Electronic Supplementary Information for

Ring-opening radical clock reactions: Many density functionals have difficulty keeping time

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Table S1. Activation energies (kcal/mol) and ring-opening rate constants for CPC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	8.2	8.5	8.2E+06	12.21
B3LYP	6-31+G(d,p)-DCP[†]	7.6	7.9	2.4E+07	4.17
B3LYP	6-311+G(d,p)	6.6	6.9	1.3E+08	0.79
B3LYP	aug-cc-pVTZ	6.5	6.9	1.4E+08	0.72
B97-D	6-31+G(d,p)	5.8	6.1	2.2E+08	0.22
B971	6-31+G(d,p)	6.7	7.0	1.0E+08	0.99
B971 (49.434)[‡]	6-31+G(d,p)	6.7	7.0	1.0E+08	0.96
B971	6-31+G(d,p)-DCP[†]	5.4	5.6	8.9E+08	0.11
B971	6-311+G(d,p)	6.3	6.6	2.0E+08	0.50
B971	aug-cc-pVTZ	6.2	6.6	2.1E+08	0.47
PBE	6-31+G(d,p)	7.1	7.4	5.6E+07	1.79
PBE	6-31+G(d,p)-DCP[†]	6.1	6.4	3.0E+08	0.33
PBE	6-311+G(d,p)	6.7	7.0	1.1E+08	0.91
PBE	aug-cc-pVTZ	6.7	7.0	1.1E+08	0.88
PBE1PBE	6-31+G(d,p)	9.9	10.2	4.7E+05	214.13
MPW1K	6-31+G(d,p)	11.2	11.5	4.7E+04	2141.22
MPW1K	6-311+G(d,p)	10.7	11.1	1.0E+05	976.30
MPW1K	aug-cc-pVTZ	10.7	11.0	1.1E+05	908.58
BB1K	6-31+G(d,p)	11.1	11.5	5.7E+04	1768.54
BB1K	6-311+G(d,p)	10.7	11.0	1.2E+05	805.69
BB1K	aug-cc-pVTZ	10.7	11.0	1.3E+05	784.99
BMK	6-31+G(d,p)	7.6	7.9	1.8E+07	5.57
BMK (99,590)[‡]	6-31+G(d,p)	7.7	8.0	1.7E+07	5.82
BMK	6-311+G(d,p)	7.3	7.6	3.7E+07	2.73
BMK	aug-cc-pVTZ	7.8	8.1	1.4E+07	7.21
CAM-B3LYP	6-31+G(d,p)	9.4	9.7	1.1E+06	87.07
CAM-B3LYP	6-311+G(d,p)	8.9	9.2	2.5E+06	39.62
CAM-B3LYP	aug-cc-pVTZ	8.8	9.2	2.8E+06	35.60
B2PLYP	6-31+G(d,p)	8.8	9.1	1.5E+06	67.25
B2PLYP	6-311+G(d,p)	8.3	8.6	3.0E+06	33.17
B2PLYP	aug-cc-pVTZ	8.0	8.4	3.1E+06	32.14
B2PLYP-D	6-31+G(d,p)	8.7	9.0	1.6E+06	62.56
B2PLYP-D	6-311+G(d,p)	8.2	8.5	3.3E+06	30.54
B2PLYP-D	aug-cc-pVTZ	8.0	8.3	3.4E+06	29.26
BHandHLYP	6-31+G(d,p)	9.5	9.8	8.6E+05	115.82
BHandHLYP	6-31+G(d,p)-DCP[†]	9.9	10.2	4.2E+05	240.37
BHandHLYP	6-311+G(d,p)	9.0	9.3	1.8E+06	54.28
BHandHLYP	aug-cc-pVTZ	9.0	9.3	2.1E+06	48.74
BLYP	6-31+G(d,p)	4.5	4.8	4.2E+09	0.02
BLYP	6-311+G(d,p)	4.2	4.5	7.1E+09	0.01
BLYP	aug-cc-pVTZ	4.2	4.5	7.6E+09	0.01

M062X	6-31+G(d,p)	11.9	12.3	1.8E+04	5626.56
M062X	6-311+G(d,p)	11.5	11.8	3.8E+04	2629.06
M062X	aug-cc-pVTZ	11.4	11.7	4.6E+04	2171.00
M062X (49,434)‡	6-31+G(d,p)	12.1	12.4	9.6E+03	10468.93
M062X (49,434)‡	6-311+G(d,p)	11.8	12.0	1.7E+04	6022.46
M062X (49,434)‡	aug-cc-pVTZ	11.6	11.9	2.2E+04	4450.15
M062X (99,302)‡	6-31+G(d,p)	12.0	12.3	1.4E+04	7302.89
M062X (99,302)‡	6-311+G(d,p)	11.5	11.8	2.8E+04	3563.01
M062X (99,302)‡	aug-cc-pVTZ	11.4	11.7	3.8E+04	2649.78
M062X (99,590)‡	6-31+G(d,p)	11.9	12.2	1.4E+04	6930.92
M062X (99,590)‡	6-311+G(d,p)	11.5	11.8	3.0E+04	3384.63
M062X (99,590)‡	aug-cc-pVTZ	11.4	11.7	3.7E+04	2691.28
M062X (250,590)‡	6-31+G(d,p)	12.0	12.3	1.3E+04	7991.35
M062X (250,590)‡	6-311+G(d,p)	11.6	11.9	2.6E+04	3875.29
M062X (250,590)‡	aug-cc-pVTZ	11.4	11.8	3.2E+04	3135.08
M062X (300,974)‡	6-31+G(d,p)	12.0	12.3	1.2E+04	8159.67
M062X (300,974)‡	6-311+G(d,p)	11.6	11.8	2.6E+04	3857.18
M062X (300,974)‡	aug-cc-pVTZ	11.4	11.7	3.3E+04	3060.78
CCSD(T)	CBS	8.5	8.8	4.1E+06	12.21

