# Interplay between the gentlest ascent dynamics method and conjugate directions to locate transition states

# Supporting Information

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## 1. Sets of internal coordinates

**Table S1.1**. Set of internal coordinates employed in the location of the TS configuration of the *sn2* reaction.

| Variable number | Type of variable | Atoms involved in the definition of the internal variable[a] | | | |
|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | |
| 2 | distance | 3 | 2 | | |
| 3 | angle[b] | 3 | 1 | 2 | |
| 4 | distance | 4 | 2 | | |
| 5 | angle | 4 | 3 | 2 | |
| 6 | dihedral | 4 | 2 | 3 | 1 |
| 7 | distance | 5 | 2 | | |
| 8 | angle | 5 | 1 | 2 | |
| 9 | dihedral | 5 | 2 | 1 | 3 |
| 10 | distance | 6 | 2 | | |
| 11 | angle | 6 | 1 | 2 | |
| 12 | dihedral | 6 | 2 | 1 | 3 |

*a*) See Figure 2 in the main text for the atom numbering.
*b*) In the definition of angles, the third atom number refers to the atom in the apex.

**Table S1.2**. Set of internal coordinates employed in the location of the TS configuration of the *sn2b* reaction.

| Variable number | Type of variable | Atoms involved in the definition of the internal variable[a] | | | |
|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | |
| 2 | distance | 3 | 2 | | |
| 3 | angle[b] | 2 | 1 | 3 | |
| 4 | distance | 4 | 2 | | |
| 5 | angle | 4 | 3 | 2 | |
| 6 | dihedral | 4 | 2 | 3 | 1 |
| 7 | distance | 5 | 4 | | |
| 8 | angle | 5 | 2 | 4 | |
| 9 | dihedral | 5 | 4 | 3 | 2 |
| 10 | distance | 6 | 2 | | |
| 11 | angle | 6 | 3 | 2 | |
| 12 | dihedral | 6 | 2 | 3 | 1 |
| 13 | distance | 7 | 2 | | |
| 14 | angle | 7 | 3 | 2 | |
| 15 | dihedral | 7 | 2 | 3 | 1 |
| 16 | distance | 8 | 4 | | |
| 17 | angle | 8 | 5 | 4 | |
| 18 | dihedral | 8 | 4 | 5 | 2 |
| 19 | distance | 9 | 4 | | |
| 20 | angle | 9 | 5 | 4 | |
| 21 | dihedral | 9 | 4 | 5 | 2 |

*a*) See Figure 3 in the main text for the atom numbering.
*b*) In the definition of angles, the third atom number refers to the atom in the apex.

**Table S1.3**. Set of internal coordinates employed in the location of the TS configuration of the *sig* reaction.

| Variable number | Type of variable | Atoms involved in the definition of the internal variable[a] | | | |
|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | |
| 2 | distance | 3 | 2 | | |
| 3 | angle[b] | 3 | 1 | 2 | |
| 4 | distance | 4 | 3 | | |
| 5 | angle | 4 | 2 | 3 | |
| 6 | dihedral | 4 | 3 | 2 | 1 |
| 7 | distance | 5 | 1 | | |
| 8 | angle | 5 | 2 | 1 | |
| 9 | dihedral | 5 | 1 | 2 | 3 |
| 10 | distance | 6 | 2 | | |
| 11 | angle | 6 | 3 | 2 | |
| 12 | dihedral | 6 | 2 | 3 | 4 |
| 13 | distance | 7 | 3 | | |
| 14 | angle | 7 | 4 | 3 | |
| 15 | dihedral | 7 | 3 | 2 | 4 |
| 16 | distance | 8 | 4 | | |
| 17 | angle | 8 | 3 | 4 | |
| 18 | dihedral | 8 | 4 | 3 | 2 |
| 19 | distance | 9 | 1 | | |
| 20 | angle | 9 | 2 | 1 | |
| 21 | dihedral | 9 | 1 | 2 | 3 |
| 22 | distance | 10 | 9 | | |
| 23 | angle | 10 | 4 | 9 | |
| 24 | dihedral | 10 | 9 | 4 | 3 |
| 25 | distance | 11 | 1 | | |
| 26 | angle | 11 | 1 | 9 | |
| 27 | dihedral | 11 | 9 | 1 | 3 |

*a*) See Figure 4 in the main text for the atom numbering.
*b*) In the definition of angles, the third atom number refers to the atom in the apex.

**Table S1.4**. Set of internal coordinates employed in the location of the TS configuration of the *dcc* reaction.

| Variable number | Type of variable | Atoms involved in the definition of the internal variable[a] | | | |
|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | |
| 2 | distance | 3 | 1 | | |
| 3 | angle[b] | 3 | 2 | 1 | |
| 4 | distance | 4 | 3 | | |
| 5 | angle | 4 | 1 | 3 | |
| 6 | dihedral | 4 | 3 | 1 | 2 |
| 7 | distance | 5 | 2 | | |
| 8 | angle | 5 | 1 | 2 | |
| 9 | dihedral | 5 | 2 | 1 | 3 |
| 10 | distance | 6 | 1 | | |
| 11 | angle | 6 | 2 | 1 | |
| 12 | dihedral | 6 | 1 | 2 | 3 |
| 13 | distance | 7 | 1 | | |
| 14 | angle | 7 | 3 | 1 | |
| 15 | dihedral | 7 | 1 | 3 | 2 |
| 16 | distance | 8 | 2 | | |
| 17 | angle | 8 | 1 | 2 | |
| 18 | dihedral | 8 | 2 | 1 | 3 |
| 19 | distance | 9 | 3 | | |
| 20 | angle | 9 | 1 | 3 | |
| 21 | dihedral | 9 | 3 | 1 | 2 |
| 22 | distance | 10 | 4 | | |
| 23 | angle | 10 | 3 | 4 | |
| 24 | dihedral | 10 | 4 | 3 | 1 |
| 25 | distance | 11 | 4 | | |
| 26 | angle | 11 | 3 | 4 | |
| 27 | dihedral | 11 | 4 | 3 | 10 |
| 28 | distance | 12 | 4 | | |
| 29 | angle | 12 | 3 | 4 | |
| 30 | dihedral | 12 | 4 | 3 | 10 |
| 31 | distance | 13 | 5 | | |
| 32 | angle | 13 | 2 | 5 | |
| 33 | dihedral | 13 | 5 | 2 | 1 |
| 34 | distance | 14 | 5 | | |
| 35 | angle | 14 | 2 | 5 | |
| 36 | dihedral | 14 | 5 | 2 | 13 |
| 37 | distance | 15 | 5 | | |
| 38 | angle | 15 | 2 | 5 | |
| 39 | dihedral | 15 | 5 | 2 | 13 |

*a*) See Figure 5 in the main text for the atom numbering.

*b*) In the definition of angles, the third atom number refers to the atom in the apex.

**Table S1.5**. Set of internal coordinates employed in the location of the TS configuration of the *bcb* reaction.

| Variable number | Type of variable | Atoms involved in the definition of the internal variable[a] | | | |
|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | |
| 2 | distance | 3 | 1 | | |
| 3 | angle[b] | 3 | 2 | 1 | |
| 4 | distance | 4 | 2 | | |
| 5 | angle | 4 | 1 | 2 | |
| 6 | dihedral | 4 | 2 | 1 | 3 |
| 7 | distance | 5 | 3 | | |
| 8 | angle | 5 | 1 | 3 | |
| 9 | dihedral | 5 | 3 | 1 | 2 |
| 10 | distance | 6 | 4 | | |
| 11 | angle | 6 | 2 | 4 | |
| 12 | dihedral | 6 | 4 | 2 | 1 |
| 13 | distance | 7 | 4 | | |
| 14 | angle | 7 | 2 | 4 | |
| 15 | dihedral | 7 | 4 | 2 | 8 |
| 16 | distance | 8 | 2 | | |
| 17 | angle | 8 | 1 | 2 | |
| 18 | dihedral | 8 | 2 | 1 | 3 |
| 19 | distance | 9 | 1 | | |
| 20 | angle | 9 | 2 | 1 | |
| 21 | dihedral | 9 | 1 | 2 | 4 |
| 22 | distance | 10 | 3 | | |
| 23 | angle | 10 | 1 | 3 | |
| 24 | dihedral | 10 | 3 | 1 | 2 |
| 25 | distance | 11 | 5 | | |
| 26 | angle | 11 | 3 | 5 | |
| 27 | dihedral | 11 | 5 | 3 | 1 |
| 28 | distance | 12 | 6 | | |
| 29 | angle | 12 | 4 | 6 | |
| 30 | dihedral | 12 | 6 | 4 | 2 |
| 31 | distance | 13 | 11 | | |
| 32 | angle | 13 | 5 | 11 | |
| 33 | dihedral | 13 | 11 | 5 | 6 |
| 34 | distance | 14 | 12 | | |
| 35 | angle | 14 | 6 | 12 | |
| 36 | dihedral | 14 | 12 | 6 | 4 |
| 37 | distance | 15 | 11 | | |
| 38 | angle | 15 | 5 | 11 | |

| | | | | | |
|---|---|---|---|---|---|
| 39 | dihedral | 15 | 11 | 5 | 3 |
| 40 | distance | 16 | 12 | | |
| 41 | angle | 16 | 6 | 12 | |
| 42 | dihedral | 16 | 12 | 6 | 5 |
| 43 | distance | 17 | 15 | | |
| 44 | angle | 17 | 11 | 15 | |
| 45 | dihedral | 17 | 15 | 11 | 5 |
| 46 | distance | 18 | 15 | | |
| 47 | angle | 18 | 11 | 15 | |
| 48 | dihedral | 18 | 15 | 11 | 7 |
| 49 | distance | 19 | 15 | | |
| 50 | angle | 19 | 11 | 15 | |
| 51 | dihedral | 19 | 15 | 11 | 17 |
| 52 | distance | 20 | 16 | | |
| 53 | angle | 20 | 12 | 16 | |
| 54 | dihedral | 20 | 16 | 12 | 6 |
| 55 | distance | 21 | 16 | | |
| 56 | angle | 21 | 12 | 16 | |
| 57 | dihedral | 21 | 16 | 12 | 20 |
| 58 | distance | 22 | 16 | | |
| 59 | angle | 22 | 12 | 16 | |
| 60 | dihedral | 22 | 16 | 12 | 20 |

*a*) See Figure 6 in the main text for the atom numbering.
*b*) In the definition of angles, the third atom number refers to the atom in the apex.

# 2. Initial configurations

## 2.1. Intial configurations for the *sn2* reactions

**Initial configuration (in cartesian coordinates) for the *sn2.1.n* reactions** (*n*=1,15)

| | | | |
|---|---|---|---|
| F | -2.4672660 | 0.0007512 | -0.0001717 |
| C | -0.6731430 | 0.0005964 | -0.0014634 |
| H | -0.5364968 | -0.8920896 | -0.5943660 |
| Cl | 1.8526759 | 0.0004861 | -0.0002772 |
| H | -0.5335207 | -0.0701768 | 1.0929060 |
| H | -0.5360983 | 0.9622929 | -0.4741287 |

**Initial configuration (in internal coordinates) for the *sn2.1.n* reactions** (*n*=1,15)
(distances in atomic units; angles and dihedrals in degree)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 3.39040 |
| 2 | distance | 3 | 2 | | | 2.04151 |
| 3 | angle | 3 | 1 | 2 | | 97.29355 |
| 4 | distance | 4 | 2 | | | 4.77311 |
| 5 | angle | 4 | 3 | 2 | | 82.74619 |
| 6 | dihedral | 4 | 2 | 3 | 1 | 179.94412 |
| 7 | distance | 5 | 2 | | | 2.08911 |
| 8 | angle | 5 | 1 | 2 | | 97.21481 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 240.11201 |
| 10 | distance | 6 | 2 | | | 2.04148 |
| 11 | angle | 6 | 1 | 2 | | 97.30180 |
| 12 | dihedral | 6 | 2 | 1 | 3 | 120.24410 |

**Initial configuration (in cartesian coordinates) for the *sn2.2.n* reactions** (*n*=1,2)

| | | | |
|---|---|---|---|
| F | -2.4279870 | 0.0007465 | -0.0002054 |
| C | -0.7557393 | 0.0005718 | -0.0009818 |
| H | -0.5447866 | -0.8847321 | -0.5895375 |
| Cl | 1.8602496 | 0.0004868 | -0.0002907 |
| H | -0.5410869 | -0.0692703 | 1.0795792 |
| H | -0.5442577 | 0.9543927 | -0.4701656 |

**Initial configuration (in internal coordinates) for the *sn2.2.n* reactions** (*n*=1,2)
(distances in atomic units; angles and dihedrals in degree)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 3.16009 |
| 2 | distance | 3 | 2 | | | 2.04812 |
| 3 | angle | 3 | 1 | 2 | | 101.24332 |
| 4 | distance | 4 | 2 | | | 4.94350 |
| 5 | angle | 4 | 3 | 2 | | 78.78323 |
| 6 | dihedral | 4 | 2 | 3 | 1 | 179.96689 |
| 7 | distance | 5 | 2 | | | 2.08604 |
| 8 | angle | 5 | 1 | 2 | | 101.18652 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 240.08418 |
| 10 | distance | 6 | 2 | | | 2.04809 |
| 11 | angle | 6 | 1 | 2 | | 101.25862 |
| 12 | dihedral | 6 | 2 | 1 | 3 | 120.20026 |

**Initial configuration (in cartesian coordinates) for the *sn2.3.n* reactions** (*n*=1,6)

| | | | |
|---|---|---|---|
| F | -2.3894780 | 0.0007449 | -0.0002117 |
| C | -0.8413690 | 0.0005793 | -0.0010560 |
| H | -0.5604436 | -0.8743733 | -0.5825627 |
| Cl | 1.8698667 | 0.0004884 | -0.0003033 |
| H | -0.5553969 | -0.0686303 | 1.0684808 |
| H | -0.5598854 | 0.9432155 | -0.4644695 |

