 |
| C | 2.89517400  | -4.78883800 | -1.77173000 |
| H | 1.86984000  | -6.55701100 | -1.05082600 |
| H | 3.67819900  | -2.85588500 | -2.34470700 |
| H | 3.71892900  | -5.34908000 | -2.21977800 |
| N | -0.33757400 | -2.58434700 | -0.02593400 |
| N | 0.33757400  | 2.58434700  | -0.02593400 |

## C2

### B3LYP/BS1

|    |             |             |            |
|----|-------------|-------------|------------|
| Be | 0.00398200  | -0.89447900 | 0.11689900 |
| Be | -0.00398200 | 0.89447900  | 0.11689900 |
| P  | 0.00376400  | -2.94771900 | 0.07645400 |
| P  | -0.00376400 | 2.94771900  | 0.07645400 |
| H  | 1.08929700  | 0.00671200  | 0.36669600 |
| H  | -1.08929700 | -0.00671200 | 0.36669600 |
| C  | -0.17640500 | 3.87583900  | 1.66894200 |
| C  | -0.99787400 | 3.32346900  | 2.66537100 |
| C  | 0.49407400  | 5.08269200  | 1.92669200 |
| C  | -1.16646400 | 3.97713500  | 3.88721100 |
| H  | -1.49115400 | 2.36406400  | 2.48437100 |
| C  | 0.33883700  | 5.72678300  | 3.15932600 |
| H  | 1.14655800  | 5.51868200  | 1.16779500 |
| C  | -0.49407400 | 5.17909200  | 4.13891400 |
| H  | -1.81299200 | 3.53904600  | 4.65125700 |
| H  | 0.87276300  | 6.66040300  | 3.35267600 |
| H  | -0.61263300 | 5.68242600  | 5.10130700 |
| C  | 0.17640500  | -3.87583900 | 1.66894200 |
| C  | 0.99787400  | -3.32346900 | 2.66537100 |
| C  | -0.49407400 | -5.08269200 | 1.92669200 |
| C  | 1.16646400  | -3.97713500 | 3.88721100 |
| H  | 1.49115400  | -2.36406400 | 2.48437100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.33883700 | -5.72678300 | 3.15932600  |
| H | -1.14655800 | -5.51868200 | 1.16779500  |
| C | 0.49407400  | -5.17909200 | 4.13891400  |
| H | 1.81299200  | -3.53904600 | 4.65125700  |
| H | -0.87276300 | -6.66040300 | 3.35267600  |
| H | 0.61263300  | -5.68242600 | 5.10130700  |
| C | 1.57185600  | 3.55444500  | -0.63327600 |
| C | 1.62566500  | 4.40611000  | -1.74795800 |
| C | 2.77501800  | 3.11117300  | -0.05095300 |
| C | 2.85951400  | 4.80458800  | -2.27235900 |
| H | 0.70265800  | 4.75262200  | -2.21513100 |
| C | 4.00338200  | 3.51152400  | -0.57802000 |
| H | 2.74670700  | 2.44433900  | 0.81378500  |
| C | 4.05010600  | 4.35966400  | -1.69095100 |
| H | 2.88690100  | 5.46590500  | -3.14157600 |
| H | 4.92888200  | 3.15697300  | -0.11850700 |
| H | 5.01252900  | 4.67176000  | -2.10272900 |
| C | -1.36825300 | 3.62158900  | -0.96042900 |
| C | -1.88772300 | 2.81245200  | -1.98466800 |
| C | -1.89635700 | 4.90976700  | -0.76861900 |
| C | -2.91208900 | 3.28800000  | -2.80781700 |
| H | -1.48053700 | 1.80604400  | -2.12358200 |
| C | -2.91738700 | 5.38332400  | -1.59719600 |
| H | -1.51846700 | 5.54263600  | 0.03574200  |
| C | -3.42596400 | 4.57442000  | -2.61880600 |
| H | -3.31152400 | 2.64625700  | -3.59658600 |
| H | -3.32021400 | 6.38655900  | -1.43931700 |
| H | -4.22663000 | 4.94575900  | -3.26303400 |
| C | -1.57185600 | -3.55444500 | -0.63327600 |
| C | -1.62566500 | -4.40611000 | -1.74795800 |
| C | -2.77501800 | -3.11117300 | -0.05095300 |
| C | -2.85951400 | -4.80458800 | -2.27235900 |
| H | -0.70265800 | -4.75262200 | -2.21513100 |
| C | -4.00338200 | -3.51152400 | -0.57802000 |
| H | -2.74670700 | -2.44433900 | 0.81378500  |
| C | -4.05010600 | -4.35966400 | -1.69095100 |
| H | -2.88690100 | -5.46590500 | -3.14157600 |
| H | -4.92888200 | -3.15697300 | -0.11850700 |