Table S2. Activation energies (kcal/mol) and ring-opening rate constants for cis-SCPC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	7.4	8.0	1.3E+08	0.13
B3LYP	6-311+G(d,p)	7.2	7.7	7.3E+07	0.23
B971	6-31+G(d,p)	7.3	7.8	4.9E+07	0.35
B971	6-311+G(d,p)	7.0	7.5	8.3E+07	0.21
PBE	6-31+G(d,p)	7.2	7.8	8.1E+07	0.21
PBE	6-311+G(d,p)	6.9	7.5	8.6E+07	0.20
BMK	6-31+G(d,p)	8.6	9.1	4.8E+06	3.57
BMK (99,590)‡	6-31+G(d,p)	8.3	8.9	4.4E+07	0.39
BMK	6-311+G(d,p)	8.2	8.7	1.3E+07	1.33
M062X	6-31+G(d,p)	12.9	13.5	5.1E+03	3312.67
M062X	6-311+G(d,p)	12.5	13.1	1.2E+04	1444.81
M062X	aug-cc-pVTZ	12.5	13.1	2.0E+04	840.72
M062X (49,434)‡	6-31+G(d,p)	12.6	13.3	2.0E+04	843.91
M062X (49,434)‡	6-311+G(d,p)	12.3	12.9	2.9E+04	583.19
M062X (49,434)‡	aug-cc-pVTZ	12.2	12.8	5.0E+04	340.98
M062X (300,974)‡	6-31+G(d,p)	12.7	13.4	1.1E+04	1588.99
M062X (300,974)‡	6-311+G(d,p)	12.3	12.9	2.6E+04	651.02
CAM-B3LYP	6-31+G(d,p)	10.2	10.7	5.1E+05	33.06
CAM-B3LYP	6-311+G(d,p)	9.8	10.3	8.7E+05	19.57
B2PLYP	6-31+G(d,p)	9.4	10.0	2.3E+06	7.24
B2PLYP	6-311+G(d,p)	8.9	9.5	5.0E+06	3.40
B2PLYP-D	6-31+G(d,p)	9.3	10.0	3.1E+06	5.46
B2PLYP-D	6-311+G(d,p)	8.9	9.5	5.8E+06	2.95
BHandHLYP	6-31+G(d,p)	10.1	10.7	1.3E+06	12.75
BHandHLYP	6-311+G(d,p)	9.7	10.3	2.9E+06	5.82
BLYP	6-31+G(d,p)	4.8	5.4	3.4E+09	0.01
BLYP	6-311+G(d,p)	4.6	5.1	3.1E+09	0.01

Table S3. Activation energies (kcal/mol) and ring-opening rate constants for trans-SCPC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	7.8	8.4	2.5E+07	0.67
B3LYP	6-311+G(d,p)	7.4	8.0	5.4E+07	0.31
B971	6-31+G(d,p)	7.5	8.1	5.9E+07	0.29
B971	6-311+G(d,p)	7.2	7.8	1.3E+08	0.13
PBE	6-31+G(d,p)	7.4	8.1	5.3E+07	0.32
PBE	6-311+G(d,p)	7.1	7.7	1.0E+08	0.16
MPW1K	6-31+G(d,p)	12.1	12.7	3.0E+04	573.89
MPW1K	6-311+G(d,p)	11.7	12.3	7.4E+04	230.26
BMK	6-31+G(d,p)	8.6	9.1	6.4E+06	2.65
BMK (99,590)[‡]	6-31+G(d,p)	8.7	9.3	4.3E+06	4.00
BMK	6-311+G(d,p)	8.3	8.8	1.7E+07	1.02
M062X	6-31+G(d,p)	12.0	13.1	1.2E+05	140.79
M062X	6-311+G(d,p)	11.5	12.7	3.2E+05	53.65
M062X	aug-cc-pVTZ	12.6	13.1	3.1E+03	5495.30
M062X (49,434)[‡]	6-31+G(d,p)	12.0	13.0	5.6E+04	304.02
M062X (49,434)[‡]	6-311+G(d,p)	11.6	12.6	8.3E+04	204.79
M062X (49,434)[‡]	aug-cc-pVTZ	11.4	12.5	1.0E+05	162.81
M062X (300,974)[‡]	6-31+G(d,p)	12.9	13.5	4.8E+03	3566.84
M062X (300,974)[‡]	6-311+G(d,p)	12.5	13.1	8.9E+03	1902.39
CAM-B3LYP	6-31+G(d,p)	9.6	10.6	3.4E+06	4.93
CAM-B3LYP	6-311+G(d,p)	9.1	10.2	9.6E+06	1.78
B2PLYP	6-31+G(d,p)	9.8	10.4	8.9E+05	19.01
B2PLYP	6-311+G(d,p)	9.3	9.9	2.2E+06	7.73
B2PLYP-D	6-31+G(d,p)	9.8	10.3	9.7E+05	17.54
B2PLYP-D	6-311+G(d,p)	9.3	9.8	2.5E+06	6.85
BHandHLYP	6-31+G(d,p)	10.6	11.2	2.7E+05	64.01
BHandHLYP	6-311+G(d,p)	10.2	10.8	5.8E+05	29.19
BLYP	6-31+G(d,p)	5.0	5.6	1.8E+09	0.01
BLYP	6-311+G(d,p)	4.8	5.3	3.4E+09	0.01