**Initial configuration (in internal coordinates) for the *sn2.3.n* reactions** (*n*=1,6)
(distances in atomic units; angles and dihedrals in degree)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.92550 |
| 2 | distance | 3 | 2 | | | 2.05504 |
| 3 | angle | 3 | 1 | 2 | | 104.99322 |
| 4 | distance | 4 | 2 | | | 5.12349 |
| 5 | angle | 4 | 3 | 2 | | 75.03638 |
| 6 | dihedral | 4 | 2 | 3 | 1 | 179.96176 |
| 7 | distance | 5 | 2 | | | 2.09622 |
| 8 | angle | 5 | 1 | 2 | | 104.90890 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 240.09772 |
| 10 | distance | 6 | 2 | | | 2.05498 |
| 11 | angle | 6 | 1 | 2 | | 105.00996 |
| 12 | dihedral | 6 | 2 | 1 | 3 | 120.22629 |

## 2.2. Intial configuration for the *sn2b* reaction

**Initial configuration (in cartesian coordinates) for the *sn2b.1.n* reactions** (*n*=1,4)

| | | | |
|---|---|---|---|
| Br | -1.0636208 | -0.0000441 | -0.0001072 |
| C | 1.7787006 | 0.0006178 | 0.0015304 |
| H | 1.4630861 | -0.9966441 | 0.3143327 |
| N | 3.4098239 | -0.0003301 | -0.0008114 |
| H | 3.7830058 | -0.7045887 | -0.6500730 |
| H | 1.4612773 | 0.2290434 | -1.0178036 |
| H | 1.4644553 | 0.7699130 | 0.7096108 |
| H | 3.7846509 | 0.9130553 | -0.2870653 |
| H | 3.7863063 | -0.2100547 | 0.9325308 |

**Initial configuration (in internal coordinates) for the *sn2b.1.n* reactions** (*n*=1,4)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 5.37121 |
| 2 | distance | 3 | 2 | | | 2.06317 |
| 3 | angle | 2 | 1 | 3 | | 84.33338 |
| 4 | distance | 4 | 2 | | | 3.08238 |
| 5 | angle | 4 | 3 | 2 | | 106.79582 |
| 6 | dihedral | 4 | 2 | 3 | 1 | 180.12947 |
| 7 | distance | 5 | 4 | | | 1.94264 |
| 8 | angle | 5 | 2 | 4 | | 111.36584 |
| 9 | dihedral | 5 | 4 | 3 | 2 | 60.04631 |
| 10 | distance | 6 | 2 | | | 2.06316 |
| 11 | angle | 6 | 3 | 2 | | 111.99699 |
| 12 | dihedral | 6 | 2 | 3 | 1 | -63.24883 |
| 13 | distance | 7 | 2 | | | 2.06313 |
| 14 | angle | 7 | 3 | 2 | | 112.00005 |
| 15 | dihedral | 7 | 2 | 3 | 1 | 63.53118 |
| 16 | distance | 8 | 4 | | | 1.94257 |
| 17 | angle | 8 | 5 | 4 | | 107.48619 |
| 18 | dihedral | 8 | 4 | 5 | 2 | 237.74951 |
| 19 | distance | 9 | 4 | | | 1.94270 |
| 20 | angle | 9 | 5 | 4 | | 107.49972 |
| 21 | dihedral | 9 | 4 | 5 | 2 | 122.29893 |

### 2.3. Intial configurations for the *sig* reactions

**Initial configuration (in cartesian coordinates) for the *sig.1.n* reactions** (*n*=1,2)

| | | | |
|---|---|---|---|
| C | -0.9439243 | -0.7589479 | -0.0483523 |
| C | 0.3858443 | -1.1540546 | -0.0098707 |
| C | 1.2012554 | 0.0113897 | -0.0035884 |
| C | 0.4105539 | 1.1486558 | -0.0084393 |
| H | -1.8411883 | -1.3729454 | -0.1257973 |
| H | 0.7415728 | -2.1838222 | 0.0381117 |
| H | 2.3253662 | 0.0038012 | 0.0602227 |
| H | 0.7495869 | 2.1835349 | 0.0264660 |
| C | -0.9669535 | 0.7320307 | 0.0003400 |
| H | -1.8378151 | 1.3510140 | -0.2291739 |
| H | -1.1778655 | 0.2671743 | 1.0667453 |

**Initial configuration (in internal coordinates) for the *sig.1.n* reactions** (*n*=1,2)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.62248 |
| 2 | distance | 3 | 2 | | | 2.68793 |
| 3 | angle | 3 | 1 | 2 | | 108.43072 |
| 4 | distance | 4 | 3 | | | 2.61753 |
| 5 | angle | 4 | 2 | 3 | | 110.21035 |
| 6 | dihedral | 4 | 3 | 2 | 1 | 1.28357 |
| 7 | distance | 5 | 1 | | | 2.05978 |
| 8 | angle | 5 | 2 | 1 | | 129.07822 |
| 9 | dihedral | 5 | 1 | 2 | 3 | 175.77855 |
| 10 | distance | 6 | 2 | | | 2.06081 |
| 11 | angle | 6 | 3 | 2 | | 125.90953 |
| 12 | dihedral | 6 | 2 | 3 | 4 | 182.99062 |
| 13 | distance | 7 | 3 | | | 2.12773 |
| 14 | angle | 7 | 4 | 3 | | 125.14506 |
| 15 | dihedral | 7 | 3 | 2 | 4 | 176.53619 |
| 16 | distance | 8 | 4 | | | 2.05897 |
| 17 | angle | 8 | 3 | 4 | | 127.02081 |
| 18 | dihedral | 8 | 4 | 3 | 2 | 177.89248 |
| 19 | distance | 9 | 1 | | | 2.81938 |
| 20 | angle | 9 | 2 | 1 | | 107.36204 |
| 21 | dihedral | 9 | 1 | 2 | 3 | -2.72046 |
| 22 | distance | 10 | 9 | | | 2.06510 |
| 23 | angle | 10 | 4 | 9 | | 126.69201 |
| 24 | dihedral | 10 | 9 | 4 | 3 | 195.12999 |
| 25 | distance | 11 | 1 | | | 2.89757 |
| 26 | angle | 11 | 1 | 9 | | 68.85452 |
| 27 | dihedral | 11 | 9 | 1 | 3 | 259.14340 |

**Initial configuration (in cartesian coordinates) for the *sig.2.n* reactions** (*n*=1,4)

| | | | |
|---|---|---|---|
| C | -0.9342752 | -0.7759210 | -0.0786104 |
| C | 0.3698478 | -1.1596542 | -0.0156359 |
| C | 1.2056588 | 0.0274456 | -0.0028656 |
| C | 0.4290301 | 1.1457096 | -0.0103722 |
| H | -1.8242523 | -1.4063528 | -0.0872598 |
| H | 0.7392685 | -2.1852146 | 0.0386752 |
| H | 2.3321572 | 0.0099758 | 0.0526422 |
| H | 0.7630856 | 2.1829416 | 0.0225020 |
| C | -0.9861406 | 0.7141360 | 0.0421940 |
| H | -1.8004730 | 1.3178177 | -0.3822355 |
| H | -1.2186614 | 0.6543064 | 1.1372637 |

**Initial configuration (in internal coordinates) for the *sig.2.n* reactions** (*n*=1,4)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.57166 |
| 2 | distance | 3 | 2 | | | 2.74365 |
| 3 | angle | 3 | 1 | 2 | | 108.75526 |
| 4 | distance | 4 | 3 | | | 2.57289 |
| 5 | angle | 4 | 2 | 3 | | 110.06759 |
| 6 | dihedral | 4 | 3 | 2 | 1 | 2.10953 |
| 7 | distance | 5 | 1 | | | 2.06108 |
| 8 | angle | 5 | 2 | 1 | | 128.26804 |
| 9 | dihedral | 5 | 1 | 2 | 3 | 181.14613 |
| 10 | distance | 6 | 2 | | | 2.06248 |
| 11 | angle | 6 | 3 | 2 | | 124.95984 |
| 12 | dihedral | 6 | 2 | 3 | 4 | 183.31382 |
| 13 | distance | 7 | 3 | | | 2.13161 |
| 14 | angle | 7 | 4 | 3 | | 125.63695 |
| 15 | dihedral | 7 | 3 | 2 | 4 | 177.45126 |
| 16 | distance | 8 | 4 | | | 2.06017 |
| 17 | angle | 8 | 3 | 4 | | 127.33577 |
| 18 | dihedral | 8 | 4 | 3 | 2 | 178.23726 |
| 19 | distance | 9 | 1 | | | 2.82674 |
| 20 | angle | 9 | 2 | 1 | | 108.08191 |
| 21 | dihedral | 9 | 1 | 2 | 3 | -6.11754 |
| 22 | distance | 10 | 9 | | | 2.07673 |
| 23 | angle | 10 | 4 | 9 | | 122.30878 |
| 24 | dihedral | 10 | 9 | 4 | 3 | 207.68121 |
| 25 | distance | 11 | 1 | | | 3.58788 |
| 26 | angle | 11 | 1 | 9 | | 91.88631 |
| 27 | dihedral | 11 | 9 | 1 | 5 | 75.42335 |

**Initial configuration (in cartesian coordinates) for the *sig.3.n* reactions** (*n*=1,6)

| | | | |
|---|---|---|---|
| C | -0.9320234 | -0.7863220 | -0.0331547 |
| C | 0.3673617 | -1.1638013 | -0.0527704 |
| C | 1.2164020 | 0.0335404 | -0.0160395 |
| C | 0.4387754 | 1.1379411 | 0.0272826 |
| H | -1.8039778 | -1.4421811 | -0.0510860 |
| H | 0.7409614 | -2.1893208 | -0.0927854 |
| H | 2.3603997 | 0.0156048 | -0.0261657 |
| H | 0.7744463 | 2.1757911 | 0.0619081 |
| C | -1.0050492 | 0.7141450 | 0.0609271 |
| H | -1.6166523 | 1.1751886 | -0.7377528 |
| H | -1.4807859 | 1.0227942 | 1.0141455 |

**Initial configuration (in internal coordinates) for the *sig.3.n* reactions** (*n*=1,6)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.55727 |
| 2 | distance | 3 | 2 | | | 2.77465 |
| 3 | angle | 3 | 1 | 2 | | 109.11142 |
| 4 | distance | 4 | 3 | | | 2.55378 |
| 5 | angle | 4 | 2 | 3 | | 109.54134 |
| 6 | dihedral | 4 | 3 | 2 | 1 | 0.06470 |
| 7 | distance | 5 | 1 | | | 2.06212 |
| 8 | angle | 5 | 2 | 1 | | 126.82430 |
| 9 | dihedral | 5 | 1 | 2 | 3 | 180.00669 |
| 10 | distance | 6 | 2 | | | 2.06393 |
| 11 | angle | 6 | 3 | 2 | | 124.66742 |
| 12 | dihedral | 6 | 2 | 3 | 4 | 179.87918 |
| 13 | distance | 7 | 3 | | | 2.16219 |
| 14 | angle | 7 | 4 | 3 | | 126.04525 |
| 15 | dihedral | 7 | 3 | 2 | 4 | 180.15638 |
| 16 | distance | 8 | 4 | | | 2.06232 |
| 17 | angle | 8 | 3 | 4 | | 126.95638 |
| 18 | dihedral | 8 | 4 | 3 | 2 | 179.97599 |
| 19 | distance | 9 | 1 | | | 2.84439 |
| 20 | angle | 9 | 2 | 1 | | 108.99951 |
| 21 | dihedral | 9 | 1 | 2 | 3 | -1.69902 |
| 22 | distance | 10 | 9 | | | 2.09112 |
| 23 | angle | 10 | 4 | 9 | | 113.37489 |
| 24 | dihedral | 10 | 9 | 4 | 3 | 234.26860 |
| 25 | distance | 11 | 1 | | | 4.08412 |
| 26 | angle | 11 | 1 | 9 | | 110.60541 |
| 27 | dihedral | 11 | 9 | 1 | 3 | 242.96632 |

## 2.4. Intial configurations for the *dcc* reactions

**Initial configuration (in cartesian coordinates) for the *dcc.1.n* reactions** (*n*=1,5)

| | | | |
|---|---|---|---|
| C | 0.0501798 | 0.1804853 | -0.1292330 |
| C | -1.1066651 | 0.1016331 | -1.0077937 |
| C | 0.7177559 | -0.7175706 | -1.0408016 |
| C | 1.6412108 | -1.8283596 | -0.6078733 |
| C | -2.5463769 | -0.0303780 | -0.5673896 |
| Cl | -0.3053665 | -0.6150558 | 1.4553818 |
| Cl | 0.9859143 | 1.8796327 | 0.1203746 |
| H | -0.9638291 | 0.6107239 | -1.9670141 |
| H | 0.9718964 | -0.2491656 | -1.9948637 |
| H | 1.2197783 | -2.4670395 | 0.1802190 |
| H | 1.9685466 | -2.4511880 | -1.4528529 |
| H | 2.5371788 | -1.3345950 | -0.1803985 |
| H | -2.8718124 | 0.9682959 | -0.2131112 |
| H | -3.2043400 | -0.3155868 | -1.4018481 |
| H | -2.6839228 | -0.7318124 | 0.2655242 |

