Supporting Information

Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantum-Chemical Assessment
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1. Computational Details

The calculations of the electronic structures were performed with ORCA, Gaussian and MRCC.[1]

We used the B3LYP[2] density functional in combination with the aug-cc-pVTZ[3] basis set for the structural optimization to model the potential energy surfaces of the thermal reactions. Harmonic vibrational frequencies were computed to verify the nature of the stationary points. The minimum structures reported in this paper show only positive eigenvalues of the Hessian matrix, whereas the transition states (TSs) have only one negative eigenvalue. Intrinsic reaction coordinate[4] calculations were also performed to confirm that the transition states correlate with designated intermediates. The thermodynamic functions (ΔH) were estimated within the ideal gas, rigid-rotor, and harmonic oscillator approximations at 4K and 1 atm.

As commonly accepted, the geometries of molecular structures are less dependent on the level of theory than the energies. Therefore, for further energetic refinements, single-point energy calculations by using the CCSD(T) method in combination with various basis sets such as aug-cc-pVTZ (AVTZ), aug-cc-pVQZ (AVQZ), and ANO-pVTZ:ANO-pVQZ[5] extrapolated complete basis set (CBS)[5-6] were performed for the structures as optimized by the aid of the B3LYP functional. The energetic information is given in Table S1.

Quite elaborate multireference (MR) calculations were conducted to determine the relative energies of low-lying electronic states of Be2. To treat dynamic correlation without the problems of intruder states or level shifts,[7] CASPT2[8] in conjunction with the aug-cc-pVQZ basis set, as implemented in ORCA, was employed to optimize the geometries of Be2; the active space (4e,8o) with 4-electron in 8 orbitals has been considered in these calculations.

For the calculations of the different spin states of Be2, the state-specific complete active space self-consistent field (CASSCF)[9] approach in conjunction with the aug-cc-pVTZ basis set was conducted to obtain the electronic configuration. An active space (14e,16o) has been considered; for the selection of the active space, see Figure S1. In addition, we also optimized the structures by using the CCSD(T) method with various basis sets such as aug-cc-pVTZ (AVTZ), aug-cc-pVQZ (AVQZ), cc-pVTZ (VTZ), aug-cc-pVQZ (VQZ), and refined the energy by using aug-cc-pV5Z (AV5Z) and CBS basis sets, respectively. The energetic information is given in Table 1.

In addition, single-point energy, vibrational frequencies (cm\(^{-1}\)), IR intensities (km mol\(^{-1}\)) of selected isomers by various DFT and MP2 methods in conjunction with the aug-cc-pVTZ basis set were also performed; the data is given in Tables S2, S3 and S5.
2. Figures

Figure S1. The selected active spaces considered in the CASSCF(14e,16o)/aug-cc-pVTZ calculations for the triplet and quintet states of BeOBeC. Natural orbital partial occupation numbers and roots are given.
Figure S2. Simplified PES ($\Delta H_{4K}$ in kJ mol$^{-1}$) and optimized structures (bond lengths in Å) for the reactions of Be$_2$ with CO as obtained at the B3LYP/aug-cc-pVTZ level of theory. The insets display the MECPs. Color codes: singlet: blue; triplet: brown; quintet: red, MECP: purple.
Figure S3. IR spectra of $^3$S$_5$ and the assignment of vibrational modes as obtained at the B3LYP/aug-cc-pVTZ level of theory.
### 3. Tables

**Table S1.** Energetics (in kJ mol\(^{-1}\)) as obtained at the B3LYP/aug-cc-pVTZ level by using Gaussian and ORCA and at the CCSD(T)/aug-cc-pVTZ (AVTZ), CCSD(T)/aug-cc-pVQZ (AVQZ), CCSD(T)/ANO-cc-pVTZ:ANO-cc-pVQZ (CBS) levels by ORCA. ΔΔ\(H\) gives the errors of B3LYP as compared with CCSD(T)/CBS. The T1 diagnostic values of the CCSD(T) calculations are provided as well. Numbers given in red suggest that the data based on the CCSD(T) approaches should be viewed with caution.