| H | -5.01252900 | -4.67176000 | -2.10272900 |
| C | 1.36825300  | -3.62158900 | -0.96042900 |
| C | 1.89635700  | -4.90976700 | -0.76861900 |
| C | 1.88772300  | -2.81245200 | -1.98466800 |
| C | 2.91738700  | -5.38332400 | -1.59719600 |
| H | 1.51846700  | -5.54263600 | 0.03574200  |
| C | 2.91208900  | -3.28800000 | -2.80781700 |
| H | 1.48053700  | -1.80604400 | -2.12358200 |
| C | 3.42596400  | -4.57442000 | -2.61880600 |
| H | 3.32021400  | -6.38655900 | -1.43931700 |
| H | 3.31152400  | -2.64625700 | -3.59658600 |
| H | 4.22663000  | -4.94575900 | -3.26303400 |

**A2'**  
B3LYP/BS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.00000000  | 2.64338400  | -0.00811800 |
| C  | 0.72809900  | 4.78627400  | -0.26441000 |
| C  | -0.57076600 | 4.84325000  | 0.13119900  |
| C  | 0.00000000  | -2.64338400 | -0.00811800 |
| C  | -0.72809900 | -4.78627400 | -0.26441000 |
| C  | 0.57076600  | -4.84325000 | 0.13119900  |
| N  | -0.99599500 | 3.52863100  | 0.28529000  |
| N  | -1.05692700 | -3.43575700 | -0.34868700 |
| N  | 1.05692700  | 3.43575700  | -0.34868700 |
| N  | 0.99599500  | -3.52863100 | 0.28529000  |
| H  | -1.22707500 | 5.68618600  | 0.31358800  |
| H  | -1.44170800 | -5.56825800 | -0.49736600 |
| H  | 1.44170800  | 5.56825800  | -0.49736600 |
| H  | 1.22707500  | -5.68618600 | 0.31358800  |
| Be | -0.02873800 | 0.90429100  | 0.26901400  |
| Be | 0.02873800  | -0.90429100 | 0.26901400  |
| C  | -2.32763100 | 3.16846800  | 0.71467600  |
| C  | -2.60722500 | 3.14136000  | 2.09858900  |
| C  | -3.91751400 | 2.82431000  | 2.48329700  |
| C  | -4.90083400 | 2.54281100  | 1.53537100  |
| C  | -4.59430900 | 2.57596200  | 0.17662200  |
| C  | -3.30138200 | 2.89139800  | -0.26669700 |
| C  | -1.56014900 | 3.48736800  | 3.15403800  |
| C  | -3.00512500 | 2.94759800  | -1.76249800 |
| C  | -3.76040700 | 4.11002500  | -2.43462800 |
| C  | -3.30383700 | 1.60732700  | -2.45646300 |
| C  | -2.35483200 | -2.97390800 | -0.78530300 |
| C  | -2.59464600 | -2.86658700 | -2.17176000 |
| C  | -3.87666900 | -2.46954400 | -2.57687600 |
| C  | -4.87338400 | -2.19588400 | -1.64135100 |
| C  | -4.60433600 | -2.30286400 | -0.27798400 |
| C  | -3.33842000 | -2.69071000 | 0.18458500  |
| C  | -1.50279900 | -3.11682200 | -3.20889600 |
| C  | -0.92154100 | -1.78149900 | -3.71300300 |
| C  | -1.97886800 | -3.99558000 | -4.37793000 |
| C  | -3.07072600 | -2.82212900 | 1.68116600  |
| C  | -3.63777800 | -4.14956300 | 2.22173900  |
| C  | -3.60528200 | -1.62491700 | 2.48423500  |
| C  | -1.51439300 | 2.46873000  | 4.30474200  |
| C  | -1.78292000 | 4.91522800  | 3.69193600  |
| C  | 2.35483200  | 2.97390800  | -0.78530300 |
| C  | 2.32763100  | -3.16846800 | 0.71467600  |
| C  | 2.59464600  | 2.86658700  | -2.17176000 |
| C  | 3.33842000  | 2.69071000  | 0.18458500  |
| C  | 4.60433600  | 2.30286400  | -0.27798400 |
| C  | 3.07072600  | 2.82212900  | 1.68116600  |
| C  | 3.63777800  | 4.14956300  | 2.22173900  |
| C  | 3.60528200  | 1.62491700  | 2.48423500  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 4. 87338400  | 2. 19588400  | -1. 64135100 |
| C | 3. 87666900  | 2. 46954400  | -2. 57687600 |
| C | 1. 50279900  | 3. 11682200  | -3. 20889600 |
| C | 0. 92154100  | 1. 78149900  | -3. 71300300 |
| C | 1. 97886800  | 3. 99558000  | -4. 37793000 |