Table S4. Activation energies (kcal/mol) and ring-opening rate constants for cis-MSCPC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	7.6/7.6	8.2/8.2	3.3E+07	0.72
B3LYP	6-311+G(d,p)	7.2/7.2	7.8/7.8	5.8E+07	0.41
B971	6-31+G(d,p)	7.4/7.8	8.0/8.3	2.5E+07	0.96
B971	6-31+G(d,p)-DCP[†]	6.2/6.5	6.7/7.0	2.1E+08	0.11
B971	6-311+G(d,p)	7.0/7.4	7.6/7.9	5.3E+07	0.46
PBE	6-31+G(d,p)	7.4/7.6	8.0/8.2	4.6E+07	0.52
PBE	6-311+G(d,p)	7.1/7.2	7.6/7.8	9.0E+07	0.27
BMK	6-31+G(d,p)	8.5/9.3	9.1/9.7	3.4E+06	7.03
BMK (99,590)[‡]	6-31+G(d,p)	8.6/8.8	9.1/9.4	5.4E+06	4.43
BMK	6-311+G(d,p)	8.2/8.6	8.7/9.1	7.7E+06	3.13
M062X	6-31+G(d,p)	12.5/12.8	13.1/13.3	5.6E+03	4323.26
M062X	6-311+G(d,p)	12.1/12.2	12.7/12.7	9.6E+03	2502.59
M062X (300,974)[‡]	6-31+G(d,p)	12.5/12.8	13.1/13.3	5.3E+03	4500.15
M062X (300,974)[‡]	6-311+G(d,p)	12.0/12.2	12.7/12.7	1.1E+04	2250.48
CAM-B3LYP	6-31+G(d,p)	10.3/10.7	10.9/11.3	2.2E+05	111.10
CAM-B3LYP	6-311+G(d,p)	9.9/10.2	10.4/10.8	4.9E+05	49.01
B2PLYP	6-31+G(d,p)	9.5/10.0	10.1/10.6	8.4E+05	28.67
B2PLYP	6-311+G(d,p)	8.9/9.4	9.5/9.9	2.0E+06	11.92
B2PLYP-D	6-31+G(d,p)	9.4/9.6	10.0/10.2	1.0E+06	23.33

B2PLYP-D	6-311+G(d,p)	8.9/9.0	9.5/9.5	2.5E+06	9.68
BHandHLYP	6-31+G(d,p)	10.3/10.8	10.9/11.5	2.0E+05	119.95
BHandHLYP	6-311+G(d,p)	9.9/10.4	10.5/11.0	4.3E+05	55.83
BLYP	6-31+G(d,p)	5.0/4.9	5.6/5.5	3.5E+09	0.01
BLYP	6-311+G(d,p)	4.7/4.7	5.3/5.2	4.0E+09	0.01

Table S5. Activation energies (kcal/mol) and ring-opening rate constants for trans-MSCPC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	7.9/7.9	8.5/9.1	1.9E+07	1.26
B3LYP	6-311+G(d,p)	7.0/7.5	7.6/8.7	7.3E+07	0.33
B971	6-31+G(d,p)	7.8/7.8	8.3/8.9	2.4E+07	1.01
B971	6-31+G(d,p)-DCP[†]	6.5/6.5	7.1/7.7	1.9E+08	0.12
B971	6-311+G(d,p)	7.4/7.3	7.9/8.5	4.7E+07	0.51
PBE	6-31+G(d,p)	7.7/7.8	8.3/8.9	1.9E+07	1.27
PBE	6-311+G(d,p)	7.3/7.3	7.9/8.5	4.8E+07	0.50
MPW1K	6-31+G(d,p)	12.1/-	12.8/-	9.2E+03	2607.87
MPW1K	6-311+G(d,p)	11.6/-	12.3/-	2.5E+04	944.22
BMK	6-31+G(d,p)	8.2/8.2	9.2/9.8	3.0E+07	0.79
BMK (99,590)[‡]	6-31+G(d,p)	8.8/9.0	9.4/9.6	3.7E+06	6.56
BMK	6-311+G(d,p)	8.2/8.2	9.1/9.6	2.1E+07	1.15
M062X	6-31+G(d,p)	12.1/12.5	12.7/14.0	4.0E+04	595.58
M062X	6-311+G(d,p)	11.6/12.1	12.2/13.6	7.4E+04	323.38
M062X (300,974)[‡]	6-31+G(d,p)	12.2/12.9	12.8/14.2	8.3E+03	3005.87
M062X (300,974)[‡]	6-311+G(d,p)	11.7/12.5	12.3/13.7	7.2E+03	1272.60
CAM-B3LYP	6-31+G(d,p)	10.2/10.6	10.8/11.9	3.1E+05	76.51
CAM-B3LYP	6-311+G(d,p)	9.6/10.2	10.2/11.4	7.9E+05	30.25
B2PLYP	6-31+G(d,p)	9.2/9.8	9.7/11.0	1.6E+06	15.22
B2PLYP	6-311+G(d,p)	8.6/9.2	9.1/10.4	4.7E+06	5.06
B2PLYP-D	6-31+G(d,p)	9.2/9.9	9.7/11.1	1.4E+06	17.11
B2PLYP-D	6-311+G(d,p)	8.6/9.3	9.2/10.5	3.5E+06	6.88
BHandHLYP	6-31+G(d,p)	10.1/10.7	10.7/11.9	3.5E+05	69.17
BHandHLYP	6-311+G(d,p)	9.6/10.2	10.2/11.4	1.2E+06	19.70
BLYP	6-31+G(d,p)	4.9/5.2	5.5/6.4	2.5E+09	0.01
BLYP	6-311+G(d,p)	4.4/4.8	5.0/6.0	6.3E+09	0.00