|        | B3LYP       |       |       | CCSD(T)     |       |       |      |
|--------|-------------|-------|-------|-------------|-------|-------|------|
|        | Gaussian    | ORCA  | AVTZ  | AVQZ        | CBS   | ΔΔ\(H\) | T1   |
| \(^1\)Be\(_2\)+CO | 185         | 186   | 172   | 198         | 199   | 13     | 0.094|
| \(^3\)Be\(_2\)+CO | 242         | 242   | 245   | 274         | 277   | 35     | 0.014|
| \(^1\)1 | 96          | 96    | 106   | 119         | 119   | 23     | 0.020|
| \(^3\)1 | 91          | 91    | 100   | 113         | 113   | 22     | 0.020|
| \(^1\)TS1/2 | 183         | 183   | 198   | 199         | 199   | 16     | 0.053|
| \(^3\)TS1/2 | 181         | 181   | 200   | 193         | 193   | 12     | 0.064|
| \(^1\)2 | 142         | 142   | 156   | 152         | 152   | 11     | 0.057|
| \(^3\)2 | 138         | 138   | 165   | 157         | 157   | 19     | 0.085|
| \(^1\)TS2/3 | 170         | 170   | 179   | 179         | 179   | 9      | 0.074|
| \(^3\)TS2/3 | 169         | 169   | 180   | 179         | 179   | 10     | 0.073|
| \(^1\)3 | 159         | 159   | 165   | 166         | 166   | 6      | 0.020|
| \(^3\)3 | 158         | 158   | 164   | 165         | 165   | 6      | 0.036|
| \(^1\)TS3/4 | 179         | 179   | 177   | 177         | 177   | -3     | 0.020|
| \(^3\)TS3/4 | 181         | 180   | 179   | 177         | 177   | -3     | 0.019|
| \(^1\)4 | 163         | 163   | 159   | 150         | 150   | -13    | 0.019|
| \(^3\)4 | 165         | 164   | 161   | 151         | 151   | -13    | 0.018|
| \(^1\)TS4/5\(^*\) | 172         | 172   | 201   | 187         | 187   | 15     | 0.071|
| \(^3\)TS4/5 | 175         | 175   | 180   | 169         | 169   | -6     | 0.040|
| \(^1\)5 | 29          | 29    | 34    | 34          | 34    | 5      | 0.022|
| \(^3\)5 | 0           | 0     | 0     | 0           | 0     | 0      | 0.024|
| \(^1\)TS5/6 | 133         | 133   | 146   | 164         | 164   | 31     | 0.031|
| \(^3\)TS5/6 | 106         | 106   | 101   | 117         | 117   | 11     | 0.027|
| \(^1\)6 | 73          | 73    | 76    | 91          | 91    | 19     | 0.015|
| \(^3\)6 | 39          | 39    | 24    | 39          | 38.51 | 0      | 0.017|
| \(^1\)TS3/7 | 39          | 39    | 24    | 38          | 38.36 | 0      | 0.016|
| \(^3\)TS3/7 | 196         | 195   | 220   | 229         | 229   | 33     | 0.022|
| \(^1\)7 | 178         | 178   | 195   | 203         | 203   | 25     | 0.020|
| \(^3\)7 | 168         | 168   | 198   | 208         | 208   | 40     | 0.021|
| \(^5\)7 | 151         | 151   | 174   | 183         | 183   | 32     | 0.020|
| CP1    | 181         | 181   | 201   | 205         | 205   | 23     | 0.059|
| CP2    | 115         | 115   | 110   | 112         | 112   | -3     | 0.045|
| CP3    | 39          | 39    | 24    | 39          | 39    | 0      | 0.017|
Table S2. Energy differences (in kJ mol⁻¹ without zero-point energy corrections) between \(^3\text{6}\) and \(^6\text{6}\) relative to the latter. Note, the AVTZ basis set was used in these single point energy calculations by using the geometries optimized at the B3LYP/AVTZ level.