| C | 2. 60722500  | -3. 14136000 | 2. 09858900  |
| C | 3. 30138200  | -2. 89139800 | -0. 26669700 |
| C | 3. 91751400  | -2. 82431000 | 2. 48329700  |
| C | 1. 56014900  | -3. 48736800 | 3. 15403800  |
| C | 4. 59430900  | -2. 57596200 | 0. 17662200  |
| C | 3. 00512500  | -2. 94759800 | -1. 76249800 |
| C | 4. 90083400  | -2. 54281100 | 1. 53537100  |
| C | 1. 51439300  | -2. 46873000 | 4. 30474200  |
| C | 1. 78292000  | -4. 91522800 | 3. 69193600  |
| C | 3. 76040700  | -4. 11002500 | -2. 43462800 |
| C | 3. 30383700  | -1. 60732700 | -2. 45646300 |
| H | -5. 91450400 | 2. 29516000  | 1. 85975800  |
| H | -5. 37240100 | 2. 35362800  | -0. 55608800 |
| H | -0. 57413500 | 3. 45539600  | 2. 66950900  |
| H | -1. 93024600 | 3. 13920000  | -1. 88791500 |
| H | -4. 85249900 | 3. 97359900  | -2. 36759100 |
| H | -3. 49706900 | 4. 17329300  | -3. 50351500 |
| H | -3. 51619700 | 5. 07717200  | -1. 96600100 |
| H | -2. 74409400 | 0. 78830000  | -1. 98122300 |
| H | -4. 37706200 | 1. 35836200  | -2. 41959100 |
| H | -5. 39170000 | -2. 07846000 | 0. 44309800  |
| H | -0. 68432800 | -3. 66026700 | -2. 71479000 |
| H | -0. 53789000 | -1. 17539100 | -2. 87882900 |
| H | -2. 40516500 | -4. 94781000 | -4. 02347000 |
| H | -1. 98174100 | -2. 83199500 | 1. 82870900  |
| H | -4. 73412300 | -4. 18975600 | 2. 10710800  |
| H | -3. 40633900 | -4. 25948500 | 3. 29417400  |
| H | -3. 21487500 | -5. 01943800 | 1. 69385100  |
| H | -3. 20929600 | -0. 67738900 | 2. 09152700  |
| H | -3. 28721400 | -1. 71216800 | 3. 53525400  |
| H | -4. 70647000 | -1. 57683500 | 2. 47596400  |
| H | -4. 17110800 | 2. 79493800  | 3. 54415900  |
| H | -3. 01128100 | 1. 65758400  | -3. 51859500 |
| H | -4. 09774300 | -2. 37038900 | -3. 64095200 |
| H | -5. 86743100 | -1. 89189600 | -1. 97820700 |
| H | -1. 69050100 | -1. 18848800 | -4. 23539600 |
| H | -0. 09503200 | -1. 96365500 | -4. 41986800 |
| H | -1. 13274400 | -4. 22800000 | -5. 04486900 |
| H | -2. 74445600 | -3. 49155000 | -4. 98985400 |
| H | -2. 44951400 | 2. 45804600  | 4. 88870400  |
| H | -0. 69890900 | 2. 72902500  | 4. 99942400  |
| H | -1. 32043500 | 1. 45847100  | 3. 91651900  |
| H | -1. 77053100 | 5. 66602500  | 2. 88558700  |
| H | -0. 99449000 | 5. 18211400  | 4. 41502100  |
| H | -2. 75444200 | 4. 99801500  | 4. 20749100  |
| H | 1. 98174100  | 2. 83199500  | 1. 82870900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.20929600  | 0.67738900  | 2.09152700  |
| H | 3.28721400  | 1.71216800  | 3.53525400  |
| H | 4.70647000  | 1.57683500  | 2.47596400  |
| H | 5.39170000  | 2.07846000  | 0.44309800  |
| H | 5.86743100  | 1.89189600  | -1.97820700 |
| H | 0.68432800  | 3.66026700  | -2.71479000 |
| H | 1.69050100  | 1.18848800  | -4.23539600 |
| H | 0.09503200  | 1.96365500  | -4.41986800 |
| H | 0.53789000  | 1.17539100  | -2.87882900 |
| H | 2.40516500  | 4.94781000  | -4.02347000 |
| H | 1.13274400  | 4.22800000  | -5.04486900 |
| H | 2.74445600  | 3.49155000  | -4.98985400 |
| H | 4.73412300  | 4.18975600  | 2.10710800  |
| H | 3.40633900  | 4.25948500  | 3.29417400  |
| H | 3.21487500  | 5.01943800  | 1.69385100  |
| H | 4.09774300  | 2.37038900  | -3.64095200 |
| H | 4.17110800  | -2.79493800 | 3.54415900  |
| H | 0.57413500  | -3.45539600 | 2.66950900  |
| H | 5.37240100  | -2.35362800 | -0.55608800 |