**Initial configuration (in internal coordinates) for the *dcc.1.n* reactions** (*n*=1,5)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.74913 |
| 2 | distance | 3 | 1 | | | 2.72744 |
| 3 | angle | 3 | 2 | 1 | | 87.28657 |
| 4 | distance | 4 | 3 | | | 2.84970 |
| 5 | angle | 4 | 1 | 3 | | 124.07322 |
| 6 | dihedral | 4 | 3 | 1 | 2 | 218.56552 |
| 7 | distance | 5 | 2 | | | 2.85602 |
| 8 | angle | 5 | 1 | 2 | | 125.89275 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 137.65226 |
| 10 | distance | 6 | 1 | | | 3.41738 |
| 11 | angle | 6 | 2 | 1 | | 110.42578 |
| 12 | dihedral | 6 | 1 | 2 | 3 | 247.77135 |
| 13 | distance | 7 | 1 | | | 3.69585 |
| 14 | angle | 7 | 3 | 1 | | 113.57127 |
| 15 | dihedral | 7 | 1 | 3 | 2 | 237.96010 |
| 16 | distance | 8 | 2 | | | 2.06981 |
| 17 | angle | 8 | 1 | 2 | | 113.57759 |
| 18 | dihedral | 8 | 2 | 1 | 3 | -70.52016 |
| 19 | distance | 9 | 3 | | | 2.06510 |
| 20 | angle | 9 | 1 | 3 | | 113.09542 |
| 21 | dihedral | 9 | 3 | 1 | 2 | 70.90974 |
| 22 | distance | 10 | 4 | | | 2.07578 |
| 23 | angle | 10 | 3 | 4 | | 113.53537 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 24 | dihedral | 10 | 4 | 3 | 1 | 49.56721 |
| 25 | distance | 11 | 4 | | | 2.07789 |
| 26 | angle | 11 | 3 | 4 | | 112.26645 |
| 27 | dihedral | 11 | 4 | 3 | 10 | 125.07139 |
| 28 | distance | 12 | 4 | | | 2.09521 |
| 29 | angle | 12 | 3 | 4 | | 106.11149 |
| 30 | dihedral | 12 | 4 | 3 | 10 | 242.75953 |
| 31 | distance | 13 | 5 | | | 2.09476 |
| 32 | angle | 13 | 2 | 5 | | 107.10397 |
| 33 | dihedral | 13 | 5 | 2 | 1 | 76.49553 |
| 34 | distance | 14 | 5 | | | 2.07920 |
| 35 | angle | 14 | 2 | 5 | | 111.79596 |
| 36 | dihedral | 14 | 5 | 2 | 13 | 117.48467 |
| 37 | distance | 15 | 5 | | | 2.07412 |
| 38 | angle | 15 | 2 | 5 | | 113.34913 |
| 39 | dihedral | 15 | 5 | 2 | 13 | 241.92346 |

**Initial configuration (in cartesian coordinates) for the *dcc.2.n* reactions** (*n*=1,8)

| | | | |
|---|---|---|---|
| C | 0.1041371 | 0.2710712 | -0.0698725 |
| C | -0.9814904 | 0.0457930 | -1.0400369 |
| C | 0.5962197 | -0.6810691 | -1.0683612 |
| C | 1.4996951 | -1.8485435 | -0.6598501 |
| C | -2.4444812 | -0.1184447 | -0.6194347 |
| Cl | -0.2800434 | -0.5742462 | 1.4796551 |
| Cl | 0.9554914 | 1.8568574 | 0.1387620 |
| H | -0.9004352 | 0.7080936 | -1.9115574 |
| H | 1.0165965 | -0.1636718 | -1.9371749 |
| H | 1.0805328 | -2.4892782 | 0.1265274 |
| H | 1.7848592 | -2.4728324 | -1.5199218 |
| H | 2.4209624 | -1.3873338 | -0.2581493 |
| H | -2.7833869 | 0.8724957 | -0.2651300 |
| H | -3.0838781 | -0.4045833 | -1.4684900 |
| H | -2.5937071 | -0.8335382 | 0.1987803 |

**Initial configuration (in internal coordinates) for the *dcc.2.n* reactions** (*n*=1,8)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.78410 |
| 2 | distance | 3 | 1 | | | 2.76811 |
| 3 | angle | 3 | 2 | 1 | | 72.49928 |
| 4 | distance | 4 | 3 | | | 2.89452 |
| 5 | angle | 4 | 1 | 3 | | 120.78300 |
| 6 | dihedral | 4 | 3 | 1 | 2 | 217.77546 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 7 | distance | 5 | 2 | | | 2.89333 |
| 8 | angle | 5 | 1 | 2 | | 122.65711 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 138.43780 |
| 10 | distance | 6 | 1 | | | 3.41366 |
| 11 | angle | 6 | 2 | 1 | | 109.66912 |
| 12 | dihedral | 6 | 1 | 2 | 3 | 253.78605 |
| 13 | distance | 7 | 1 | | | 3.42403 |
| 14 | angle | 7 | 3 | 1 | | 119.30958 |
| 15 | dihedral | 7 | 1 | 3 | 2 | 240.56651 |
| 16 | distance | 8 | 2 | | | 2.07419 |
| 17 | angle | 8 | 1 | 2 | | 112.09731 |
| 18 | dihedral | 8 | 2 | 1 | 3 | -86.06076 |
| 19 | distance | 9 | 3 | | | 2.06945 |
| 20 | angle | 9 | 1 | 3 | | 111.26257 |
| 21 | dihedral | 9 | 3 | 1 | 2 | 86.24083 |
| 22 | distance | 10 | 4 | | | 2.07408 |
| 23 | angle | 10 | 3 | 4 | | 114.25398 |
| 24 | dihedral | 10 | 4 | 3 | 1 | 55.16226 |
| 25 | distance | 11 | 4 | | | 2.07937 |
| 26 | angle | 11 | 3 | 4 | | 112.13790 |
| 27 | dihedral | 11 | 4 | 3 | 10 | 124.85004 |
| 28 | distance | 12 | 4 | | | 2.08967 |
| 29 | angle | 12 | 3 | 4 | | 105.68781 |
| 30 | dihedral | 12 | 4 | 3 | 10 | 241.97271 |
| 31 | distance | 13 | 5 | | | 2.08928 |
| 32 | angle | 13 | 2 | 5 | | 106.54644 |
| 33 | dihedral | 13 | 5 | 2 | 1 | 70.01142 |
| 34 | distance | 14 | 5 | | | 2.08007 |
| 35 | angle | 14 | 2 | 5 | | 111.77963 |
| 36 | dihedral | 14 | 5 | 2 | 13 | 117.26531 |
| 37 | distance | 15 | 5 | | | 2.07277 |
| 38 | angle | 15 | 2 | 5 | | 113.88190 |
| 39 | dihedral | 15 | 5 | 2 | 13 | 241.45253 |

**Initial configuration (in cartesian coordinates) for the *dcc.3.n* reactions** (*n*=1,6)

| | | | |
|---|---|---|---|
| C | 0.1474413 | 0.3203373 | 0.0113191 |
| C | -0.8462702 | 0.0737190 | -1.0818081 |
| C | 0.5617195 | -0.5878190 | -1.1015437 |
| C | 1.0731100 | -1.9894105 | -0.8385490 |
| C | -2.2383492 | -0.4541721 | -0.7977997 |
| Cl | -0.2146868 | -0.4661391 | 1.5721114 |
| Cl | 0.9373385 | 1.9009045 | 0.1945968 |
| H | -0.8682168 | 0.9069161 | -1.8091960 |
| H | 1.1932406 | -0.0622822 | -1.8278294 |
| H | 0.4612341 | -2.5447608 | -0.1149487 |
| H | 1.1346200 | -2.5751747 | -1.7693977 |
| H | 2.0926641 | -1.9126846 | -0.4238110 |
| H | -2.8449752 | 0.3643220 | -0.3742850 |
| H | -2.7317001 | -0.7915401 | -1.7233693 |
| H | -2.2464239 | -1.2817609 | -0.0764872 |

**Initial configuration (in internal coordinates) for the *dcc.3.n* reactions** (*n*=1,6)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.83031 |
| 2 | distance | 3 | 1 | | | 2.82502 |
| 3 | angle | 3 | 2 | 1 | | 62.64614 |
| 4 | distance | 4 | 3 | | | 2.86289 |
| 5 | angle | 4 | 1 | 3 | | 121.75835 |
| 6 | dihedral | 4 | 3 | 1 | 2 | 234.34889 |
| 7 | distance | 5 | 2 | | | 2.86418 |
| 8 | angle | 5 | 1 | 2 | | 122.00331 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 124.43833 |
| 10 | distance | 6 | 1 | | | 3.37291 |
| 11 | angle | 6 | 2 | 1 | | 115.53482 |
| 12 | dihedral | 6 | 1 | 2 | 3 | 252.46638 |
| 13 | distance | 7 | 1 | | | 3.35698 |
| 14 | angle | 7 | 3 | 1 | | 119.60959 |
| 15 | dihedral | 7 | 1 | 3 | 2 | 247.95792 |
| 16 | distance | 8 | 2 | | | 2.09051 |
| 17 | angle | 8 | 1 | 2 | | 111.65652 |
| 18 | dihedral | 8 | 2 | 1 | 3 | 260.01488 |
| 19 | distance | 9 | 3 | | | 2.07225 |
| 20 | angle | 9 | 1 | 3 | | 111.19219 |
| 21 | dihedral | 9 | 3 | 1 | 2 | 99.99406 |
| 22 | distance | 10 | 4 | | | 2.07561 |
| 23 | angle | 10 | 3 | 4 | | 113.20949 |
| 24 | dihedral | 10 | 4 | 3 | 1 | 45.77298 |
| 25 | distance | 11 | 4 | | | 2.08160 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 26 | angle | 11 | 3 | 4 | | 111.35368 |
| 27 | dihedral | 11 | 4 | 3 | 10 | 122.70134 |
| 28 | distance | 12 | 4 | | | 2.08503 |
| 29 | angle | 12 | 3 | 4 | | 108.23041 |
| 30 | dihedral | 12 | 4 | 3 | 10 | 240.82168 |
| 31 | distance | 13 | 5 | | | 2.08495 |
| 32 | angle | 13 | 2 | 5 | | 108.57474 |
| 33 | dihedral | 13 | 5 | 2 | 1 | 75.12640 |
| 34 | distance | 14 | 5 | | | 2.08204 |
| 35 | angle | 14 | 2 | 5 | | 111.13121 |
| 36 | dihedral | 14 | 5 | 2 | 13 | 118.23317 |
| 37 | distance | 15 | 5 | | | 2.07462 |
| 38 | angle | 15 | 2 | 5 | | 113.10545 |
| 39 | dihedral | 15 | 5 | 2 | 13 | 240.60138 |

## 2.5. Intial configurations for the *bcb* reactions

**Initial configuration (in cartesian coordinates) for the *bcb.1.n* reactions** (*n*=1,14)

| | | | |
|---|---|---|---|
| C | 2.2775993 | -1.0294153 | 0.3945519 |
| C | 2.6247237 | 0.2790740 | 0.0005532 |
| C | 0.9565349 | -1.4813882 | 0.3303552 |
| C | 1.6485087 | 1.2177177 | -0.3543473 |
| C | 0.0058725 | -0.5686427 | -0.1374678 |
| C | 0.3158738 | 0.7944940 | -0.2928589 |
| H | 1.9238978 | 2.2503393 | -0.5951831 |
| H | 3.6776927 | 0.5751542 | 0.0154238 |
| H | 3.0677398 | -1.7151586 | 0.7118063 |
| H | 0.7061383 | -2.5206600 | 0.5588773 |
| C | -1.3605770 | -0.6721625 | -0.6490454 |
| C | -1.0082747 | 1.4269168 | -0.3707194 |
| H | -1.4240714 | -0.5326814 | -1.7363040 |
| H | -1.1584949 | 2.2011698 | -1.1458856 |
| C | -2.3722056 | -1.6563686 | -0.0852217 |
| C | -1.8520006 | 1.6761159 | 0.8591584 |
| H | -3.2479061 | -1.1325731 | 0.3414219 |
| H | -2.7607963 | -2.3410212 | -0.8580190 |
| H | -1.9390635 | -2.2575520 | 0.7308583 |
| H | -1.7131435 | 0.8850256 | 1.6119050 |
| H | -1.6152060 | 2.6436037 | 1.3444186 |
| H | -2.9212773 | 1.7105553 | 0.5883382 |

**Initial configuration (in internal coordinates) for the *bcb.1.n* reactions** (*n*=1,14)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.66436 |
| 2 | distance | 3 | 1 | | | 2.64130 |
| 3 | angle | 3 | 2 | 1 | | 121.33001 |
| 4 | distance | 4 | 2 | | | 2.64562 |
| 5 | angle | 4 | 1 | 2 | | 121.42559 |
| 6 | dihedral | 4 | 2 | 1 | 3 | 5.92321 |
| 7 | distance | 5 | 3 | | | 2.64273 |
| 8 | angle | 5 | 1 | 3 | | 116.53980 |
| 9 | dihedral | 5 | 3 | 1 | 2 | -0.25268 |
| 10 | distance | 6 | 4 | | | 2.64482 |
| 11 | angle | 6 | 2 | 4 | | 116.74781 |
| 12 | dihedral | 6 | 4 | 2 | 1 | 0.26314 |
| 13 | distance | 7 | 4 | | | 2.07022 |
| 14 | angle | 7 | 2 | 4 | | 120.82470 |
| 15 | dihedral | 7 | 4 | 2 | 8 | -1.39324 |
| 16 | distance | 8 | 2 | | | 2.06718 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 17 | angle | 8 | 1 | 2 | | 118.97193 |
| 18 | dihedral | 8 | 2 | 1 | 3 | 183.26962 |
| 19 | distance | 9 | 1 | | | 2.06596 |
| 20 | angle | 9 | 2 | 1 | | 119.03056 |
| 21 | dihedral | 9 | 1 | 2 | 4 | 183.05004 |
| 22 | distance | 10 | 3 | | | 2.06578 |
| 23 | angle | 10 | 1 | 3 | | 120.95183 |
| 24 | dihedral | 10 | 3 | 1 | 2 | 174.93572 |
| 25 | distance | 11 | 5 | | | 2.76418 |
| 26 | angle | 11 | 3 | 5 | | 134.89765 |
| 27 | dihedral | 11 | 5 | 3 | 1 | 163.14611 |
| 28 | distance | 12 | 6 | | | 2.77693 |
| 29 | angle | 12 | 4 | 6 | | 136.51275 |
| 30 | dihedral | 12 | 6 | 4 | 2 | 169.25271 |
| 31 | distance | 13 | 11 | | | 2.07493 |
| 32 | angle | 13 | 5 | 11 | | 113.03826 |
| 33 | dihedral | 13 | 11 | 5 | 6 | 69.57733 |
| 34 | distance | 14 | 12 | | | 2.08976 |
| 35 | angle | 14 | 6 | 12 | | 117.44294 |
| 36 | dihedral | 14 | 12 | 6 | 4 | 42.88077 |
| 37 | distance | 15 | 11 | | | 2.87210 |
| 38 | angle | 15 | 5 | 11 | | 122.53932 |
| 39 | dihedral | 15 | 11 | 5 | 3 | 37.47374 |
| 40 | distance | 16 | 12 | | | 2.85753 |
| 41 | angle | 16 | 6 | 12 | | 122.04684 |
| 42 | dihedral | 16 | 12 | 6 | 5 | 77.97038 |
| 43 | distance | 17 | 15 | | | 2.09004 |
| 44 | angle | 17 | 11 | 15 | | 111.31107 |
| 45 | dihedral | 17 | 15 | 11 | 5 | 118.58210 |
| 46 | distance | 18 | 15 | | | 2.08468 |
| 47 | angle | 18 | 11 | 15 | | 112.11597 |
| 48 | dihedral | 18 | 15 | 11 | 7 | 119.27757 |
| 49 | distance | 19 | 15 | | | 2.08301 |
| 50 | angle | 19 | 11 | 15 | | 111.48656 |
| 51 | dihedral | 19 | 15 | 11 | 17 | 241.25062 |
| 52 | distance | 20 | 16 | | | 2.08019 |
| 53 | angle | 20 | 12 | 16 | | 111.55298 |
| 54 | dihedral | 20 | 16 | 12 | 6 | -33.92907 |
| 55 | distance | 21 | 16 | | | 2.09375 |
| 56 | angle | 21 | 12 | 16 | | 112.38794 |
| 57 | dihedral | 21 | 16 | 12 | 20 | 120.85114 |
| 58 | distance | 22 | 16 | | | 2.08546 |
| 59 | angle | 22 | 12 | 16 | | 110.25347 |
| 60 | dihedral | 22 | 16 | 12 | 20 | 239.74588 |