| Method       | Energy Difference (kJ mol⁻¹) |
|--------------|------------------------------|
| VWN          | -0.04                        |
| VWN3         | 0.02                         |
| PWLDA        | -0.03                        |
| BP86         | 0.10                         |
| BLYP         | -0.45                        |
| OLYP         | -0.22                        |
| XLYP         | -0.57                        |
| PW91         | 0.14                         |
| mPW PW       | 0.21                         |
| mPW WL       | -0.62                        |
| PBE          | 0.14                         |
| RPBE         | 0.05                         |
| REV PBE      | 0.13                         |
| PWP          | -0.09                        |
| B1LYP        | -0.01                        |
| B3LYP        | 0.01                         |
| O3LYP        | 0.04                         |
| X3LYP        | 0.00                         |
| B1P          | 0.15                         |
| B3P          | 0.15                         |
| B3PW         | 0.21                         |
| PW1 PW       | 0.17                         |
| mPW1 PW      | 0.19                         |
| mPW1 LW      | -0.03                        |
| PBE0         | 0.18                         |
| BHand HLYP   | 0.01                         |
| TPSS         | 0.08                         |
| TPSSH        | 0.11                         |
| TPSS0        | 0.10                         |
| M06          | 0.05                         |
| **M062X**    | **-0.58**                    |
| B97 M-D3BJ   | 0.22                         |
| wB97         | -0.01                        |
| wB97 X       | 0.06                         |
| wB97 X-D3BJ  | 0.09                         |
| CAM-B3LYP    | 0.07                         |
| LC-B3LYP     | 0.12                         |
| B2 PLYP      | 0.09                         |
| mPW2 PLYP    | 0.07                         |
| B2 GP-PLOY   | 0.10                         |
| B2 K-PLOY    | 0.12                         |
| B2 T-PLOY    | 0.10                         |
| DSD-BLYP     | 0.13                         |
| DSD-PBE P86  | 0.16                         |
| wB2 PLOY     | 0.12                         |
| wB2 GP-PLOY  | 0.13                         |
| **Average**  | **0.03**                     |
Table S3. Calculated vibrational frequencies (cm$^{-1}$) and IR intensities (km mol$^{-1}$) of [2Be,C,O] isomers at the B3LYP/aug-cc-pVTZ level of theory.

|     | $\nu_1$ (cm$^{-1}$) | $I$ (km mol$^{-1}$) | $\nu_2$ (cm$^{-1}$) | $I$ (km mol$^{-1}$) |
|-----|---------------------|---------------------|---------------------|---------------------|
| CO  | 2207.3              | 80                  |                     |                     |
| $^1$| 2028.9              | 773                 |                     |                     |
| $^3$| 2030.6              | 835                 |                     |                     |
| $^2$| 1396.8              | 450                 |                     |                     |
| $^3$| 1370.6              | 303                 |                     |                     |
| $^3$| 926.9               | 205                 | 1461.1              | 43.4                |
| $^3$| 923.6               | 212                 | 1460.8              | 38.6                |
| $^4$| 998.8               | 224                 | 1123.9              | 19.6                |
| $^4$| 1003.9              | 252                 | 1139.0              | 21.8                |
| $^5$| 1156.0              | 120                 |                     |                     |
| $^5$| 1157.1              | 110                 |                     |                     |
| $^6$| 1155.4              | 0.4                 | 1485.5              | 792                 |
| $^6$| 1190.1              | 0.7                 | 1495.5              | 890                 |
| $^5$| 1190.3              | 0.1                 | 1497.1              | 919                 |
| $^7$| 1170.5              | 458                 | 1678.8              | 253                 |
| $^7$| 1159.4              | 415                 | 1666.7              | 87.2                |
| $^5$| 1150.9              | 412                 | 1662.8              | 147                 |
Table S4. Calculated vibrational frequencies (cm\(^{-1}\)), IR intensities (km mol\(^{-1}\)) of selected isomers by various methods in conjunction with the aug-cc-pVTZ basis set.