| H | 1.93024600  | -3.13920000 | -1.88791500 |
| H | 5.91450400  | -2.29516000 | 1.85975800  |
| H | 2.44951400  | -2.45804600 | 4.88870400  |
| H | 0.69890900  | -2.72902500 | 4.99942400  |
| H | 1.32043500  | -1.45847100 | 3.91651900  |
| H | 1.77053100  | -5.66602500 | 2.88558700  |
| H | 0.99449000  | -5.18211400 | 4.41502100  |
| H | 2.75444200  | -4.99801500 | 4.20749100  |
| H | 4.85249900  | -3.97359900 | -2.36759100 |
| H | 3.49706900  | -4.17329300 | -3.50351500 |
| H | 3.51619700  | -5.07717200 | -1.96600100 |
| H | 2.74409400  | -0.78830000 | -1.98122300 |
| H | 3.01128100  | -1.65758400 | -3.51859500 |
| H | 4.37706200  | -1.35836200 | -2.41959100 |
| H | -1.02520900 | -0.01262400 | -0.42059900 |
| H | 1.02520900  | 0.01262400  | -0.42059900 |
| C | 0.00000000  | 0.00000000  | 1.77872800  |
| H | 0.89004400  | 0.05106000  | 2.40914200  |
| H | -0.89004400 | -0.05106000 | 2.40914200  |

## B2'

### B3LYP/BS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Be | 0.65067600  | 0.62059200  | 0.60959600  |
| Be | -0.65067600 | -0.62059200 | 0.60959600  |
| H  | 0.72247700  | -0.72565700 | -0.08454100 |
| H  | -0.72247700 | 0.72565700  | -0.08454100 |
| C  | -1.65962800 | -2.22772200 | -1.33834000 |
| C  | -1.53155100 | -1.17616100 | -2.25476900 |
| C  | -1.61636100 | -3.55013200 | -1.78862400 |
| C  | -1.36579900 | -1.45197700 | -3.61190900 |
| H  | -1.55827000 | -0.14814500 | -1.89608600 |
| C  | -1.43630100 | -3.81777900 | -3.15147700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.71897900 | -4.37618800 | -1.08745900 |
| C | -1.31297500 | -2.77392800 | -4.06871800 |
| H | -1.27097400 | -0.62175400 | -4.31477500 |
| H | -1.39923100 | -4.85565400 | -3.48920900 |
| H | -1.17585800 | -2.98599500 | -5.13118500 |
| C | 1.65962800  | 2.22772200  | -1.33834000 |
| C | 1.53155100  | 1.17616100  | -2.25476900 |
| C | 1.61636100  | 3.55013200  | -1.78862400 |
| C | 1.36579900  | 1.45197700  | -3.61190900 |
| H | 1.55827000  | 0.14814500  | -1.89608600 |
| C | 1.43630100  | 3.81777900  | -3.15147700 |
| H | 1.71897900  | 4.37618800  | -1.08745900 |
| C | 1.31297500  | 2.77392800  | -4.06871800 |
| H | 1.27097400  | 0.62175400  | -4.31477500 |
| H | 1.39923100  | 4.85565400  | -3.48920900 |
| H | 1.17585800  | 2.98599500  | -5.13118500 |
| C | -1.61115900 | -3.05292200 | 0.98046400  |
| C | -2.65327800 | -3.79444300 | 1.53975100  |
| C | -0.28150100 | -3.41629300 | 1.22106000  |
| C | -2.36203900 | -4.89774200 | 2.35207600  |
| H | -3.68972500 | -3.51641800 | 1.35441600  |
| C | 0.00000000  | -4.52320100 | 2.02189200  |
| H | 0.52511800  | -2.83063100 | 0.78024300  |
| C | -1.03834100 | -5.26601700 | 2.59561600  |
| H | -3.18288900 | -5.46847700 | 2.79142400  |
| H | 1.04061300  | -4.79633000 | 2.20773900  |
| H | -0.81392500 | -6.12481400 | 3.23181100  |
| C | -3.20080400 | -1.28222900 | 0.34257200  |
| C | -3.38741700 | -0.60513000 | 1.55428000  |
| C | -4.25319500 | -1.39590700 | -0.56936800 |
| C | -4.62660000 | -0.02976000 | 1.83871100  |
| H | -2.54662300 | -0.52439600 | 2.24746500  |
| C | -5.49123500 | -0.81144600 | -0.27469700 |
| H | -4.11920600 | -1.93185700 | -1.50748400 |
| C | -5.68298700 | -0.12581200 | 0.92596300  |
| H | -4.76169500 | 0.50130900  | 2.78339200  |
| H | -6.30747600 | -0.90126400 | -0.99470400 |