**Initial configuration (in cartesian coordinates) for the *bcb.2.n* reactions** (*n*=1,5)

| | | | |
|---|---|---|---|
| C | 2.2911304 | -1.0283543 | 0.3922468 |
| C | 2.6305240 | 0.2793658 | 0.0083299 |
| C | 0.9687822 | -1.4910568 | 0.3134198 |
| C | 1.6463761 | 1.2260449 | -0.3306864 |
| C | 0.0302169 | -0.5738212 | -0.1379185 |
| C | 0.3268431 | 0.7859266 | -0.2827026 |
| H | 1.9216774 | 2.2588442 | -0.5641759 |
| H | 3.6825177 | 0.5780943 | 0.0178251 |
| H | 3.0833701 | -1.7108707 | 0.7127625 |
| H | 0.7205324 | -2.5333666 | 0.5333455 |
| C | -1.3646099 | -0.5740557 | -0.6475986 |
| C | -1.0804571 | 1.2872230 | -0.3948771 |
| H | -1.3583148 | -0.6095333 | -1.7476596 |
| H | -1.2985564 | 1.9739564 | -1.2334930 |
| C | -2.3764798 | -1.5981570 | -0.0821617 |
| C | -1.8423114 | 1.6806975 | 0.8635892 |
| H | -3.2722022 | -1.1180779 | 0.3478438 |
| H | -2.7281265 | -2.2887216 | -0.8660223 |
| H | -1.9216541 | -2.1998685 | 0.7217882 |
| H | -1.6987657 | 0.9287700 | 1.6559527 |
| H | -1.5435290 | 2.6614756 | 1.2754573 |
| H | -2.9198654 | 1.7342164 | 0.6348338 |

**Initial configuration (in internal coordinates) for the *bcb.2.n* reactions** (*n*=1,5)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.65418 |
| 2 | distance | 3 | 1 | | | 2.65162 |
| 3 | angle | 3 | 2 | 1 | | 121.29132 |
| 4 | distance | 4 | 2 | | | 2.65887 |
| 5 | angle | 4 | 1 | 2 | | 121.55353 |
| 6 | dihedral | 4 | 2 | 1 | 3 | 7.08886 |
| 7 | distance | 5 | 3 | | | 2.62252 |
| 8 | angle | 5 | 1 | 3 | | 115.95545 |
| 9 | dihedral | 5 | 3 | 1 | 2 | -1.20154 |
| 10 | distance | 6 | 4 | | | 2.63017 |
| 11 | angle | 6 | 2 | 4 | | 116.23559 |
| 12 | dihedral | 6 | 4 | 2 | 1 | -0.93584 |
| 13 | distance | 7 | 4 | | | 2.06749 |
| 14 | angle | 7 | 2 | 4 | | 120.70162 |
| 15 | dihedral | 7 | 4 | 2 | 8 | -1.23412 |
| 16 | distance | 8 | 2 | | | 2.06666 |
| 17 | angle | 8 | 1 | 2 | | 118.97286 |
| 18 | dihedral | 8 | 2 | 1 | 3 | 184.29745 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 19 | distance | 9 | 1 | | | 2.06681 |
| 20 | angle | 9 | 2 | 1 | | 119.08402 |
| 21 | dihedral | 9 | 1 | 2 | 4 | 184.12498 |
| 22 | distance | 10 | 3 | | | 2.06699 |
| 23 | angle | 10 | 1 | 3 | | 121.11917 |
| 24 | dihedral | 10 | 3 | 1 | 2 | 174.84941 |
| 25 | distance | 11 | 5 | | | 2.80630 |
| 26 | angle | 11 | 3 | 5 | | 138.30903 |
| 27 | dihedral | 11 | 5 | 3 | 1 | 165.00261 |
| 28 | distance | 12 | 6 | | | 2.83104 |
| 29 | angle | 12 | 4 | 6 | | 141.46167 |
| 30 | dihedral | 12 | 6 | 4 | 2 | 172.80804 |
| 31 | distance | 13 | 11 | | | 2.07993 |
| 32 | angle | 13 | 5 | 11 | | 109.73443 |
| 33 | dihedral | 13 | 11 | 5 | 6 | 82.03927 |
| 34 | distance | 14 | 12 | | | 2.08936 |
| 35 | angle | 14 | 6 | 12 | | 116.73919 |
| 36 | dihedral | 14 | 12 | 6 | 4 | 45.86287 |
| 37 | distance | 15 | 11 | | | 2.92290 |
| 38 | angle | 15 | 5 | 11 | | 119.28131 |
| 39 | dihedral | 15 | 11 | 5 | 3 | 34.29142 |
| 40 | distance | 16 | 12 | | | 2.87771 |
| 41 | angle | 16 | 6 | 12 | | 119.63962 |
| 42 | dihedral | 16 | 12 | 6 | 5 | 89.55859 |
| 43 | distance | 17 | 15 | | | 2.08530 |
| 44 | angle | 17 | 11 | 15 | | 112.67007 |
| 45 | dihedral | 17 | 15 | 11 | 5 | 123.14798 |
| 46 | distance | 18 | 15 | | | 2.08297 |
| 47 | angle | 18 | 11 | 15 | | 111.31799 |
| 48 | dihedral | 18 | 15 | 11 | 7 | 120.07979 |
| 49 | distance | 19 | 15 | | | 2.08321 |
| 50 | angle | 19 | 11 | 15 | | 110.98269 |
| 51 | dihedral | 19 | 15 | 11 | 17 | 240.35121 |
| 52 | distance | 20 | 16 | | | 2.08199 |
| 53 | angle | 20 | 12 | 16 | | 110.65956 |
| 54 | dihedral | 20 | 16 | 12 | 6 | -44.59679 |
| 55 | distance | 21 | 16 | | | 2.08798 |
| 56 | angle | 21 | 12 | 16 | | 113.71093 |
| 57 | dihedral | 21 | 16 | 12 | 20 | 121.24469 |
| 58 | distance | 22 | 16 | | | 2.08412 |
| 59 | angle | 22 | 12 | 16 | | 109.26487 |
| 60 | dihedral | 22 | 16 | 12 | 20 | 241.16550 |

**Initial configuration (in cartesian coordinates) for the *bcb.3.n* reactions** (*n*=1,20)

| | | | |
|---|---|---|---|
| C | 2.3646289 | -1.0178083 | 0.3348790 |
| C | 2.6288333 | 0.3411663 | 0.1052319 |
| C | 1.0720146 | -1.5515026 | 0.1778588 |
| C | 1.6012701 | 1.2578548 | -0.1935271 |
| C | 0.0850732 | -0.6473700 | -0.1890537 |
| C | 0.3185330 | 0.7280700 | -0.2795061 |
| H | 1.8241887 | 2.3224794 | -0.3264513 |
| H | 3.6682257 | 0.7034686 | 0.1912483 |
| H | 3.1904295 | -1.6794174 | 0.6149283 |
| H | 0.8834730 | -2.6204062 | 0.3147572 |
| C | -1.3613830 | -0.5287487 | -0.6391148 |
| C | -1.1663013 | 1.0512264 | -0.4469009 |
| H | -1.3971040 | -0.7068897 | -1.7286600 |
| H | -1.4365531 | 1.6449876 | -1.3387014 |
| C | -2.4708268 | -1.3505375 | 0.0207533 |
| C | -1.8253804 | 1.6512260 | 0.7975510 |
| H | -3.4021819 | -0.7715938 | 0.1335346 |
| H | -2.7138536 | -2.2351731 | -0.5896008 |
| H | -2.1801535 | -1.7082957 | 1.0212078 |
| H | -1.6001816 | 1.0527970 | 1.6950514 |
| H | -1.4611519 | 2.6756300 | 0.9804987 |
| H | -2.9212318 | 1.7025213 | 0.6854411 |

**Initial configuration (in internal coordinates) for the *bcb.3.n* reactions** (*n*=1,20)

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.65192 |
| 2 | distance | 3 | 1 | | | 2.65931 |
| 3 | angle | 3 | 2 | 1 | | 121.46198 |
| 4 | distance | 4 | 2 | | | 2.66274 |
| 5 | angle | 4 | 1 | 2 | | 121.83005 |
| 6 | dihedral | 4 | 2 | 1 | 3 | 4.91180 |
| 7 | distance | 5 | 3 | | | 2.62266 |
| 8 | angle | 5 | 1 | 3 | | 115.82574 |
| 9 | dihedral | 5 | 3 | 1 | 2 | -1.21615 |
| 10 | distance | 6 | 4 | | | 2.62766 |
| 11 | angle | 6 | 2 | 4 | | 115.97506 |
| 12 | dihedral | 6 | 4 | 2 | 1 | -1.55416 |
| 13 | distance | 7 | 4 | | | 2.07077 |
| 14 | angle | 7 | 2 | 4 | | 120.62539 |
| 15 | dihedral | 7 | 4 | 2 | 8 | -0.83557 |
| 16 | distance | 8 | 2 | | | 2.08641 |
| 17 | angle | 8 | 1 | 2 | | 118.83331 |
| 18 | dihedral | 8 | 2 | 1 | 3 | 183.08325 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 19 | distance | 9 | 1 | | | 2.06845 |
| 20 | angle | 9 | 2 | 1 | | 119.02325 |
| 21 | dihedral | 9 | 1 | 2 | 4 | 183.17685 |
| 22 | distance | 10 | 3 | | | 2.06737 |
| 23 | angle | 10 | 1 | 3 | | 120.98987 |
| 24 | dihedral | 10 | 3 | 1 | 2 | 177.20171 |
| 25 | distance | 11 | 5 | | | 2.87143 |
| 26 | angle | 11 | 3 | 5 | | 143.71753 |
| 27 | dihedral | 11 | 5 | 3 | 1 | 171.39287 |
| 28 | distance | 12 | 6 | | | 2.88899 |
| 29 | angle | 12 | 4 | 6 | | 145.30722 |
| 30 | dihedral | 12 | 6 | 4 | 2 | 174.03124 |
| 31 | distance | 13 | 11 | | | 2.08737 |
| 32 | angle | 13 | 5 | 11 | | 108.08042 |
| 33 | dihedral | 13 | 11 | 5 | 6 | 94.87936 |
| 34 | distance | 14 | 12 | | | 2.08804 |
| 35 | angle | 14 | 6 | 12 | | 116.07304 |
| 36 | dihedral | 14 | 12 | 6 | 4 | 55.36334 |
| 37 | distance | 15 | 11 | | | 2.89173 |
| 38 | angle | 15 | 5 | 11 | | 114.33257 |
| 39 | dihedral | 15 | 11 | 5 | 3 | 43.27588 |
| 40 | distance | 16 | 12 | | | 2.89261 |
| 41 | angle | 16 | 6 | 12 | | 114.33257 |
| 42 | dihedral | 16 | 12 | 6 | 5 | 105.25182 |
| 43 | distance | 17 | 15 | | | 2.08326 |
| 44 | angle | 17 | 11 | 15 | | 111.99972 |
| 45 | dihedral | 17 | 15 | 11 | 5 | 141.54166 |
| 46 | distance | 18 | 15 | | | 2.08228 |
| 47 | angle | 18 | 11 | 15 | | 110.62152 |
| 48 | dihedral | 18 | 15 | 11 | 7 | 119.24005 |
| 49 | distance | 19 | 15 | | | 2.08161 |
| 50 | angle | 19 | 11 | 15 | | 112.00880 |
| 51 | dihedral | 19 | 15 | 11 | 17 | 239.13795 |
| 52 | distance | 20 | 16 | | | 2.08242 |
| 53 | angle | 20 | 12 | 16 | | 111.17929 |
| 54 | dihedral | 20 | 16 | 12 | 6 | -49.54163 |
| 55 | distance | 21 | 16 | | | 2.08345 |
| 56 | angle | 21 | 12 | 16 | | 110.90795 |
| 57 | dihedral | 21 | 16 | 12 | 20 | 119.64541 |
| 58 | distance | 22 | 16 | | | 2.08392 |
| 59 | angle | 22 | 12 | 16 | | 111.31258 |
| 60 | dihedral | 22 | 16 | 12 | 20 | 239.38056 |

# 3. Transition state configurations

## 3.1. TS configuration for the *sn2* reaction

### Cartesian coordinates

| | | | |
|---|---|---|---|
| F | -2.6318067 | -0.0000242 | 0.0000595 |
| C | -0.4599682 | 0.0000377 | -0.0001588 |
| H | -0.6404202 | 0.5663719 | -0.9041343 |
| Cl | 1.6207714 | -0.0000067 | 0.0000342 |
| H | -0.6400560 | -1.0660802 | -0.0384852 |
| H | -0.6405552 | 0.4999510 | 0.9421885 |