|       | \(^{31}\) vib | \(^{36}\) vib1 | \(^{36}\) vib2 | \(^{56}\) vib1 | \(^{56}\) vib2 | \(^{57}\) vib1 | \(^{57}\) vib2 | \(^{35}\) vib | \(^{35}\) int |
|-------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| B3LYP | 2031           | 835            | 1495           | 890            | 1190           | 1              | 1497           | 919            | 1190           | 0              |
| BP86  |                |                |                |                |                |                |                |                |                | 1663           |
| TPSS  |                |                |                |                |                |                |                |                |                | 147            |
| TPSSH | 2011           | 826            | 1486           | 873            | 1183           | 0              | 1489           | 893            | 1186           | 0              |
| BH&HLYP |             |                |                |                |                |                |                |                |                | 1640           |
| BMK   |                | 1468           | 796            | 1169           | 0              | 1470           | 863            | 1169           | 0              | 1610           |
| CAM-B3LYP |            |                |                |                |                |                |                |                |                | 1166           |
| M062X | 2115           | 1028           | 1541           | 972            | 1228           | 1              | 1542           | 976            | 1228           | 1              |
| M06L  | 2035           | 1757           |                |                |                |                |                |                |                |                |
| M11   | 2069           | 783            | 1466           | 954            | 1162           | 0              | 1466           | 955            | 1162           | 0              |
| M11L  | 1471           | 727            | 1168           | 8              | 1476           | 935            | 1170           | 0              | 1695           |
| PBE1PBE |             |                |                |                |                |                |                |                |                | 1100           |
| X3LYP | 2036           | 845            | 1499           | 892            | 1193           | 1              | 1500           | 920            | 1194           | 0              |
| wB97  | 2058           | 777            | 1474           | 961            | 1176           | 1              | 1475           | 963            | 1176           | 1              |
| B2LYP | 1984           | 775            | 1494           | 923            | 1187           | 0              | 1496           | 926            | 1189           | 0              |
| B2GP-PLYP |            |                |                |                |                |                |                |                |                |                |
| MP2   | 1957           | 836            | 1479           | 942            | 1176           | 0              | 1479           | 940            | 1176           | 0              |

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Table S5. Relative energies (in kJ mol\(^{-1}\)) of isomers 5 and 6 at 4K as obtained at the CCSD(T)/CBS(ANO-pVTZ:ANO-pVQZ)//B3LYP/aug-cc-pVTZ level of theory.

| CCSD(T) | \(\Delta H\) | \(\Delta E\) |
|---------|--------------|--------------|
| \(^1\text{S}5\) | 38 | 35.8 |
| \(^3\text{S}5\) | 0.0 | 0.0 |
| \(^1\text{S}6\) | 82 | 87.0 |
| \(^3\text{S}6\) | 40 | 43.3 |
| \(^5\text{S}6\) | 40 | 43.1 |

Table S6. Relative energies (in kJ mol\(^{-1}\)) for selected isomers as obtained by various methods in conjunction with the aug-cc-pVTZ basis set.

|       | \(^3\text{S}1\) | \(^5\text{S}5\) | \(^5\text{S}6\) | \(^5\text{S}6\) | \(^5\text{S}7\) |
|-------|----------------|----------------|----------------|----------------|----------------|
| B3LYP | 96             | 31             | 0              | 43             | 43             | 154           |
| BP86  | 31             | 0              | 67             | 67             | 144            |
| TPSS  | 36             | 0              | 57             | 56             | 155            |
| TPSSH | 91             | 38             | 0              | 48             | 48             | 154           |
| BH&HLYP | 102         | 33             | 0              | 17             | 17             | 151           |
| BMK   | 118            | 45             | 0              | 48             | 48             | 160           |
| CAM-B3LYP | 101        | 33             | 0              | 37             | 37             | 155           |
| M062X | 121            | 54             | 0              | 41             | 42             | 176           |
| M06L  | 128            | 54             | 0              | 51             |
| M11   | 85             | 42             | 0              | 34             | 33             | 158           |
| M11L  | 42             | 0              | 46             | 46             | 171           |
| PBE1PBE | 91          | 37             | 0              | 44             | 43             | 139           |
| X3LYP | 97             | 31             | 0              | 44             | 44             | 155           |
| wB97  | 95             | 37             | 0              | 53             | 53             | 190           |
| B2PLYP | 98           | 36             | 0              | 39             | 39             | 165           |
| B2GP-PLYP | 101        | 39             | 0              | 32             | 32             | 164           |
| MP2   | 104            | 72             | 0              | 22             | 23             | 167           |
| CCSDT | 0              | 28             | 28             |                |                |                |
4. Coordinates of key isomers of [2Be,C,O] as obtained at the B3LYP/AVTZ level of theory