| H | -6.64968500 | 0.32989800  | 1.15120200  |
| C | 1.61115900  | 3.05292200  | 0.98046400  |
| C | 2.65327800  | 3.79444300  | 1.53975100  |
| C | 0.28150100  | 3.41629300  | 1.22106000  |
| C | 2.36203900  | 4.89774200  | 2.35207600  |
| H | 3.68972500  | 3.51641800  | 1.35441600  |
| C | 0.00000000  | 4.52320100  | 2.02189200  |
| H | -0.52511800 | 2.83063100  | 0.78024300  |
| C | 1.03834100  | 5.26601700  | 2.59561600  |
| H | 3.18288900  | 5.46847700  | 2.79142400  |
| H | -1.04061300 | 4.79633000  | 2.20773900  |
| H | 0.81392500  | 6.12481400  | 3.23181100  |
| C | 3.20080400  | 1.28222900  | 0.34257200  |
| C | 4.25319500  | 1.39590700  | -0.56936800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.38741700  | 0.60513000  | 1.55428000  |
| C | 5.49123500  | 0.81144600  | -0.27469700 |
| H | 4.11920600  | 1.93185700  | -1.50748400 |
| C | 4.62660000  | 0.02976000  | 1.83871100  |
| H | 2.54662300  | 0.52439600  | 2.24746500  |
| C | 5.68298700  | 0.12581200  | 0.92596300  |
| H | 6.30747600  | 0.90126400  | -0.99470400 |
| H | 4.76169500  | -0.50130900 | 2.78339200  |
| H | 6.64968500  | -0.32989800 | 1.15120200  |
| C | 0.00000000  | 0.00000000  | 2.08997900  |
| H | 0.58897600  | -0.66557400 | 2.72868800  |
| H | -0.58897600 | 0.66557400  | 2.72868800  |
| N | 1.86861700  | 1.89257000  | 0.09055000  |
| N | -1.86861700 | -1.89257000 | 0.09055000  |

**C2'**  
B3LYP/BS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Be | -0.67076500 | -0.58720100 | 0.67700100  |
| Be | 0.67076500  | 0.58720100  | 0.67700100  |
| P  | -2.19608800 | -1.97984700 | 0.12559600  |
| P  | 2.19608800  | 1.97984700  | 0.12559600  |
| H  | -0.67623800 | 0.76092900  | -0.03692400 |
| H  | 0.67623800  | -0.76092900 | -0.03692400 |
| C  | 2.62174800  | 2.09707100  | -1.65596700 |
| C  | 2.61303000  | 0.90468300  | -2.40223300 |
| C  | 2.92752800  | 3.30639000  | -2.30072700 |
| C  | 2.92769100  | 0.92181400  | -3.76284600 |
| H  | 2.34403500  | -0.03480100 | -1.91405300 |
| C  | 3.23268000  | 3.32049900  | -3.66562000 |
| H  | 2.92007500  | 4.24194300  | -1.73906400 |
| C  | 3.23791600  | 2.12944100  | -4.39746800 |
| H  | 2.91820000  | -0.01098600 | -4.33115100 |
| H  | 3.46627800  | 4.26777900  | -4.15728300 |
| H  | 3.47571700  | 2.14287700  | -5.46369100 |
| C  | -2.62174800 | -2.09707100 | -1.65596700 |
| C  | -2.61303000 | -0.90468300 | -2.40223300 |
| C  | -2.92752800 | -3.30639000 | -2.30072700 |
| C  | -2.92769100 | -0.92181400 | -3.76284600 |
| H  | -2.34403500 | 0.03480100  | -1.91405300 |
| C  | -3.23268000 | -3.32049900 | -3.66562000 |
| H  | -2.92007500 | -4.24194300 | -1.73906400 |
| C  | -3.23791600 | -2.12944100 | -4.39746800 |
| H  | -2.91820000 | 0.01098600  | -4.33115100 |
| H  | -3.46627800 | -4.26777900 | -4.15728300 |
| H  | -3.47571700 | -2.14287700 | -5.46369100 |
| C  | 1.74942400  | 3.68196900  | 0.63711700  |
| C  | 2.69050200  | 4.60878400  | 1.11217400  |
| C  | 0.39758400  | 4.05672300  | 0.54736500  |
| C  | 2.28728100  | 5.89699000  | 1.47738000  |
| H  | 3.73910900  | 4.32166900  | 1.20861000  |
| C  | 0.00000000  | 5.34655500  | 0.90730400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.34317900 | 3.32963300  | 0.20681600  |
| C | 0.94359100  | 6.26866400  | 1.37188700  |
| H | 3.02655300  | 6.61005500  | 1.84948300  |