### Internal coordinates

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 4.10774 |
| 2 | distance | 3 | 2 | | | 2.04458 |
| 3 | angle | 3 | 1 | 2 | | 80.35772 |
| 4 | distance | 4 | 2 | | | 3.92891 |
| 5 | angle | 4 | 3 | 2 | | 99.65339 |
| 6 | dihedral | 4 | 2 | 3 | 1 | 179.99600 |
| 7 | distance | 5 | 2 | | | 2.04437 |
| 8 | angle | 5 | 1 | 2 | | 80.31107 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 239.98503 |
| 10 | distance | 6 | 2 | | | 2.04459 |
| 11 | angle | 6 | 1 | 2 | | 80.33776 |
| 12 | dihedral | 6 | 2 | 1 | 3 | 119.98246 |

### 3.2. TS configuration for the *sn2b* reaction

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| Br | -1.0538771 | 0.0000011 | 0.0000186 |
| C | 1.7111907 | -0.0000226 | -0.0002853 |
| H | 1.4463561 | -1.0430044 | 0.1695814 |
| N | 3.4155720 | 0.0000062 | 0.0001362 |
| H | 3.7856908 | -0.6077663 | -0.7394539 |
| H | 1.4466281 | 0.3743758 | -0.9883772 |
| H | 1.4461737 | 0.6685919 | 0.8179942 |
| H | 3.7852178 | 0.9446136 | -0.1562076 |
| H | 3.7848509 | -0.3367163 | 0.8964969 |

**Internal coordinates**

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 5.22626 |
| 2 | distance | 3 | 2 | | | 2.05859 |
| 3 | angle | 2 | 1 | 3 | | 81.20361 |
| 4 | distance | 4 | 2 | | | 3.22051 |
| 5 | angle | 4 | 3 | 2 | | 104.08484 |
| 6 | dihedral | 4 | 2 | 3 | 1 | 180.03760 |
| 7 | distance | 5 | 4 | | | 1.93947 |
| 8 | angle | 5 | 2 | 4 | | 111.10536 |
| 9 | dihedral | 5 | 4 | 3 | 2 | 59.88672 |
| 10 | distance | 6 | 2 | | | 2.05871 |
| 11 | angle | 6 | 3 | 2 | | 114.26399 |
| 12 | dihedral | 6 | 2 | 3 | 1 | -67.11382 |
| 13 | distance | 7 | 2 | | | 2.05872 |
| 14 | angle | 7 | 3 | 2 | | 114.29643 |
| 15 | dihedral | 7 | 2 | 3 | 1 | 67.20039 |
| 16 | distance | 8 | 4 | | | 1.93948 |
| 17 | angle | 8 | 5 | 4 | | 107.78620 |
| 18 | dihedral | 8 | 4 | 5 | 2 | 238.06408 |
| 19 | distance | 9 | 4 | | | 1.93947 |
| 20 | angle | 9 | 5 | 4 | | 107.78626 |
| 21 | dihedral | 9 | 4 | 5 | 2 | 121.97009 |

### 3.3. TS configuration for the *sig* reaction

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.9548335 | -0.7453027 | -0.0241861 |
| C | 0.3980492 | -1.1508283 | -0.0086476 |
| C | 1.2031930 | -0.0002091 | -0.0036150 |
| C | 0.3984363 | 1.1506887 | -0.0086441 |
| H | -1.8437599 | -1.3603633 | -0.1670599 |
| H | 0.7436499 | -2.1836223 | 0.0315322 |
| H | 2.2932808 | -0.0004238 | 0.0588786 |
| H | 0.7444470 | 2.1833348 | 0.0315928 |
| C | -0.9545634 | 0.7456397 | -0.0242114 |
| H | -1.8432519 | 1.3610540 | -0.1669850 |
| H | -1.1701761 | 0.0001597 | 1.0378822 |

**Internal coordinates**

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.66910 |
| 2 | distance | 3 | 2 | | | 2.65383 |
| 3 | angle | 3 | 1 | 2 | | 108.29746 |
| 4 | distance | 4 | 3 | | | 2.65383 |
| 5 | angle | 4 | 2 | 3 | | 110.05449 |
| 6 | dihedral | 4 | 3 | 2 | 1 | 0.30287 |
| 7 | distance | 5 | 1 | | | 2.06050 |
| 8 | angle | 5 | 2 | 1 | | 128.34174 |
| 9 | dihedral | 5 | 1 | 2 | 3 | 170.89704 |
| 10 | distance | 6 | 2 | | | 2.05945 |
| 11 | angle | 6 | 3 | 2 | | 126.47471 |
| 12 | dihedral | 6 | 2 | 3 | 4 | 182.48759 |
| 13 | distance | 7 | 3 | | | 2.06334 |
| 14 | angle | 7 | 4 | 3 | | 124.92070 |
| 15 | dihedral | 7 | 3 | 2 | 4 | 176.43502 |
| 16 | distance | 8 | 4 | | | 2.05945 |
| 17 | angle | 8 | 3 | 4 | | 126.47466 |
| 18 | dihedral | 8 | 4 | 3 | 2 | 177.51235 |
| 19 | distance | 9 | 1 | | | 2.81749 |
| 20 | angle | 9 | 2 | 1 | | 106.67480 |
| 21 | dihedral | 9 | 1 | 2 | 3 | -0.18120 |
| 22 | distance | 10 | 9 | | | 2.06050 |
| 23 | angle | 10 | 4 | 9 | | 128.34178 |
| 24 | dihedral | 10 | 9 | 4 | 3 | 189.10285 |
| 25 | distance | 11 | 1 | | | 2.48569 |
| 26 | angle | 11 | 1 | 9 | | 55.47657 |
| 27 | dihedral | 11 | 9 | 1 | 3 | 259.07740 |

### 3.4. TS configuration for the *dcc* reaction

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.1793308 | -0.0678738 | -0.2681056 |
| C | -1.0965801 | 0.6492242 | -1.0621722 |
| C | 0.4282588 | -1.0342060 | -1.0919926 |
| C | 0.7633947 | -2.4230114 | -0.7122408 |
| C | -2.4230530 | 1.1569878 | -0.6395954 |
| Cl | -0.6836043 | -0.5506372 | 1.3471619 |
| Cl | 1.6928890 | 1.2492621 | 0.1437098 |
| H | -0.7256267 | 0.9306212 | -2.0507384 |
| H | 0.7313596 | -0.6687183 | -2.0756162 |
| H | 0.0573574 | -2.8321662 | 0.0255715 |
| H | 0.8414696 | -3.0847371 | -1.5867528 |
| H | 1.7561576 | -2.3979723 | -0.2182169 |
| H | -2.2962542 | 2.1817781 | -0.2320757 |
| H | -3.1191427 | 1.2323066 | -1.4888147 |
| H | -2.8670032 | 0.5488571 | 0.1616258 |

**Internal coordinates**

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.66342 |
| 2 | distance | 3 | 1 | | | 2.66023 |
| 3 | angle | 3 | 2 | 1 | | 107.47335 |
| 4 | distance | 4 | 3 | | | 2.79314 |
| 5 | angle | 4 | 1 | 3 | | 126.33194 |
| 6 | dihedral | 4 | 3 | 1 | 2 | 219.64650 |
| 7 | distance | 5 | 2 | | | 2.80074 |
| 8 | angle | 5 | 1 | 2 | | 126.59774 |
| 9 | dihedral | 5 | 2 | 1 | 3 | 142.69519 |
| 10 | distance | 6 | 1 | | | 3.32534 |
| 11 | angle | 6 | 2 | 1 | | 118.03896 |
| 12 | dihedral | 6 | 1 | 2 | 3 | 223.20882 |
| 13 | distance | 7 | 1 | | | 4.39424 |
| 14 | angle | 7 | 3 | 1 | | 98.25828 |
| 15 | dihedral | 7 | 1 | 3 | 2 | 246.22580 |
| 16 | distance | 8 | 2 | | | 2.06513 |
| 17 | angle | 8 | 1 | 2 | | 114.83001 |
| 18 | dihedral | 8 | 2 | 1 | 3 | -43.79701 |
| 19 | distance | 9 | 3 | | | 2.06385 |
| 20 | angle | 9 | 1 | 3 | | 114.64966 |
| 21 | dihedral | 9 | 3 | 1 | 2 | 44.15490 |
| 22 | distance | 10 | 4 | | | 2.07881 |
| 23 | angle | 10 | 3 | 4 | | 112.10047 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 24 | dihedral | 10 | 4 | 3 | 1 | 31.34152 |
| 25 | distance | 11 | 4 | | | 2.07754 |
| 26 | angle | 11 | 3 | 4 | | 112.16682 |
| 27 | dihedral | 11 | 4 | 3 | 10 | 125.39967 |
| 28 | distance | 12 | 4 | | | 2.09587 |
| 29 | angle | 12 | 3 | 4 | | 107.21993 |
| 30 | dihedral | 12 | 4 | 3 | 10 | 243.44605 |
| 31 | distance | 13 | 5 | | | 2.09790 |
| 32 | angle | 13 | 2 | 5 | | 108.59936 |
| 33 | dihedral | 13 | 5 | 2 | 1 | 89.84550 |
| 34 | distance | 14 | 5 | | | 2.07996 |
| 35 | angle | 14 | 2 | 5 | | 111.67827 |
| 36 | dihedral | 14 | 5 | 2 | 13 | 117.75691 |
| 37 | distance | 15 | 5 | | | 2.07779 |
| 38 | angle | 15 | 2 | 5 | | 112.31303 |
| 39 | dihedral | 15 | 5 | 2 | 13 | 242.10017 |

### 3.5. TS configuration for the *bcb* reaction

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.2186974 | -1.0139515 | 0.3964655 |
| C | 2.5601381 | 0.3061585 | -0.0037797 |
| C | 0.9078988 | -1.4695644 | 0.3490866 |
| C | 1.5840154 | 1.2257940 | -0.3671827 |
| C | -0.0741968 | -0.5690749 | -0.1307104 |
| C | 0.2358871 | 0.8077246 | -0.2916076 |
| H | 1.8471799 | 2.2599006 | -0.6103635 |
| H | 3.6106622 | 0.6096379 | 0.0165038 |
| H | 3.0166651 | -1.6944415 | 0.7073186 |
| H | 0.6673618 | -2.5099627 | 0.5871057 |
| C | -1.4065885 | -0.7589156 | -0.6185802 |
| C | -1.0021386 | 1.5378429 | -0.3130044 |
| H | -1.6065382 | -0.3613130 | -1.6150599 |
| H | -1.0688345 | 2.4114824 | -0.9849937 |
| C | -2.4126162 | -1.7139881 | -0.0604597 |
| C | -1.9271443 | 1.6514397 | 0.8735908 |
| H | -3.2651616 | -1.1557814 | 0.3763480 |
| H | -2.8422709 | -2.3803233 | -0.8290254 |
| H | -1.9909050 | -2.3276561 | 0.7519711 |
| H | -1.7820356 | 0.8349133 | 1.5959762 |
| H | -1.7445661 | 2.6067844 | 1.4066458 |
| H | -2.9916547 | 1.6654665 | 0.5778237 |

**Internal coordinates**

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | distance | 2 | 1 | | | 2.68545 |
| 2 | distance | 3 | 1 | | | 2.62394 |
| 3 | angle | 3 | 2 | 1 | | 121.46710 |
| 4 | distance | 4 | 2 | | | 2.62572 |
| 5 | angle | 4 | 1 | 2 | | 121.31322 |
| 6 | dihedral | 4 | 2 | 1 | 3 | 4.70958 |
| 7 | distance | 5 | 3 | | | 2.67621 |
| 8 | angle | 5 | 1 | 3 | | 117.23130 |
| 9 | dihedral | 5 | 3 | 1 | 2 | 0.76252 |
| 10 | distance | 6 | 4 | | | 2.67111 |
| 11 | angle | 6 | 2 | 4 | | 117.40595 |
| 12 | dihedral | 6 | 4 | 2 | 1 | 1.52565 |
| 13 | distance | 7 | 4 | | | 2.06818 |
| 14 | angle | 7 | 2 | 4 | | 120.96882 |
| 15 | dihedral | 7 | 4 | 2 | 8 | -1.54578 |
| 16 | distance | 8 | 2 | | | 2.06674 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 17 | angle | 8 | 1 | 2 | | 118.90422 |
| 18 | dihedral | 8 | 2 | 1 | 3 | 182.17279 |
| 19 | distance | 9 | 1 | | | 2.06702 |
| 20 | angle | 9 | 2 | 1 | | 118.86104 |
| 21 | dihedral | 9 | 1 | 2 | 4 | 182.08519 |
| 22 | distance | 10 | 3 | | | 2.06744 |
| 23 | angle | 10 | 1 | 3 | | 120.80879 |
| 24 | dihedral | 10 | 3 | 1 | 2 | 175.32959 |
| 25 | distance | 11 | 5 | | | 2.70518 |
| 26 | angle | 11 | 3 | 5 | | 132.57488 |
| 27 | dihedral | 11 | 5 | 3 | 1 | 162.43004 |
| 28 | distance | 12 | 6 | | | 2.71642 |
| 29 | angle | 12 | 4 | 6 | | 132.09909 |
| 30 | dihedral | 12 | 6 | 4 | 2 | 165.09742 |
| 31 | distance | 13 | 11 | | | 2.06233 |
| 32 | angle | 13 | 5 | 11 | | 115.68264 |
| 33 | dihedral | 13 | 11 | 5 | 6 | 50.89174 |
| 34 | distance | 14 | 12 | | | 2.08669 |
| 35 | angle | 14 | 6 | 12 | | 117.57372 |
| 36 | dihedral | 14 | 12 | 6 | 4 | 37.85730 |
| 37 | distance | 15 | 11 | | | 2.82558 |
| 38 | angle | 15 | 5 | 11 | | 125.71241 |
| 39 | dihedral | 15 | 11 | 5 | 3 | 39.53494 |
| 40 | distance | 16 | 12 | | | 2.85132 |
| 41 | angle | 16 | 6 | 12 | | 123.68323 |
| 42 | dihedral | 16 | 12 | 6 | 5 | 66.21895 |
| 43 | distance | 17 | 15 | | | 2.09511 |
| 44 | angle | 17 | 11 | 15 | | 110.05162 |
| 45 | dihedral | 17 | 15 | 11 | 5 | 114.54725 |
| 46 | distance | 18 | 15 | | | 2.08671 |
| 47 | angle | 18 | 11 | 15 | | 112.78979 |
| 48 | dihedral | 18 | 15 | 11 | 7 | 118.37321 |
| 49 | distance | 19 | 15 | | | 2.08250 |
| 50 | angle | 19 | 11 | 15 | | 111.92901 |
| 51 | dihedral | 19 | 15 | 11 | 17 | 241.75895 |
| 52 | distance | 20 | 16 | | | 2.07836 |
| 53 | angle | 20 | 12 | 16 | | 112.31997 |
| 54 | dihedral | 20 | 16 | 12 | 6 | -22.53577 |
| 55 | distance | 21 | 16 | | | 2.09597 |
| 56 | angle | 21 | 12 | 16 | | 109.99281 |
| 57 | dihedral | 21 | 16 | 12 | 20 | 119.79604 |
| 58 | distance | 22 | 16 | | | 2.08801 |
| 59 | angle | 22 | 12 | 16 | | 112.39856 |
| 60 | dihedral | 22 | 16 | 12 | 20 | 237.69745 |