1

|   |   |   |   |
|---|---|---|---|
| Be | 0.000000 | 0.000000 | 2.669266 |
| Be | 0.000000 | 0.000000 | 0.601658 |
| C  | 0.000000 | 0.000000 | -1.057542 |
| O  | 0.000000 | 0.000000 | -2.213382 |

3

|   |   |   |   |
|---|---|---|---|
| Be | 0.000000 | 0.000000 | 0.000053 |
| Be | 0.000000 | 0.000000 | 2.072110 |
| C  | 0.000000 | 0.000000 | 3.734123 |
| O  | 0.000000 | 0.000000 | 4.888714 |

1

|   |   |   |
|---|---|---|
| Be | -0.307534 | 1.375789 | -0.469048 |
| Be | -0.716676 | -0.234509 | 0.747356 |
| C  | 0.490252 | -0.084298 | -0.545904 |
| O  | 0.533958 | -1.056982 | 0.267596 |

3

|   |   |   |
|---|---|---|
| Be | -1.216498 | 10.331511 | -10.196017 |
| Be | -2.472730 | 9.549852 | -8.880513 |
| C  | -1.259964 | 10.483217 | -8.498108 |
| O  | -0.329871 | 11.094461 | -9.187565 |

3

|   |   |   |
|---|---|---|
| C  | 0.098802 | 0.019165 | 0.369641 |
| Be | -0.723015 | 0.021133 | 1.886690 |
| Be | 1.217935 | 0.044921 | -0.901330 |
| O  | -0.351547 | -0.051898 | -0.826025 |

3

|   |   |   |
|---|---|---|
| C  | 0.093548 | 0.018841 | 0.368857 |
| Be | -0.720532 | 0.020528 | 1.887939 |
| Be | 1.218521 | 0.045431 | -0.898268 |
| O  | -0.349362 | -0.051478 | -0.829552 |

1

|   |   |   |
|---|---|---|
| C  | -0.628109 | 0.000678 | -0.461342 |
| Be | -0.873291 | -0.000316 | 1.231892 |
| Be | 0.914243 | -0.000304 | -1.201820 |
| O  | 0.471023 | -0.000035 | 0.345958 |

3

|   |   |   |
|---|---|---|
| C  | -0.626838 | 0.000470 | -0.460409 |
| Be | -0.872921 | -0.000064 | 1.230784 |
Be  0.913297  -0.000052  -1.201136
O  0.470328  -0.000332  0.345449

Be  0.000000  0.376342  0.859315
Be  0.000000  -0.228593  -0.909887
C  0.000000  -1.281029  0.438038
O  0.000000  1.133280  -0.387466

C  0.000000  0.000000  0.000000
Be  0.000000  0.000000  1.681462
Be  1.561445  0.000000  0.623862
O  1.406943  0.000000  2.077216

C  -2.267351  0.004630  0.000000
Be  2.255255  0.018415  0.000011
Be  -0.557950  -0.016301  0.000013
O  0.851193  -0.003382  -0.000003

Be  0.000000  0.000000  -0.000130
O  0.000000  0.000000  1.402398
Be  0.000000  0.000000  2.813987
C  0.000000  0.000000  4.462744

Be  0.000000  0.000000  0.000000
O  0.000000  0.000000  1.403000
Be  0.000000  0.000000  2.814000
C  0.000000  0.000000  4.462000

Be  0.000000  0.000000  1.677739
Be  0.000000  0.000000  -2.592112
C  0.000000  0.000000  -1.007682
O  0.000000  0.000000  0.264410

Be  0.000000  0.000000  1.677865
Be  0.000000  0.000000  -2.591669
C  0.000000  0.000000  -1.004757
O  0.000000  0.000000  0.260916

Be  0.000000  0.000000  0.000000
C  0.000000  0.000000  1.590000
O  0.000000  0.000000  2.853000
Be  0.000000  0.000000  4.272000
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