Table S6. Activation energies (kcal/mol) and ring-opening rate constants for PMCPC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	4.4	4.5	1.8E+09	2.58
B3LYP	6-31+G(d,p)-DCP[†]	5.4	5.5	3.2E+08	14.73
B3LYP	6-311+G(d,p)	3.9	4.1	7.9E+09	0.59
B971	6-31+G(d,p)	4.1	4.1	2.3E+09	2.07
B971	6-31+G(d,p)-DCP[†]	3.0	3.1	1.9E+10	0.24
B971	6-311+G(d,p)	3.8	4.3	1.7E+10	0.28
PBEPBE	6-31+G(d,p)	3.9	3.9	2.2E+09	2.10
PBEPBE	6-311+G(d,p)	3.4	3.5	1.6E+10	0.30
MPW1K	6-31+G(d,p)	8.4	8.3	5.2E+05	9094.02
MPW1K	6-311+G(d,p)	7.8	7.9	8.5E+06	552.64
BMK	6-31+G(d,p)	3.9	3.9	2.5E+09	1.86
BMK (99,590)[‡]	6-31+G(d,p)	3.8	3.8	4.3E+09	1.10
BMK	6-311+G(d,p)	3.4	3.6	2.1E+10	0.22
M06-2X	6-31+G(d,p)	8.0	8.0	5.3E+06	879.85
M06-2X	6-311+G(d,p)	7.7	7.7	2.5E+06	1904.71

M06-2X (300,974)‡	6-31+G(d,p)	8.1	8.1	4.5E+06	1053.32
M06-2X (300,974)‡	6-311+G(d,p)	7.7	7.7	1.1E+07	436.33
CAM-B3LYP	6-31+G(d,p)	6.6	6.6	3.1E+07	153.98
CAM-B3LYP	6-311+G(d,p)	6.2	6.2	6.7E+07	69.79
B2PLYP	6-31+G(d,p)	7.2	7.3	1.4E+07	332.33
B2PLYP	6-311+G(d,p)	6.9	6.9	7.7E+06	609.36
B2PLYP-D	6-31+G(d,p)	6.0	6.1	7.9E+07	59.73
B2PLYP-D	6-311+G(d,p)	5.6	5.6	5.5E+07	84.86
BHandHLYP	6-31+G(d,p)	7.1	7.2	2.7E+07	175.45
BHandHLYP	6-311+G(d,p)	6.7	6.8	3.4E+07	136.37
BLYP	6-31+G(d,p)	2.3	2.3	3.3E+10	0.14
BLYP	6-311+G(d,p)	1.7	1.9	3.8E+11	0.01

