

**Supporting Information**  
**of**  
**One Electron Be-Be  $\pi$  bond**

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Cartesian coordinates and electronic energies calculated at CCSD(T)/aug-cc-pVQZ, CASSCF(5,6)/aug-cc-pVTZ and NEVPT2/aug-cc-pVQZ levels.

**Be<sub>2</sub> (Neutral)@CCSD(T)**

E= -29.239976

|   |             |             |             |
|---|-------------|-------------|-------------|
| 4 | 0.000000000 | 0.000000000 | 1.271177000 |
|---|-------------|-------------|-------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 4 | 0.000000000 | 0.000000000 | -1.271177000 |
|---|-------------|-------------|--------------|

**Be<sub>2</sub> (Anion)@CCSD(T)**

E = -29.256243

|   |             |             |             |
|---|-------------|-------------|-------------|
| 4 | 0.000000000 | 0.000000000 | 1.116921000 |
|---|-------------|-------------|-------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 4 | 0.000000000 | 0.000000000 | -1.116921000 |
|---|-------------|-------------|--------------|

**Be<sub>2</sub> (Neutral)@CASSCF**

E= -29.196719

|   |             |             |             |
|---|-------------|-------------|-------------|
| 4 | 0.000000000 | 0.000000000 | 1.149320000 |
|---|-------------|-------------|-------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 4 | 0.000000000 | 0.000000000 | -1.149320000 |
|---|-------------|-------------|--------------|

**Be<sub>2</sub> (Anion)@CASSCF**

E= -29.184974

|   |             |             |             |
|---|-------------|-------------|-------------|
| 4 | 0.000000000 | 0.000000000 | 1.089387000 |
|---|-------------|-------------|-------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 4 | 0.000000000 | 0.000000000 | -1.089387000 |
|---|-------------|-------------|--------------|

**Be<sub>2</sub> (Neutral)@NEVPT2**

E=-29.2415395

|   |             |             |             |
|---|-------------|-------------|-------------|
| 4 | 0.000000000 | 0.000000000 | 1.154592000 |
|---|-------------|-------------|-------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 4 | 0.000000000 | 0.000000000 | -1.154592000 |
|---|-------------|-------------|--------------|

**Be<sub>2</sub> (Anion)@NEVPT2**

E= -29.2568143

|   |              |              |             |
|---|--------------|--------------|-------------|
| 4 | 0.0000000000 | 0.0000000000 | 1.083743000 |
|---|--------------|--------------|-------------|

|   |              |              |              |
|---|--------------|--------------|--------------|
| 4 | 0.0000000000 | 0.0000000000 | -1.083743000 |
|---|--------------|--------------|--------------|