## 4. Initial $v_1$ vectors

**sn2.1.1**

0.739151 -0.011375 -0.183260 -0.543787 0.147278 0.026465 -0.010066 -0.252423
0.001575 -0.010454 -0.194667 0.004509

**sn2.1.2**

0.739151 -0.011375 -0.183260 -0.543787 0.147278 0.026465 -0.010066 -0.252423
0.001575 -0.010454 -0.194667 0.004509

**sn2.1.3**

-0.653836 0.000000 0.181062 0.653836 -0.160944 0.000000 0.000000 0.231357
0.000000 0.000000 0.181062 0.000000

**sn2.1.4**

-0.666667 0.000000 0.166667 0.666667 -0.166667 0.000000 0.000000 0.166667
0.000000 0.000000 0.166667 0.000000

**sn2.1.5**

-0.680414 0.000000 0.136083 0.680414 -0.136083 0.000000 0.000000 0.136083
0.000000 0.000000 0.136083 0.000000

**sn2.1.6**

-0.688247 0.000000 0.114708 0.688247 -0.114708 0.000000 0.000000 0.114708
0.000000 0.000000 0.114708 0.000000

**sn2.1.7**

-0.693103 0.000000 0.099015 0.693103 -0.099015 0.000000 0.000000 0.099015
0.000000 0.000000 0.099015 0.000000

**sn2.1.8**

-0.707107 0.000000 0.000000 0.707107 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000

**sn2.1.9**

-0.639602 0.000000 0.213201 0.639602 -0.213201 0.000000 0.000000 0.213201
0.000000 0.000000 0.213201 0.000000

**sn2.1.10**

-0.577350 0.000000 0.288675 0.577350 -0.288675 0.000000 0.000000 0.288675
0.000000 0.000000 0.288675 0.000000

**sn2.1.11**

-0.549972 0.000000 0.314270 0.549972 -0.314270 0.000000 0.000000 0.314270
0.000000 0.000000 0.314270 0.000000

**sn2.1.12**

-0.514496 0.000000 0.342997 0.514496 -0.342997 0.000000 0.000000 0.342997
0.000000 0.000000 0.342997 0.000000

**sn2.1.13**

-0.737865 0.000000 0.210819 0.527046 -0.210819 0.000000 0.000000 0.210819
0.000000 0.000000 0.210819 0.000000

**sn2.1.14**

-0.527046 0.000000 0.210819 0.737865 -0.210819 0.000000 0.000000 0.210819
0.000000 0.000000 0.210819 0.000000

**sn2.1.15**

0.693582 0.011854 -0.205179 -0.588039 0.197100 -0.000043 0.012272 -0.214266
0.000419 0.012269 -0.214137 -0.000777

**sn2.2.1**

-0.648346 0.017198 0.188205 0.649794 -0.166694 -0.035063 0.016684 0.237323 -0.002697 0.017085 0.189073 -0.005778

**sn2.2.2**

-0.648346 0.017198 0.188205 0.649794 -0.166694 -0.035063 0.016684 0.237323 -0.002697 0.017085 0.189073 -0.005778

**sn2.3.1**

-0.351205 0.019090 0.146423 0.882329 -0.150704 -0.069432 0.019284 0.176189 -0.004156 0.020967 0.130005 -0.006385

**sn2.3.2**

0.693690 0.011900 -0.204824 -0.588030 0.197068 -0.000208 0.012286 -0.214363 0.000678 0.012301 -0.214078 -0.000875

**sn2.3.3**

-0.351205 0.019090 0.146423 0.882329 -0.150704 -0.069432 0.019284 0.176189 -0.004156 0.020967 0.130005 -0.006385

**sn2.3.4**

-0.351205 0.019090 0.146423 0.882329 -0.150704 -0.069432 0.019284 0.176189 -0.004156 0.020967 0.130005 -0.006385

**sn2.3.5**

0.693690 0.011900 -0.204824 -0.588030 0.197068 -0.000208 0.012286 -0.214363 0.000678 0.012301 -0.214078 -0.000875

**sn2.3.6**

-0.351205 0.019090 0.146423 0.882329 -0.150704 -0.069432 0.019284 0.176189 -0.004156 0.020967 0.130005 -0.006385

**sn2b.1.1**

0.682593 0.016569 0.271637 -0.523295 0.185401 0.011263 0.010719 0.016313
-0.008679 0.017408 -0.154767 0.236908 0.017147 -0.152238 -0.213232 0.011259
-0.018805 -0.024179 0.010860 -0.020414 0.017072

**sn2b.1.2**

0.682593 0.016569 0.271637 -0.523295 0.185401 0.011263 0.010719 0.016313
-0.008679 0.017408 -0.154767 0.236908 0.017147 -0.152238 -0.213232 0.011259
-0.018805 -0.024179 0.010860 -0.020414 0.017072

**sn2b.1.3**

0.555879 0.015939 0.176629 -0.670693 0.170498 -0.001192 0.011917 0.015259
-0.000835 0.015073 -0.141069 0.261840 0.014936 -0.140454 -0.264821 0.011774
-0.016772 -0.017913 0.011903 -0.016144 0.018946

**sn2b.1.4**

0.601102 0.000000 0.185795 -0.601102 0.185795 -0.000000 0.000000 0.000000
0.000000 0.000000 -0.153008 0.284157 0.000000 -0.153008 -0.284157 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000

**sig.1.1**

-0.082207 0.086863 0.010976 -0.070034 -0.005809 -0.000318 0.001452 -0.019233
0.110330 0.003081 -0.025965 0.006801 0.000594 0.006450 0.031093 0.000568
0.012457 0.016119 -0.002926 0.018226 -0.061989 0.010107 -0.071857 0.318262
0.799190 0.463233 -0.043705

**sig.1.2**

-0.082207 0.086863 0.010976 -0.070034 -0.005809 -0.000318 0.001452 -0.019233
0.110330 0.003081 -0.025965 0.006801 0.000594 0.006450 0.031093 0.000568
0.012457 0.016119 -0.002926 0.018226 -0.061989 0.010107 -0.071857 0.318262
0.799190 0.463233 -0.043705

**sig.2.1**

0.079667 -0.127467 0.000000 0.079667 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
-0.478000 -0.717001 -0.478000 0.000000

**sig.2.2**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 -0.346844
-0.780399 -0.520266 0.000000

**sig.2.3**

0.196740 -0.149740 -0.036699 0.158465 -0.003594 0.007403 0.009388 -0.045975
-0.203198 -0.002208 0.016376 -0.017683 0.000838 -0.002319 -0.007854 0.001893
-0.019516 -0.012855 -0.016594 -0.049317 0.133500 -0.002622 0.020489
-0.192692 -0.671761 -0.591522 0.091671

**sig.2.4**

0.079667 -0.127467 0.000000 0.079667 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 -0.478000
-0.717001 -0.478000 0.000000

**sig.3.1**

0.006675 -0.012321 0.003362 0.004639 -0.006718 -0.088993 -0.003424 -0.000926
0.089647 -0.002674 0.005628 -0.069315 0.001529 0.006149 0.106813 0.002215
0.006934 -0.030790 -0.094285 0.005039 -0.098074 -0.035901 0.132625 -0.410401
-0.615602 -0.615602 0.051872

**sig.3.2**

0.006675 -0.012321 0.003362 0.004639 -0.006718 -0.088993 -0.003424 -0.000926
0.089647 -0.002674 0.005628 -0.069315 0.001529 0.006149 0.106813 0.002215
0.006934 -0.030790 -0.094285 0.005039 -0.098074 -0.035901 0.132625 -0.410401
-0.615602 -0.615602 0.051872

**sig.3.3**

0.198257 -0.147638 -0.035054 0.156772 -0.004412 -0.007756 0.008547 -0.050964
-0.245192 -0.002073 0.015469 -0.018867 0.000662 -0.002110 -0.008525 0.001939
-0.019427 -0.013559 -0.018721 -0.049946 0.144965 -0.003240 0.023344
-0.203918 -0.663003 -0.584727 -0.038783

**sig.3.4**

0.006675 -0.012321 0.003362 0.004639 -0.006718 -0.088993 -0.003424 -0.000926
0.089647 -0.002674 0.005628 -0.069315 0.001529 0.006149 0.106813 0.002215
0.006934 -0.030790 -0.094285 0.005039 -0.098074 -0.035901 0.132625 -0.410401
-0.615602 -0.615602 0.051872

**sig.3.5**

0.006675 -0.012321 0.003362 0.004639 -0.006718 -0.088993 -0.003424 -0.000926
0.089647 -0.002674 0.005628 -0.069315 0.001529 0.006149 0.106813 0.002215
0.006934 -0.030790 -0.094285 0.005039 -0.098074 -0.035901 0.132625 -0.410401
-0.615602 -0.615602 0.051872

**sig.3.6**

0.198257 -0.147638 -0.035054 0.156772 -0.004412 -0.007756 0.008547 -0.050964
-0.245192 -0.002073 0.015469 -0.018867 0.000662 -0.002110 -0.008525 0.001939
-0.019427 -0.013559 -0.018721 -0.049946 0.144965 -0.003240 0.023344
-0.203918 -0.663003 -0.584727 -0.038783

**dcc.1.1**

-0.032483 -0.027418 0.582014 -0.029426 -0.036112 -0.144038 -0.044062
-0.003425 0.193511 0.057281 -0.036247 -0.150531 0.313388 -0.207633 -0.203075
0.004656 -0.003446 0.432737 0.000938 0.045825 -0.431801 0.004076 -0.004208
0.075042 -0.001780 0.025853 0.027695 0.009620 -0.006976 0.044535 0.009620 -
0.012243 -0.031241 -0.001837 0.015404 0.002948 0.002932 -0.009107 0.026149

**dcc.1.2**

-0.032483 -0.027418 0.582014 -0.029426 -0.036112 -0.144038 -0.044062

-0.003425  0.193511  0.057281 -0.036247 -0.150531  0.313388 -0.207633 -0.203075
0.004656  -0.003446  0.432737  0.000938  0.045825 -0.431801  0.004076 -0.004208
0.075042 -0.001780  0.025853  0.027695  0.009620 -0.006976  0.044535  0.009620 -
0.012243  -0.031241 -0.001837  0.015404  0.002948  0.002932 -0.009107  0.026149

**dcc.1.3**

0.048183  0.049164 -0.323162  0.011839 -0.010178  0.105983 -0.011552 -0.005011
-0.250609  0.006130  0.002114  0.300314 -0.444274  0.631441  0.079721 -0.007644
0.000539 -0.236637 -0.004590  0.013547  0.248249 -0.001022  0.014478 -0.013447
0.001920  0.009900 -0.009667  0.010443  0.012899 -0.011246 -0.002091 -0.059267
-0.015399 -0.001152  0.018717 -0.011555 -0.001143  0.004910  0.023758

**dcc.1.4**

-0.032483 -0.027418  0.582014 -0.029426 -0.036112 -0.144038 -0.044062
-0.003425  0.193511  0.057281 -0.036247 -0.150531  0.313388 -0.207633 -0.203075
0.004656  -0.003446  0.432737  0.000938  0.045825 -0.431801  0.004076 -0.004208
0.075042 -0.001780  0.025853  0.027695  0.009620 -0.006976  0.044535  0.009620 -
0.012243  -0.031241 -0.001837  0.015404  0.002948  0.002932 -0.009107  0.026149

**dcc.1.5**

-0.032483 -0.027418  0.582014 -0.029426 -0.036112 -0.144038 -0.044062
-0.003425  0.193511  0.057281 -0.036247 -0.150531  0.313388 -0.207633 -0.203075
0.004656  -0.003446  0.432737  0.000938  0.045825 -0.431801  0.004076 -0.004208
0.075042 -0.001780  0.025853  0.027695  0.009620 -0.006976  0.044535  0.009620 -
0.012243  -0.031241 -0.001837  0.015404  0.002948  0.002932 -0.009107  0.026149

**dcc.2.1**

-0.041922 -0.041922  0.838444  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000 -0.041922  0.251533 -0.041922  0.041922  0.000000
0.000000  0.335377  0.000000  0.000000 -0.335377  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000

**dcc.2.2**

-0.041922 -0.041922  0.838444  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000 -0.041922  0.251533 -0.041922  0.041922  0.000000

0.000000 0.335377 0.000000 0.000000 -0.335377 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.2.3**

0.000000 0.000000 0.812329 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.045129 0.270776 -0.045129 0.045129 0.000000
0.000000 0.361035 0.000000 0.000000 -0.361035 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.2.4**

0.000000 0.000000 1.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0. 000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.2.5**

0.000000 0.000000 0.812329 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.045129 0.270776 -0.045129 0.045129 0.000000
0.000000 0.361035 0.000000 0.000000 -0.361035 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.2.6**