Table S7. Activation energies (kcal/mol) and ring-opening rate constants for CBC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	12.4	12.1	3.9E+03	1.20
B3LYP	6-31+G(d,p)-DCP†	13.6	13.3	5.7E+02	8.21
B3LYP	6-311+G(d,p)	11.7	11.4	1.0E+04	0.45
B971	6-31+G(d,p)	13.6	13.3	3.2E+02	14.58
B971 (99,590)‡	6-31+G(d,p)	13.6	13.9	4.5E+02	10.54
B971	6-31+G(d,p)-DCP†	11.6	11.2	1.0E+04	0.46
B971	6-311+G(d,p)	13.0	12.6	4.7E+02	10.08
PBE	6-31+G(d,p)	12.2	12.0	6.5E+03	0.72
PBE	6-311+G(d,p)	11.6	11.3	1.6E+04	0.30
MPW1K	6-31+G(d,p)	15.9	16.2	1.4E+01	333.18
MPW1K	6-311+G(d,p)	15.4	15.7	3.4E+01	138.49
BB1K	6-31+G(d,p)	14.9	15.3	9.0E+01	52.34
BB1K	6-311+G(d,p)	14.4	14.8	2.0E+02	24.05
BMK	6-31+G(d,p)	18.5	18.7	4.8E-01	9862.66
BMK (99,590)‡	6-31+G(d,p)	18.4	18.7	8.3E-02	56640.75
BMK	6-311+G(d,p)	17.6	17.8	2.1E+00	2243.52
M062X	6-31+G(d,p)	16.2	16.1	1.4E+01	335.08
M062X	6-311+G(d,p)	15.8	15.7	2.7E+01	176.23
M062X (49,434)‡	6-31+G(d,p)	16.5	16.2	4.0E+00	1182.17
M062X (49,434)‡	6-311+G(d,p)	16.0	15.7	1.2E+01	408.06
M062X (99,302)‡	6-31+G(d,p)	16.4	16.2	7.0E+00	667.66
M062X (99,302)‡	6-311+G(d,p)	16.0	15.7	1.4E+01	328.40
M062X (99,590)‡	6-31+G(d,p)	16.5	16.2	3.9E+00	1190.51
M062X (99,590)‡	6-311+G(d,p)	15.9	15.6	1.1E+01	440.81
M062X (250,590)‡	6-31+G(d,p)	16.6	16.2	2.2E+00	2100.80
M062X (250,590)‡	6-311+G(d,p)	16.0	15.6	6.1E+00	765.62
M062X (300,974)‡	6-31+G(d,p)	16.6	16.2	2.7E+00	1735.66
M062X (300,974)‡	6-311+G(d,p)	16.0	15.7	7.3E+00	647.61
CAM-B3LYP	6-31+G(d,p)	15.3	15.0	2.5E+01	189.00
CAM-B3LYP	6-311+G(d,p)	14.6	14.3	7.6E+01	61.87
B2PLYP	6-31+G(d,p)	14.7	15.0	7.9E+01	59.73
B2PLYP	6-311+G(d,p)	14.2	14.4	1.6E+02	29.37
B2PLYP-D	6-31+G(d,p)	14.7	14.4	1.6E+03	2.91
B2PLYP-D	6-311+G(d,p)	14.2	13.9	3.6E+03	1.32
BHandHLYP	6-31+G(d,p)	15.7	15.3	9.7E+00	482.29
BHandHLYP	6-311+G(d,p)	15.1	14.7	2.4E+01	197.30
BLYP	6-31+G(d,p)	9.2	8.9	1.1E+06	0.00
BLYP	6-311+G(d,p)	8.5	8.2	2.7E+06	0.00

Table S8. Activation energies (kcal/mol) and ring-opening rate constants for cis-CBEC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	13.0	12.9	3.3E+03	0.46
B3LYP	6-31+G(d,p)-DCP[†]	14.4	14.3	3.3E+02	4.54
B3LYP	6-311+G(d,p)	12.4	12.3	9.9E+03	0.15
B971	6-31+G(d,p)	14.3	14.2	3.6E+02	4.22
B971	6-31+G(d,p)-DCP[†]	12.4	12.2	5.3E+03	0.28
B971	6-311+G(d,p)	13.8	13.7	7.4E+02	2.02
PBE	6-31+G(d,p)	12.9	12.8	4.6E+03	0.33
PBE	6-311+G(d,p)	12.3	12.2	1.1E+04	0.14
MPW1K	6-31+G(d,p)	17.6	18.0	9.3E-01	1614.25
MPW1K	6-311+G(d,p)	17.1	17.5	2.1E+00	724.00
BMK	6-31+G(d,p)	19.3	19.2	8.3E-02	18013.09
BMK (99,590)[‡]	6-31+G(d,p)	19.1	19.6	1.1E-01	13352.15
BMK	6-311+G(d,p)	18.6	18.5	2.6E-01	5822.89
M062X	6-31+G(d,p)	17.0	17.1	1.1E+01	142.62
M062X	6-311+G(d,p)	16.7	16.7	1.1E+01	130.52
M062X (49,434)[‡]	6-31+G(d,p)	17.2	17.1	5.5E+00	270.54
M062X (49,434)[‡]	6-311+G(d,p)	16.7	16.7	9.9E+00	151.52
M062X (300,974)[‡]	6-31+G(d,p)	17.2	17.2	6.9E+00	217.29
M062X (300,974)[‡]	6-311+G(d,p)	16.8	16.8	1.8E+01	81.53
CAM-B3LYP	6-31+G(d,p)	16.1	16.0	1.6E+01	96.56
CAM-B3LYP	6-311+G(d,p)	15.5	15.3	4.7E+01	32.02
B2PLYP	6-31+G(d,p)	15.1	15.0	1.0E+02	14.72
B2PLYP	6-311+G(d,p)	14.6	14.5	2.0E+02	7.38
B2PLYP-D	6-31+G(d,p)	15.3	15.2	2.2E+02	6.83
B2PLYP-D	6-311+G(d,p)	14.9	14.7	6.3E+02	2.35
BHandHLYP	6-31+G(d,p)	16.3	16.2	1.1E+01	132.71
BHandHLYP	6-311+G(d,p)	15.7	15.6	2.8E+01	53.92
BLYP	6-31+G(d,p)	9.7	9.6	6.7E+05	0.00
BLYP	6-311+G(d,p)	9.1	9.0	1.3E+06	0.00

Table S9. Activation energies (kcal/mol) and ring-opening rate constants for trans-CBEC.