| H | -1.05334000 | 5.62648400  | 0.83612000  |
| H | 0.62987900  | 7.27444200  | 1.66095300  |
| C | 3.77041300  | 1.59767000  | 0.98138300  |
| C | 3.68520000  | 1.07821700  | 2.28624700  |
| C | 5.03086500  | 1.79429900  | 0.39476200  |
| C | 4.85115400  | 0.77768900  | 2.99486000  |
| H | 2.70012100  | 0.89737200  | 2.72633200  |
| C | 6.19328400  | 1.48613300  | 1.10836000  |
| H | 5.10688100  | 2.17992900  | -0.62342400 |
| C | 6.10523600  | 0.98146000  | 2.40952000  |
| H | 4.77633100  | 0.37325900  | 4.00683100  |
| H | 7.17000200  | 1.63964000  | 0.64352100  |
| H | 7.01480200  | 0.74061000  | 2.96500900  |
| C | -1.74942400 | -3.68196900 | 0.63711700  |
| C | -2.69050200 | -4.60878400 | 1.11217400  |
| C | -0.39758400 | -4.05672300 | 0.54736500  |
| C | -2.28728100 | -5.89699000 | 1.47738000  |
| H | -3.73910900 | -4.32166900 | 1.20861000  |
| C | 0.00000000  | -5.34655500 | 0.90730400  |
| H | 0.34317900  | -3.32963300 | 0.20681600  |
| C | -0.94359100 | -6.26866400 | 1.37188700  |
| H | -3.02655300 | -6.61005500 | 1.84948300  |
| H | 1.05334000  | -5.62648400 | 0.83612000  |
| H | -0.62987900 | -7.27444200 | 1.66095300  |
| C | -3.77041300 | -1.59767000 | 0.98138300  |
| C | -5.03086500 | -1.79429900 | 0.39476200  |
| C | -3.68520000 | -1.07821700 | 2.28624700  |
| C | -6.19328400 | -1.48613300 | 1.10836000  |
| H | -5.10688100 | -2.17992900 | -0.62342400 |
| C | -4.85115400 | -0.77768900 | 2.99486000  |
| H | -2.70012100 | -0.89737200 | 2.72633200  |
| C | -6.10523600 | -0.98146000 | 2.40952000  |
| H | -7.17000200 | -1.63964000 | 0.64352100  |
| H | -4.77633100 | -0.37325900 | 4.00683100  |
| H | -7.01480200 | -0.74061000 | 2.96500900  |
| C | 0.00000000  | 0.00000000  | 2.16969800  |
| H | -0.57828800 | 0.67981100  | 2.79988800  |
| H | 0.57828800  | -0.67981100 | 2.79988800  |

## A1''

### B3LYP/BS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.02596400 | 2.65170800  | -0.90910800 |
| C  | 0.02596400  | -2.65170800 | -0.90910800 |
| Be | -0.17879600 | 0.90789800  | -0.86274200 |
| Be | 0.17879600  | -0.90789800 | -0.86274200 |
| H  | -1.03368000 | -0.07997100 | -1.51836700 |
| H  | 1.03368000  | 0.07997100  | -1.51836700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.00000000  | 0.00000000  | 0.59683500  |
| Cl | 1.43620700  | 0.42336300  | 1.69675900  |
| Cl | -1.43620700 | -0.42336300 | 1.69675900  |
| C  | 0.00000000  | 4.91272000  | -1.13409100 |
| C  | 0.68719700  | 4.59999600  | 0.00284700  |
| H  | 1.18324300  | 5.23545800  | 0.72812100  |
| N  | 0.64949400  | 3.22228800  | 0.10859100  |
| C  | 0.00000000  | -4.91272000 | -1.13409100 |
| H  | 0.22236700  | -5.86908000 | -1.59391500 |
| N  | 0.41991800  | -3.69927300 | -1.66575100 |
| N  | -0.41991800 | 3.69927300  | -1.66575100 |
| H  | -0.22236700 | 5.86908000  | -1.59391500 |
| N  | -0.64949400 | -3.22228800 | 0.10859100  |
| C  | -0.68719700 | -4.59999600 | 0.00284700  |
| H  | -1.18324300 | -5.23545800 | 0.72812100  |
| H  | 0.96019800  | -3.58777800 | -2.51263400 |
| H  | 1.04520900  | 2.64042000  | 0.85459000  |
| H  | -0.96019800 | 3.58777800  | -2.51263400 |
| H  | -1.04520900 | -2.64042000 | 0.85459000  |

## A2''

### B3LYP/BS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.19955300  | 2.67105600  | -0.11952900 |
| C  | -0.19955300 | -2.67105600 | -0.11952900 |