0.000000 0.000000 0.812329 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.045129 0.270776 -0.045129 0.045129 0.000000
0.000000 0.361035 0.000000 0.000000 -0.361035 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.2.7**

0.000000 0.000000 0.812329 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.045129 0.270776 -0.045129 0.045129 0.000000
0.000000 0.361035 0.000000 0.000000 -0.361035 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.2.8**

0.000000 0.000000 1.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0. 000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.3.1**

-0.041922 -0.041922 0.838444 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.041922 0.251533 -0.041922 0.041922 0.000000
0.000000 0.335377 0.000000 0.000000 -0.335377 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.3.2**

-0.041922 -0.041922 0.838444 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.041922 0.251533 -0.041922 0.041922 0.000000
0.000000 0.335377 0.000000 0.000000 -0.335377 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.3.3**

0.000000 0.000000 1.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0. 000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.3.4**

-0.041922 -0.041922 0.838444 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.041922 0.251533 -0.041922 0.041922 0.000000
0.000000 0.335377 0.000000 0.000000 -0.335377 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.3.5**

-0.041922 -0.041922 0.838444 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 -0.041922 0.251533 -0.041922 0.041922 0.000000
0.000000 0.335377 0.000000 0.000000 -0.335377 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**dcc.3.6**

0.000000 0.000000 1.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0. 000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

**bcb.1.1**

-0.052277 -0.046441 -0.023822 -0.067894 -0.034278 0.056020 0.062263 0.162993
0.041703 0.063472 0.175220 0.042005 0.003642 -0.019996 0.001999 0.000216
0.009152 -0.016736 0.000879 0.012399 0.007741 0.002642 -0.023594 0.004103
-0.156916 -0.535400 -0.063645 -0.173493 -0.551865 0.013921 -0.015922
0.058348 -0.325768 -0.001454 -0.020005 -0.123526 -0.040384 -0.046767 -0.139376
-0.059453 0.090933 -0.317482 0.001607 -0.011886 0.015141 0.008353 0.005723
-0.008226 0.002262 0.003911 0.012728 -0.001455 0.013091 0.008956 0.007630
-0.046969 0.007036 0.002300 0.023548 -0.007276

**bcb.1.2**

-0.052277 -0.046441 -0.023822 -0.067894 -0.034278 0.056020 0.062263 0.162993
0.041703 0.063472 0.175220 0.042005 0.003642 -0.019996 0.001999 0.000216
0.009152 -0.016736 0.000879 0.012399 0.007741 0.002642 -0.023594 0.004103
-0.156916 -0.535400 -0.063645 -0.173493 -0.551865 0.013921 -0.015922
0.058348 -0.325768 -0.001454 -0.020005 -0.123526 -0.040384 -0.046767 -0.139376
-0.059453 0.090933 -0.317482 0.001607 -0.011886 0.015141 0.008353 0.005723
-0.008226 0.002262 0.003911 0.012728 -0.001455 0.013091 0.008956 0.007630
-0.046969 0.007036 0.002300 0.023548 -0.007276

**bcb.1.3**

-0.052277 -0.046441 -0.023822 -0.067894 -0.034278 0.056020 0.062263 0.162993

0.041703 0.063472 0.175220 0.042005 0.003642 -0.019996 0.001999 0.000216
0.009152 -0.016736 0.000879 0.012399 0.007741 0.002642 -0.023594 0.004103
-0.156916 -0.535400 -0.063645 -0.173493 -0.551865 0.013921 -0.015922
0.058348 -0.325768 -0.001454 -0.020005 -0.123526 -0.040384 -0.046767 -0.139376
-0.059453 0.090933 -0.317482 0.001607 -0.011886 0.015141 0.008353 0.005723
-0.008226 0.002262 0.003911 0.012728 -0.001455 0.013091 0.008956 0.007630
-0.046969 0.007036 0.002300 0.023548 -0.007276

**bcb.1.4**

-0.014277 0.077887 0.017164 0.075703 0.014726 -0.019625 -0.090326 -0.121424
-0.051635 -0.087900 -0.130771 -0.032700 -0.003001 0.012111 -0.009859
0.000500 -0.008153 0.005019 0.000526 -0.008132 0.010683 -0.001282 0.017234
-0.004146 0.170472 0.383960 -0.039170 0.164856 0.426228 -0.009138 -0.000642
-0.036277 0.471289 0.006089 0.064517 0.254617 0.021112 0.018789 0.215351
0.037169 -0.103971 0.436294 0.000903 0.024908 -0.000590 -0.007622 -0.019323
0.015255 0.000665 -0.010476 -0.004086 0.001275 -0.012213 -0.017522 -0.000034
0.049996 -0.009626 -0.000787 -0.034085 0.006404

**bcb.1.5**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.364474 0.000000 0.000000 0.364474 0.000000 0.000000 0.000000
0.546711 0.000000 0.000000 0.364474 0.000000 0.000000 0.060746 0.000000
0.000000 0.546711 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000

**bcb.1.6**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.500000 0.000000 0.000000 0.500000 0.000000 0.000000 0.000000
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0.000000 0.000000 0.000000 0.000000

**bcb.1.7**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.392232 0.000000 0.000000 0.392232 0.000000 0.000000 0.000000
0.588348 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.588348 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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0.000000 0.000000 0.000000 0.000000

**bcb.1.8**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.316228 0.000000 0.000000 0.316228 0.000000 0.000000 0.000000
0.632456 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.1.9**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.223607 0.000000 0.000000 0.223607 0.000000 0.000000 0.000000
0.670820 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.670820 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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0.000000 0.000000 0.000000 0.000000

**bcb.1.10**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.588348 0.000000 0.000000 0.588348 0.000000 0.000000 0.000000
0.392232 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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0.000000 0.000000 0.000000 0.000000

**bcb.1.11**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.632456 0.000000 0.000000 0.632456 0.000000 0.000000 0.000000
0.316228 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.316228 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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0.000000 0.000000 0.000000 0.000000

**bcb.1.12**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.670820 0.000000 0.000000 0.670820 0.000000 0.000000 0.000000
0.223607 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.223607 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.1.13**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.685994 0.000000 0.000000 0.685994 0.000000 0.000000 0.000000
0.171499 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.171499 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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0.000000 0.000000 0.000000 0.000000

**bcb.1.14**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.707107 0.000000 0.000000 0.707107 0.000000 0.000000 0.000000
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**bcb.2.1**

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0.000000 0.354713 0.000000 0.000000 0.390184 0.000000 0.000000 0.000000
0.532070 0.000000 0.000000 0.390184 0.000000 0.000000 0.059119 0.000000
0.000000 0.532070 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000

**bcb.2.2**

-0.014245 0.077916 0.017186 0.075670 0.014749 -0.019457 -0.090399
-0.121556 -0.051432 -0.087913 -0.130867 -0.032807 -0.002996 0.012137
-0.009875 0.00049 -0.008152 0.005025 0.000520 -0.008138 0.010738 -0.001278
0.017268 -0.004150 0.170468 0.384091 -0.039214 0.164759 0.426228 -0.009441
-0.000632 -0.036433 0.471376 0.006089 0.064497 0.254535 0.021168 0.018945
0.215469 0.037183 -0.103889 0.436052 0.000882 0.024704 -0.000794 -0.007615
-0.019244 0.015184 0.000663 -0.010541 -0.004134 0.001281 -0.012168 -0.017514
-0.000036 0.050013 -0.009609 -0.000778 -0.034087 0.006394

**bcb.2.3**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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0.568075 0.000000 0.000000 0.252478 0.000000 0.000000 0.063119 0.000000
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**bcb.2.4**

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**bcb.2.5**

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**bcb.3.1**

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**bcb.3.2**

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**bcb.3.3**

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**bcb.3.4**

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**bcb.3.5**

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**bcb.3.6**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.309016 0.000000 0.000000 0.309016 0.000000 0.000000 0.000000
0.618031 0.000000 0.000000 0.206010 0.000000 0.000000 0.051503 0.000000
0.000000 0.618031 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.3.7**

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0.000000 0.392232 0.000000 0.000000 0.392232 0.000000 0.000000 0.000000
0.588348 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.588348 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.3.8**

-0.014277 0.077887 0.017164 0.075703 0.014726 -0.019625 -0.090326 -0.121424
-0.051635 -0.087900 -0.130771 -0.032700 -0.003001 0.012111 -0.009859 0.000500
-0.008153 0.005019 0.000526 -0.008132 0.010683 -0.001282 0.017234 -0.004146
0.170472 0.383960 -0.039170 0.164856 0.426228 -0.009138 -0.000642 -0.036277
0.471289 0.006089 0.064517 0.254617 0.021112 0.018789 0.215351 0.037169
-0.103971 0.436294 0.000903 0.024908 -0.000590 -0.007622 -0.019323 0.015255
0.000665 -0.010476 -0.004086 0.001275 -0.012213 -0.017522 -0.000034 0.049996
-0.009626 -0.000787 -0.034085 0.006404

**bcb.3.9**

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0.568075 0.000000 0.000000 0.252478 0.000000 0.000000 0.063119 0.000000
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**bcb.3.10**

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0.632456 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.3.11**

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0.000000 0.262613 0.000000 0.000000 0.262613 0.000000 0.000000 0.000000
0.656532 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.3.12**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.223607 0.000000 0.000000 0.223607 0.000000 0.000000 0.000000
0.670820 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.670820 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.3.13**

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0.000000 0.668503 0.000000 0.000000 0.668503 0.000000 0.000000 0.000000
0.222834 0.000000 0.000000 0.074278 0.000000 0.000000 0.037139 0.000000
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**bcb.3.14**

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0.000000 0.484182 0.000000 0.000000 0.484182 0.000000 0.000000 0.000000
0.484182 0.000000 0.000000 0.242091 0.000000 0.000000 0.060523 0.000000
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**bcb.3.15**

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**bcb.3.16**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.568075 0.000000 0.000000 0.568075 0.000000 0.000000 0.000000
0.378717 0.000000 0.000000 0.252478 0.000000 0.000000 0.063119 0.000000
0.000000 0.378717 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000

**bcb.3.17**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.588348 0.000000 0.000000 0.588348 0.000000 0.000000 0.000000
0.392232 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.392232 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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0.000000 0.000000 0.000000 0.000000

**bcb.3.18**

0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.628109 0.000000 0.000000 0.628109 0.000000 0.000000 0.000000
0.314054 0.000000 0.000000 0.104685 0.000000 0.000000 0.052342 0.000000
0.000000 0.314054 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

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**bcb.3.19**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.653410 0.000000 0.000000 0.653410 0.000000 0.000000 0.000000
0.261364 0.000000 0.000000 0.087121 0.000000 0.000000 0.043561 0.000000
0.000000 0.261364 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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**bcb.3.20**

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.171499 0.000000 0.000000 0.171499 0.000000 0.000000 0.000000
0.685994 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
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## 5. TS eigenvectors

### TS eigenvector at the TS configuration for the *sn2* reaction

0.692729 0.011749 -0.205353 -0.588689 0.197221 -0.000006 0.012196
-0.214723 0.000744 0.012200 -0.214390 -0.000542

### TS eigenvector at the TS configuration for the *sn2b* reaction

0.556081 0.015955 0.177469 -0.670210 0.170722 -0.001969 0.011922
0.014780 0.001220 0.015055 -0.141272 0.260197 0.014970 -0.140552
-0.266386 0.011791 -0.016754 -0.018049 0.011876 -0.016196 0.018811

### TS eigenvector at the TS configuration for the *sig* reaction

-0.198318 0.147666 0.035068 -0.156812 0.004416 0.007746 -0.008556
0.051025 0.245191 0.002071 -0.015459 0.018850 -0.000663 0.002104
0.008518 -0.001940 0.019438 0.013552 0.018676 0.049962 -0.144970 0.003235
-0.023311 0.203875 0.662863 0.584857 0.038770

### TS eigenvector at the TS configuration for the *dcc* reaction

0.047894 0.048986 -0.323207 0.011664 -0.010667 0.106250 -0.011684
-0.005056 -0.250039 0.005908 0.002456 0.299933 -0.443695 0.631986
0.080513 -0.007649 0.000500 -0.236783 -0.004593 0.013545 0.248535
-0.000973 0.014176 -0.011025 0.001828 0.010073 -0.009355 0.010423
0.012676 -0.010459 -0.002056 -0.059614 -0.015174 -0.001164 0.018748
-0.011674 -0.001189 0.005020 0.023888

**TS eigenvector at the TS configuration for the *bcb* reaction**

-0.014277 0.077887 0.017164 0.075703 0.014726 -0.019625 -0.090326
-0.121424 -0.051635 -0.087900 -0.130771 -0.032700 -0.003001 0.012111
-0.009859 0.000500 -0.008153 0.005019 0.000526 -0.008132 0.010683
-0.001282 0.017234 -0.004146 0.170472 0.383960 -0.039170 0.164856
0.426228 -0.009138 -0.000642 -0.036277 0.471289 0.006089 0.064517
0.254617 0.021112 0.018789 0.215351 0.037169 -0.103971 0.436294
0.000903 0.024908 -0.000590 -0.007622 -0.019323 0.015255 0.000665
-0.010476 -0.004086 0.001275 -0.012213 -0.017522 -0.000034 0.049996
-0.009626 -0.000787 -0.034085 0.006404