| Be | -0.00134400 | 0.93151300  | 0.19090800  |
| Be | 0.00134400  | -0.93151300 | 0.19090800  |
| H  | -1.02412800 | 0.04186200  | -0.44576300 |
| H  | 1.02412800  | -0.04186200 | -0.44576300 |
| C  | 0.00000000  | 0.00000000  | 1.65993400  |
| Cl | 1.48511500  | 0.10830500  | 2.74188100  |
| Cl | -1.48511500 | -0.10830500 | 2.74188100  |
| C  | 1.09027000  | 4.68438100  | -0.68900100 |
| C  | 0.00000000  | 4.92474400  | 0.08539300  |
| C  | -1.09027000 | -4.68438100 | -0.68900100 |
| C  | 0.00000000  | -4.92474400 | 0.08539300  |
| N  | -0.52357300 | 3.68618300  | 0.43070000  |
| N  | -1.19510500 | -3.30307000 | -0.80334600 |
| N  | 1.19510500  | 3.30307000  | -0.80334600 |
| N  | 0.52357300  | -3.68618300 | 0.43070000  |
| H  | -0.45248000 | 5.85178400  | 0.41592200  |
| H  | -1.78952400 | -5.35663100 | -1.17232200 |
| H  | 1.78952400  | 5.35663100  | -1.17232200 |
| H  | 0.45248000  | -5.85178400 | 0.41592200  |
| C  | -1.73100400 | 3.54605600  | 1.21965800  |
| C  | -1.63424800 | 3.58702600  | 2.62758700  |
| C  | -2.83097100 | 3.50021500  | 3.35141500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.06069000 | 3.37654900  | 2.70700900  |
| C | -4.12355700 | 3.34433900  | 1.31598900  |
| C | -2.96062100 | 3.43579500  | 0.53749300  |
| C | -0.30235700 | 3.76019700  | 3.35458300  |
| C | -3.07101500 | 3.44686800  | -0.98527100 |
| C | -3.83829600 | 4.68847400  | -1.47865400 |
| C | -3.69795700 | 2.15036900  | -1.52623500 |
| C | -2.18176400 | -2.67094500 | -1.65187900 |
| C | -1.89158400 | -2.55902800 | -3.02753600 |
| C | -2.86567900 | -1.96910300 | -3.84664300 |
| C | -4.07733600 | -1.53026300 | -3.31747600 |
| C | -4.34172100 | -1.67145100 | -1.95523700 |
| C | -3.40209100 | -2.24333700 | -1.08623400 |
| C | -0.57970900 | -3.04920900 | -3.63735500 |
| C | 0.30773000  | -1.87497000 | -4.08612200 |
| C | -0.81817400 | -4.04093900 | -4.79061700 |
| C | -3.72241100 | -2.43221600 | 0.39453800  |
| C | -4.45860100 | -3.76915600 | 0.61969100  |
| C | -4.52472300 | -1.26929600 | 0.99714300  |
| C | -0.19780900 | 2.92076200  | 4.63832200  |
| C | -0.04496100 | 5.24775800  | 3.67485500  |
| C | 2.18176400  | 2.67094500  | -1.65187900 |
| C | 1.73100400  | -3.54605600 | 1.21965800  |
| C | 1.89158400  | 2.55902800  | -3.02753600 |
| C | 3.40209100  | 2.24333700  | -1.08623400 |
| C | 4.34172100  | 1.67145100  | -1.95523700 |
| C | 3.72241100  | 2.43221600  | 0.39453800  |
| C | 4.45860100  | 3.76915600  | 0.61969100  |
| C | 4.52472300  | 1.26929600  | 0.99714300  |
| C | 4.07733600  | 1.53026300  | -3.31747600 |
| C | 2.86567900  | 1.96910300  | -3.84664300 |
| C | 0.57970900  | 3.04920900  | -3.63735500 |
| C | -0.30773000 | 1.87497000  | -4.08612200 |
| C | 0.81817400  | 4.04093900  | -4.79061700 |
| C | 1.63424800  | -3.58702600 | 2.62758700  |
| C | 2.96062100  | -3.43579500 | 0.53749300  |
| C | 2.83097100  | -3.50021500 | 3.35141500  |
| C | 0.30235700  | -3.76019700 | 3.35458300  |
| C | 4.12355700  | -3.34433900 | 1.31598900  |
| C | 3.07101500  | -3.44686800 | -0.98527100 |
| C | 4.06069000  | -3.37654900 | 2.70700900  |
| C | 0.19780900  | -2.92076200 | 4.63832200  |
| C | 0.04496100  | -5.24775800 | 3.67485500  |
| C | 3.83829600  | -4.68847400 | -1.47865400 |
| C | 3.69795700  | -2.15036900 | -1.52623500 |
| H | -4.97778000 | 3.30159800  | 3.29606900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.09308600 | 3.25107900  | 0.82267300  |
| H | 0.49384100  | 3.41001400  | 2.68074100  |
| H | -2.05576500 | 3.50706300  | -1.40218800 |
| H | -4.88335200 | 4.68363400  | -1.12808600 |
| H | -3.85700000 | 4.71646900  | -2.58080900 |
| H | -3.37212900 | 5.62102600  | -1.12168100 |
| H | -3.11456400 | 1.27035700  | -1.21834900 |
| H | -4.73251900 | 2.01962500  | -1.16895400 |
| H | -5.29694700 | -1.32735900 | -1.55784800 |
| H | -0.02342200 | -3.59268500 | -2.86092800 |
| H | 0.53222300  | -1.20065400 | -3.24633300 |
| H | -1.44003300 | -4.89225900 | -4.47040500 |
| H | -2.77077000 | -2.47133800 | 0.94398500  |
| H | -5.42942400 | -3.77678000 | 0.09596300  |
| H | -4.65142600 | -3.92401900 | 1.69387400  |
| H | -3.87533900 | -4.62937700 | 0.25537100  |
| H | -4.01664600 | -0.30814500 | 0.83776400  |
| H | -4.61723100 | -1.41271700 | 2.08455900  |
| H | -5.54555600 | -1.20981800 | 0.58433300  |
| H | -2.79756300 | 3.51777600  | 4.44091000  |
| H | -3.72646900 | 2.17130700  | -2.62825400 |
| H | -2.67283800 | -1.85683600 | -4.91528800 |
| H | -4.82544100 | -1.07684200 | -3.97214700 |
| H | -0.18187100 | -1.28365600 | -4.87682200 |
| H | 1.26326500  | -2.24972200 | -4.48888500 |
| H | 0.14277800  | -4.43879500 | -5.15568700 |
| H | -1.32211600 | -3.56246100 | -5.64606000 |
| H | -0.87609100 | 3.28912900  | 5.42597200  |
| H | 0.82770300  | 2.98386400  | 5.03555900  |
| H | -0.42058800 | 1.86367000  | 4.44152800  |
| H | -0.04958500 | 5.88025400  | 2.77374700  |
| H | 0.93452900  | 5.36964400  | 4.16609100  |
| H | -0.81647900 | 5.63844500  | 4.35953900  |
| H | 2.77077000  | 2.47133800  | 0.94398500  |
| H | 4.01664600  | 0.30814500  | 0.83776400  |
| H | 4.61723100  | 1.41271700  | 2.08455900  |
| H | 5.54555600  | 1.20981800  | 0.58433300  |
| H | 5.29694700  | 1.32735900  | -1.55784800 |
| H | 4.82544100  | 1.07684200  | -3.97214700 |
| H | 0.02342200  | 3.59268500  | -2.86092800 |
| H | 0.18187100  | 1.28365600  | -4.87682200 |
| H | -1.26326500 | 2.24972200  | -4.48888500 |
| H | -0.53222300 | 1.20065400  | -3.24633300 |
| H | 1.44003300  | 4.89225900  | -4.47040500 |
| H | -0.14277800 | 4.43879500  | -5.15568700 |
| H | 1.32211600  | 3.56246100  | -5.64606000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.42942400  | 3.77678000  | 0.09596300  |
| H | 4.65142600  | 3.92401900  | 1.69387400  |
| H | 3.87533900  | 4.62937700  | 0.25537100  |
| H | 2.67283800  | 1.85683600  | -4.91528800 |
| H | 2.79756300  | -3.51777600 | 4.44091000  |
| H | -0.49384100 | -3.41001400 | 2.68074100  |
| H | 5.09308600  | -3.25107900 | 0.82267300  |
| H | 2.05576500  | -3.50706300 | -1.40218800 |
| H | 4.97778000  | -3.30159800 | 3.29606900  |
| H | 0.87609100  | -3.28912900 | 5.42597200  |
| H | -0.82770300 | -2.98386400 | 5.03555900  |
| H | 0.42058800  | -1.86367000 | 4.44152800  |
| H | 0.04958500  | -5.88025400 | 2.77374700  |
| H | -0.93452900 | -5.36964400 | 4.16609100  |
| H | 0.81647900  | -5.63844500 | 4.35953900  |
| H | 4.88335200  | -4.68363400 | -1.12808600 |
| H | 3.85700000  | -4.71646900 | -2.58080900 |
| H | 3.37212900  | -5.62102600 | -1.12168100 |
| H | 3.11456400  | -1.27035700 | -1.21834900 |
| H | 3.72646900  | -2.17130700 | -2.62825400 |
| H | 4.73251900  | -2.01962500 | -1.16895400 |