## 5. Performance of GAD-CD as a function of the initial $\mathbf{v}_1$ vector

**Table S5.1**. Assessment of the performance of the GAD-CD method for the $S_N2$ reaction as a function of the initial $\mathbf{v}_1$ vector.[a]

| Reaction[b] | $\mathbf{v}_1$ relevant components[c] | | | | | | Angle[d] | #steps[e] |
|---|---|---|---|---|---|---|---|---|
| | $\mathbf{v}_1$ (1) | $\mathbf{v}_1$ (3) | $\mathbf{v}_1$ (4) | $\mathbf{v}_1$ (5) | $\mathbf{v}_1$ (8) | $\mathbf{v}_1$ (11) | | |
| **sn2.1.1** | 0.74 | -0.18 | -0.54 | 0.14 | -0.25 | -0.19 | 6.1 | 7 |
| **sn2.1.3** | 0.65 | -0.18 | -0.65 | 0.16 | -0.23 | -0.18 | 5.6 | 7 |
| **sn2.1.4** | 0.66 | -0.16 | -0.66 | 0.16 | -0.16 | -0.16 | 6.8 | 8 |
| **sn2.1.5** | 0.68 | -0.14 | -0.68 | 0.14 | -0.14 | -0.14 | 9.9 | 9 |
| **sn2.1.6** | 0.69 | -0.11 | -0.69 | 0.11 | -0.11 | -0.11 | 12.2 | 11 |
| **sn2.1.7** | 0.69 | -0.09 | -0.69 | 0.09 | -0.09 | -0.09 | 14.0 | 15 |
| **sn2.1.8** | 0.71 | 0.00 | -0.71 | 0.00 | 0.00 | 0.00 | 25.1 | – |
| **sn2.1.9** | 0.64 | -0.21 | -0.64 | 0.21 | -0.21 | -0.21 | 4.5 | 7 |
| **sn2.1.10** | 0.58 | -0.29 | -0.58 | 0.29 | -0.29 | -0.29 | 11.5 | 9 |
| **sn2.1.11** | 0.55 | -0.31 | -0.55 | 0.31 | -0.31 | -0.31 | 15.0 | 15 |
| **sn2.1.12** | 0.51 | -0.34 | -0.51 | 0.34 | -0.34 | -0.34 | 19.2 | – |
| **sn2.1.13** | 0.74 | -0.21 | -0.53 | 0.21 | -0.21 | -0.21 | 4.7 | 8 |
| **sn2.1.14** | 0.53 | -0.21 | -0.74 | 0.21 | -0.21 | -0.21 | 12.9 | 8 |
| **sn2.1.15** | 0.69 | -0.21 | -0.59 | 0.19 | -0.21 | -0.21 | 0.0 | 8 |

*a*) The starting configuration was the same for all the calculations and was taken from the IRC (the arc length along the IRC associated with the starting configuration is 0.58). In all the calculations, the Hessian was analytically evaluated at every point of the optimization and the $\mathbf{v}_1$ vector was updated according to Eq. 17 in the main text.
*b*) Labels used to identify the reactions studied and the initial conditions employed to locate the TS configurations.
*c*) The components of the initial v1 vector with a non-negligible weight are (see Figure 2 for the atom numbering):
$\mathbf{v}_1(1)$ = bond length {2 1} (ie., the bond length between atoms 1 and 2)
$\mathbf{v}_1(3)$ = angle {3 2 1} (ie, the angle formed between atoms 3, 2 and 1, atom 2 being the apex atom)
$\mathbf{v}_1(4)$ = bond length {4 2}
$\mathbf{v}_1(5)$ = angle {4 2 3}
$\mathbf{v}_1(8)$ = angle {5 2 1}
$\mathbf{v}_1(11)$ = angle {6 2 1}
*d*) Angle between the initial $\mathbf{v}_1$ vector and the eigenvector associated with the imaginary frequency at the TS configuration.
*e*) Number of steps needed to reach convergence. If the entry is "-", it means that convergence was not achieved due to any of the following reasons: i) the maximum number of steps (150) was reached; ii) the algorithm failed to progress after reaching a specific configuration (i.e., the molecular structure barely changed from a certain point on); iii) the optimization led to a high-energy configuration for which the SCF calculation did not converge.

**Table S5.2**. Assessment of the performance of the GAD-CD method for the *bcb* reaction as a function of the initial $\mathbf{v}_1$ vector.[a]

| Reaction[b] | $\mathbf{v}_1$ relevant components[c] | | | | | | Angle[d] | #steps[e] |
|---|---|---|---|---|---|---|---|---|
| | $\mathbf{v}_1$ (26) | $\mathbf{v}_1$ (29) | $\mathbf{v}_1$ (33) | $\mathbf{v}_1$ (36) | $\mathbf{v}_1$ (39) | $\mathbf{v}_1$ (42) | | |
| **bcb.1.3**[f] | 0.54 | 0.55 | 0.33 | 0.12 | 0.14 | 0.32 | 20.4 | 14 |
| **bcb.1.4**[f] | 0.38 | 0.42 | 0.47 | 0.25 | 0.21 | 0.44 | 0.00 | 78 |
| **bcb.1.5** | 0.36 | 0.36 | 0.55 | 0.36 | 0.06 | 0.55 | 26.2 | 8 |
| **bcb.1.6** | 0.50 | 0.50 | 0.50 | 0.00 | 0.00 | 0.50 | 30.8 | 16 |
| **bcb.1.7** | 0.39 | 0.39 | 0.59 | 0.00 | 0.00 | 0.59 | 31.6 | 10 |
| **bcb.1.8** | 0.32 | 0.32 | 0.63 | 0.00 | 0.00 | 0.63 | 33.9 | 19 |
| **bcb.1.9** | 0.22 | 0.22 | 0.67 | 0.00 | 0.00 | 0.67 | 37.8 | – |
| **bcb.1.10** | 0.59 | 0.59 | 0.39 | 0.00 | 0.00 | 0.39 | 33.6 | 23 |
| **bcb.1.11** | 0.63 | 0.63 | 0.32 | 0.00 | 0.00 | 0.32 | 36.9 | 16 |
| **bcb.1.12** | 0.67 | 0.67 | 0.22 | 0.00 | 0.00 | 0.22 | 41.7 | 32 |
| **bcb.1.13** | 0.69 | 0.69 | 0.17 | 0.00 | 0.00 | 0.17 | 44.6 | 89 |
| **bcb.1.14** | 0.71 | 0.71 | 0.00 | 0.00 | 0.00 | 0.00 | 55.0 | – |

*a*) The starting configuration was the same for all the calculations and was taken from the IRC (the arc length along the IRC associated with the starting configuration is 0.75). In all the calculations, the Hessian was analytically evaluated every 5 steps of the optimization. The Hessian was updated via Eq. 18 in between the steps in which an analytical evaluation was carried out. The $\mathbf{v}_1$ vector was updated according to Eq. 17 in all calculations.

*b*) Labels used to identify the reactions studied and the initial conditions employed to locate the TS configurations.

*c*) The components of the initial $\mathbf{v}_1$ vector with a non-negligible weight are (see Figure 6 for the atom numbering):

$\mathbf{v}_1(26)$ = angle {11 5 3} (ie., the angle formed between atoms 11, 5 and 3, atom 5 being the apex atom)

$\mathbf{v}_1(29)$ = angle {12 6 4}

$\mathbf{v}_1(33)$ = dihedral {13 11 5 6} (ie., the dihedral angle formed between atoms 13, 11, 5 and 6)

$\mathbf{v}_1(36)$ = dihedral {14 12 6 4}

$\mathbf{v}_1(39)$ = dihedral {15 11 5 3}

$\mathbf{v}_1(42)$ = dihedral {16 12 6 5}

*d*) Angle between the initial $\mathbf{v}_1$ vector and the eigenvector associated with the imaginary frequency at the TS configuration.

*e*) Number of steps needed to reach convergence. If the entry is "–", it means that convergence was not achieved due to any of the reasons mentioned in footnote *g*) of Table S5.1.

*f*) In this particular case, the $\mathbf{v}_1$ vector has other components with a non-negligible weight. The full list of components is given in Section 4 of the Supp. Info.

## 6. Comparison between the GAD-CD and TRIM algorithms

The comparison between GAD-CD and TRIM has been made using the five different reactions included in the main text (*sn2*, *sn2b*, *sig*, *dcc*, *bcb*). As done with GAD-CD, three different starting points have been considered for each reaction (except for the *sn2b* reaction, for which a single starting configuration very close to reactants was considered). For each different starting point, both analytical and updated Hessian matrices have been used. The TRIM calculations have been carried with the Turbomole package (see reference 60 in the main text) using the default settings, the same level of theory and the same sets of internal coordinates as used for GAD-CD. We note that in the cases in which TRIM failed to locate the TS, several reasonable initial following eigenvectors were tested. The following table summarizes the results of the study carried out to compare the reliability and efficiency of GAD-CD and TRIM.

**Table S6.** Comparison between the performance of the GAD-CD and TRIM methods in the location of TS configurations.

| Reaction[a] | Starting configuration[b] | Hessian[c] | #steps TRIM[d] | #steps GAD-CD[e] |
|---|---|---|---|---|
| **sn2** | 0.58 | Analytical | 8 | 7 (sn2.1.1) |
| **sn2** | 0.58 | Updated | 12 | 13 (sn2.1.2) |
| **sn2** | 0.76 | Analytical | 9 | 9 (sn2.2.1) |
| **sn2** | 0.76 | Updated | 12 | 19 (sn2.2.2) |
| **sn2** | 0.95 | Analytical | 10 | 14 (sn2.3.3) |
| **sn2** | 0.95 | Updated | 19 | 26 (sn2.3.5) |
| | | | | |
| **sn2b** | –[f] | Analytical | 8 | 10 (sn2b.1.2) |
| **sn2b** | –[f] | Updated | 9 | 13 (sn2b.1.4) |
| | | | | |
| **sig** | 0.33 | Analytical | 6 | 6 (sig.1.1) |
| **sig** | 0.33 | Updated | 11 | 7 (sig.1.2) |
| **sig** | 1.30 | Analytical | 13 | 14 (sig.2.2) |
| **sig** | 1.30 | Updated | – | 43 (sig.2.4) |
| **sig** | 2.67 | Analytical | 13 | 26 (sig.3.2) |
| **sig** | 2.67 | Updated | 42 | 45 (sig.3.5) |
| | | | | |
| **dcc** | 0.96 | Analytical | 17 | 19 (dcc.1.2) |
| **dcc** | 0.96 | Updated | 12 | 18 (dcc.1.5) |
| **dcc** | 1.96 | Analytical | – | 38 (dcc.2.3) |
| **dcc** | 1.96 | Updated (5) | – | 80 (dcc.2.7) |
| **dcc** | 5.25 | Analytical | – | 42 (dcc.3.2) |
| **dcc** | 5.25 | Updated (5) | – | 120 (dcc.3.5) |
| | | | | |
| **bcb** | 0.75 | Analytical | 9 | 13 (bcb.1.1) |
| **bcb** | 0.75 | Updated | 10 | 8 (bcb.1.5) |
| **bcb** | 1.51 | Analytical | – | 49 (bcb.2.1) |
| **bcb** | 1.51 | Updated | – | 40 (bcb.2.5) |
| **bcb** | 4.15 | Analytical | – | 39 (bcb.3.2) |
| **bcb** | 4.15 | Updated (5) | – | 24 (bcb.3.5) |

*a*) The labels used to identify the reactions are the same as those used in the main text of the article:
"*sn2*" refers to the following sn2 reaction: $Cl^- + CH_3F \rightarrow CH_3Cl + F^-$
"*sn2b*" refers to the following sn2 reaction: $Br^- + CH_3NH_3^+ \rightarrow BrCH_3 + NH_3$
"*sig*" refers to the [1,5]-hydrogen shift in 1,3-cyclopentadiene
"*dcc*" refers to the disrotatory ring-opening of 1,1-dichloro-2,3-dimethylcyclo propane
"*bcb*" refers to the conrotatory ring-opening of cis-1,2-dimethyl-benzocyclobutene
*b*) Except for the "*sn2b*" reaction, the initial configurations for all reactions were taken from the corresponding IRCs. The values collected in this column are the arc lengths along the IRC associated with the initial configuration. Smaller *s* values are associated with configurations that are closer to the TS configuration.
*c*) If the entry is "Analytical", it means that the Hessian was evaluated by means of an analytical calculation at each iteration of the optimization procedure. If the entry is "Updated", it means that the Hessian was analytically solved only at the initial configuration and that the Hessian was updated from then on. If the entry is "Updated (*n*)", it means that the Hessian was computed analytically every *n* steps. Note that the updating protocol used in the GAD-CD method is different from that used in the TRIM method implemented in Turbomole[60]: the Murtagh-Sargent-Powell formula (see Eq. 18 in the main text) is employed in the former method, while the Powell formula is employed in the latter. The Powell formula is based on Eq. 18 of the main text, but taking $\mathbf{W} = \mathbf{I}$.
*d*) Number of steps needed to reach convergence using the TRIM method. If the entry is "–", it means that convergence was not achieved due to one of the following reasons: i) the maximum number of steps (150) was reached; ii) the optimization led to a high-energy configuration for which the SCF calculation did not converge; iii) the optimization led to a minimum energy configuration instead of a TS.
*e*) Number of steps needed to reach convergence using the GAD-CD method. The label associated with the setup employed (see Tables 1-5 in the main text) appears in brackets.
*f*) In this particular case, the starting configuration was generated manually from the reactant configuration by shortening the C···Br bond by 0.02 au and stretching the C-N bond by 0.02 au.

The results gathered in the Table S6 above demonstrate that the performance of GAC-CD is similar to the performance of TRIM when considering starting configurations relatively close to the TS. In some of these cases, TRIM is faster because GAD-CD takes a few extra iterations to reach convergence. Yet, the difference in number of steps is relatively small. The slightly better performance of TRIM in some of these cases (initial configuration close to the TS) is not surprising taking into account that TRIM was designed specifically for this type of situations and that TRIM has had a large period of time for improvement.

In contrast, the performance of GAD-CD is superior (compared to TRIM) when the starting configurations of medium-sized molecular systems are very far away from the TS. While TRIM fails to locate the TS for two of the starting points of *dcc* and *bcb* reactions, GAD-CD has been always able to successfully locate the TS in reasonable number of iterations even when using an updated Hessian. Again, this is not a suprise, since it is well known that TRIM does not properly work for initial configurations that are far away from the desired TS. As a matter of fact, in the Turbomole manual (see reference 60 in the main text) it is recommended to use a "double-ended" method to generate an educated guess for TRIM.

On the whole, the results presented in the article clearly demonstrate that GAD-CD, which is, to the best of our knowledge, the first algorithm to locate TSs based on optimization control theory, is a very robust, reliable and verstaile method to locate TS. Let us stress that the main advantage of GAD-CD over TRIM is that there is no need to start close to the TS in order to locate it.