Functional	Basis set	E_0	E_a	k_{calc}	k_{exp}/k_{calc}
B3LYP	6-31+G(d,p)	13.1	14.2	1.8E+03	0.83
B3LYP	6-31+G(d,p)-DCP[†]	14.4	15.5	1.9E+02	7.71
B3LYP	6-311+G(d,p)	12.5	13.5	5.1E+03	0.30
B971	6-31+G(d,p)	14.3	15.4	2.5E+02	6.05
B971	6-31+G(d,p)-DCP[†]	10.4	11.4	7.3E+04	0.02
B971	6-311+G(d,p)	13.7	14.8	6.4E+02	2.35
PBE	6-31+G(d,p)	13.0	14.1	2.4E+03	0.63
PBE	6-311+G(d,p)	12.4	13.5	5.8E+03	0.26
BMK	6-31+G(d,p)	19.0	20.1	1.1E-01	13351.93
BMK (99,590)[‡]	6-31+G(d,p)	19.0	19.6	1.0E-01	14621.31
BMK	6-311+G(d,p)	18.2	19.4	3.1E-01	4901.72
M062X	6-31+G(d,p)	17.1	18.2	2.3E+00	657.94
M062X	6-311+G(d,p)	16.6	17.7	4.9E+00	308.70
M062X (49,434)[‡]	6-31+G(d,p)	17.0	18.1	3.0E+00	506.60
M062X (49,434)[‡]	6-311+G(d,p)	16.5	17.7	4.4E+00	343.04
M062X (300,974)[‡]	6-31+G(d,p)	17.2	18.3	1.7E+00	866.99
M062X (300,974)[‡]	6-311+G(d,p)	16.8	17.8	3.6E+00	417.60
CAM-B3LYP	6-31+G(d,p)	16.2	17.3	9.4E+00	159.07
CAM-B3LYP	6-311+G(d,p)	15.5	16.6	2.9E+01	52.32
B2PLYP	6-31+G(d,p)	15.1	16.2	6.3E+01	23.90

B2PLYP	6-311+G(d,p)	14.6	15.7	1.4E+02	10.77
B2PLYP-D	6-31+G(d,p)	15.2	16.3	4.7E+01	31.83
B2PLYP-D	6-311+G(d,p)	14.7	15.8	1.2E+02	13.03
BHandHLYP	6-31+G(d,p)	16.4	17.5	7.7E+00	193.94
BHandHLYP	6-311+G(d,p)	15.8	16.9	2.0E+01	75.93
BLYP	6-31+G(d,p)	7.9	8.9	4.8E+06	0.00
BLYP	6-311+G(d,p)	7.4	8.4	1.1E+07	0.00

Table S10. E_0, ΔE_{therm} and $Q^{\ddagger}/Q$ (energies in kcal/mol) for ring-opening of CPC.

Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$	Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$
BLYP	6-31+G(d,p)	4.5	-0.86	0.67	BLYP	6-311+G(d,p)	4.2	-0.88	0.68
PBE	6-31+G(d,p)	7.1	-0.96	0.70	PBE	6-311+G(d,p)	6.7	-0.96	0.71
PBE1PBE	6-31+G(d,p)	9.9	-1.07	0.66	B3LYP	6-311+G(d,p)	6.6	-0.97	0.67
B3LYP	6-31+G(d,p)	8.2	-0.97	0.66	B971	6-311+G(d,p)	6.3	-0.88	0.64
B3LYP	6-31+G(d,p)-DCP[†]	7.6	-0.99	0.67	CAM-B3LYP	6-311+G(d,p)	8.9	-1.08	0.67
B971	6-31+G(d,p)	6.7	-0.88	0.63	BMK	6-311+G(d,p)	7.3	-0.86	0.63
B971	6-31+G(d,p)-DCP[†]	5.4	-0.84	0.61	BB1K	6-311+G(d,p)	10.7	-1.11	0.66
CCSD(T)	CBS	8.5	-1.20	0.55	MPW1K	6-311+G(d,p)	10.7	-1.14	0.62
CAM-B3LYP	6-31+G(d,p)	9.4	-1.07	0.67	BHandHLYP	6-311+G(d,p)	9.0	-1.10	0.61
BMK	6-31+G(d,p)	7.6	-0.82	0.56	B2PLYP-D	6-311+G(d,p)	8.2	-0.94	0.64
BMK (99,590)[‡]	6-31+G(d,p)	7.7	-0.72	0.61	B2PLYP	6-311+G(d,p)	8.3	-1.01	0.64
BB1K	6-31+G(d,p)	11.1	-1.12	0.66	M062X (300,974)[‡]	6-311+G(d,p)	11.6	-1.08	0.62
MPW1K	6-31+G(d,p)	11.2	-1.15	0.62	M062X	6-31+G(d,p)	11.9	-1.05	0.77
BHandHLYP	6-31+G(d,p)	9.5	-1.10	0.60	M062X	6-311+G(d,p)	11.5	-1.10	0.77
B2PLYP-D	6-31+G(d,p)	8.7	-0.97	0.63	M062X	aug-cc-pVTZ	11.4	-1.09	0.80
B2PLYP	6-31+G(d,p)	8.8	-1.03	0.63	M062X (49,434)[‡]	6-31+G(d,p)	12.1	-0.85	0.58
M062X (300,974)[‡]	6-31+G(d,p)	12.0	-1.06	0.59	M062X (49,434)[‡]	6-311+G(d,p)	11.8	-0.80	0.57
BLYP	aug-cc-pVTZ	4.2	-0.88	0.70	M062X (49,434)[‡]	aug-cc-pVTZ	11.6	-0.85	0.60
PBE	aug-cc-pVTZ	6.7	-0.98	0.72	M062X (99,302)[‡]	6-31+G(d,p)	12.0	-1.06	0.65
B3LYP	aug-cc-pVTZ	6.5	-0.99	0.68	M062X (99,302)[‡]	6-311+G(d,p)	11.5	-1.08	0.65
B971	aug-cc-pVTZ	6.2	-0.90	0.65	M062X (99,302)[‡]	aug-cc-pVTZ	11.4	-1.10	0.71
CAM-B3LYP	aug-cc-pVTZ	8.8	-1.10	0.69	M062X (99,590)[‡]	6-31+G(d,p)	11.9	-1.09	0.64
BMK	aug-cc-pVTZ	7.8	-0.84	0.62	M062X (99,590)[‡]	6-311+G(d,p)	11.5	-1.10	0.66
BB1K	aug-cc-pVTZ	10.7	-1.13	0.68	M062X (99,590)	aug-cc-pVTZ	11.4	-1.13	0.67
MPW1K	aug-cc-pVTZ	10.7	-1.17	0.64	M062X (250,590)[‡]	6-31+G(d,p)	12.0	-1.07	0.60
BHandHLYP	aug-cc-pVTZ	9.0	-1.12	0.63	M062X (250,590)[‡]	6-311+G(d,p)	11.6	-1.07	0.62
B2PLYP-D	aug-cc-pVTZ	8.0	-0.92	0.66	M062X (250,590)[‡]	aug-cc-pVTZ	11.4	-1.10	0.63
B2PLYP	aug-cc-pVTZ	8.0	-0.99	0.66					
M062X (300,974)[‡]	aug-cc-pVTZ	11.4	-1.10	0.64					

Table S11. E_0, ΔE_{therm} and $Q^{\ddagger}/Q$ (energies in kcal/mol) for ring-opening of cis-SCPC.

Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$	Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$
B3LYP	6-31+G(d,p)	7.4	-1.40	3.02	B3LYP	6-311+G(d,p)	7.2	-1.36	1.03
B971	6-31+G(d,p)	7.3	-1.29	0.89	B971	6-311+G(d,p)	7.0	-1.27	0.87
PBE	6-31+G(d,p)	7.2	-1.32	1.33	PBE	6-311+G(d,p)	6.9	-1.27	0.84
BMK	6-31+G(d,p)	8.6	-1.10	0.75	BMK	6-311+G(d,p)	8.2	-1.21	0.99
M062X (75,302)	6-31+G(d,p)	12.9	-1.38	1.22	M062X (75,302)	6-311+G(d,p)	12.5	-1.40	1.38
M062X (49,434)	6-31+G(d,p)	12.6	-1.52	2.93	M062X (49,434)	6-311+G(d,p)	12.3	-1.45	2.32
M062X (300,974)	6-31+G(d,p)	12.7	-1.57	1.77	M062X (300,974)	6-311+G(d,p)	12.3	-1.57	2.10
CAM-B3LYP	6-31+G(d,p)	10.2	-1.54	1.15	CAM-B3LYP	6-311+G(d,p)	9.8	-1.50	1.07
B2PLYP	6-31+G(d,p)	9.4	-1.54	1.36	B2PLYP	6-311+G(d,p)	8.9	-1.48	1.38
B2PLYP-D	6-31+G(d,p)	9.3	-1.48	1.77	B2PLYP-D	6-311+G(d,p)	8.9	-1.42	1.58
BHandHLYP	6-31+G(d,p)	10.1	-1.67	2.64	BHandHLYP	6-311+G(d,p)	9.7	-1.62	3.06
BLYP	6-31+G(d,p)	4.8	-1.18	0.94	BLYP	6-311+G(d,p)	4.6	-1.15	0.63

M062X (75,302)	aug-cc-pVTZ	12.5	-1.30	2.35
M062X (49,434)	aug-cc-pVTZ	12.2	-1.42	3.30

Table S12. E_0, ΔE_{therm} and $Q^{\ddagger}/Q$ (energies in kcal/mol) for ring-opening of trans-SCPC.

Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$	Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$
B3LYP	6-31+G(d,p)	7.8	-1.48	1.04	B3LYP	6-311+G(d,p)	7.4	-1.47	1.22
B971	6-31+G(d,p)	7.5	-1.42	1.58	B971	6-311+G(d,p)	7.2	-1.41	1.97
PBE	6-31+G(d,p)	7.4	-1.38	1.23	PBE	6-311+G(d,p)	7.1	-1.37	1.38
MPW1K	6-31+G(d,p)	12.1	-1.75	1.81	MPW1K	6-311+G(d,p)	11.7	-1.72	2.20
BMK	6-31+G(d,p)	8.6	-1.46	1.00	BMK	6-311+G(d,p)	8.3	-1.46	1.52
M062X (75,302)	6-31+G(d,p)	12.0	-1.04	5.62	M062X (75,302)	6-311+G(d,p)	11.5	-1.05	6.73
M062X (49,434)	6-31+G(d,p)	12.0	-1.02	2.59	M062X (49,434)	6-311+G(d,p)	11.6	-0.96	2.14
M062X (300,974)	6-31+G(d,p)	12.9	-1.71	1.12	M062X (300,974)	6-311+G(d,p)	12.5	-1.68	1.13
CAM-B3LYP	6-31+G(d,p)	9.6	-1.06	3.01	CAM-B3LYP	6-311+G(d,p)	9.1	-1.04	3.69
B2PLYP	6-31+G(d,p)	9.8	-1.62	1.10	B2PLYP	6-311+G(d,p)	9.3	-1.58	1.18
B2PLYP-D	6-31+G(d,p)	9.8	-1.55	1.11	B2PLYP-D	6-311+G(d,p)	9.3	-1.51	1.23
BHandHLYP	6-31+G(d,p)	10.6	-1.74	1.28	BHandHLYP	6-311+G(d,p)	10.2	-1.71	1.42
BLYP	6-31+G(d,p)	5.0	-1.26	0.72	BLYP	6-311+G(d,p)	4.8	-1.27	0.83
M062X (75,302)	aug-cc-pVTZ	12.6	-1.57	0.42					
M062X (49,434)	aug-cc-pVTZ	11.4	-1.00	2.01					

Table S13. E_0, ΔE_{therm} and $Q^{\ddagger}/Q$ (energies in kcal/mol) for ring-opening of PMCPC.

Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$	Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$
B3LYP	6-31+G(d,p)	4.4	-0.61	0.25	B3LYP	6-311+G(d,p)	3.9	-0.76	0.44
B3LYP	6-31+G(d,p)-DCP[†]	5.4	-0.61	0.25	B971	6-311+G(d,p)	3.8	0.02	0.81
B971	6-31+G(d,p)	4.1	-0.50	0.18	PBEPBE	6-311+G(d,p)	3.4	-0.65	0.38
B971	6-31+G(d,p)-DCP[†]	3.0	-0.53	0.25	MPW1K	6-311+G(d,p)	7.8	-0.78	0.33
PBEPBE	6-31+G(d,p)	3.9	-0.63	0.13	BMK	6-311+G(d,p)	3.4	-0.57	0.52
MPW1K	6-31+G(d,p)	8.4	-0.72	0.06	M062X	6-311+G(d,p)	7.7	-0.71	0.10
BMK	6-31+G(d,p)	3.9	-0.60	0.15	M062X (300,974)[‡]	6-311+G(d,p)	7.7	-0.72	0.35
BMK (99,590)[‡]	6-31+G(d,p)	3.8	-0.65	0.20	CAM-B3LYP	6-311+G(d,p)	6.2	-0.73	0.18
M062X	6-31+G(d,p)	8.0	-0.78	0.29	B2PLYP	6-311+G(d,p)	6.9	-0.65	0.08
M062X (300,974)[‡]	6-31+G(d,p)	8.1	-0.68	0.31	B2PLYP-D	6-311+G(d,p)	5.6	-0.68	0.05
CAM-B3LYP	6-31+G(d,p)	6.6	-0.72	0.16	BHandHLYP	6-311+G(d,p)	6.7	-0.78	0.23
B2PLYP	6-31+G(d,p)	7.2	-0.66	0.22	BLYP	6-311+G(d,p)	1.7	-0.80	0.50
B2PLYP-D	6-31+G(d,p)	6.0	-0.71	0.17					
BHandHLYP	6-31+G(d,p)	7.1	-0.76	0.32					
BLYP	6-31+G(d,p)	2.3	-0.54	0.13					

Table S14. E_0, ΔE_{therm} and $Q^{\ddagger}/Q$ (energies in kcal/mol) for ring-opening of CBC.

Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$	Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$
B3LYP	6-31+G(d,p)	12.6	-0.65	0.74	B3LYP	6-311+G(d,p)	12.0	-0.64	0.77
B3LYP	6-31+G(d,p)-DCP[†]	14.0	-0.71	0.69	B971	6-311+G(d,p)	13.2	-0.62	0.75
B971	6-31+G(d,p)	13.9	-0.64	0.74	PBE	6-311+G(d,p)	11.9	-0.65	0.70
B971	6-31+G(d,p)-DCP[†]	10.1	-0.56	0.30	MPW1K	6-311+G(d,p)	15.4	-1.43	0.52
PBE	6-31+G(d,p)	12.5	-0.66	0.70	BB1K	6-311+G(d,p)	14.4	-1.34	0.60
MPW1K	6-31+G(d,p)	15.9	-1.43	0.52	BMK	6-311+G(d,p)	17.6	-1.41	1.37
BB1K	6-31+G(d,p)	14.9	-1.37	0.63	M062X	6-311+G(d,p)	15.8	-1.89	0.84
BMK	6-31+G(d,p)	18.5	-1.34	1.35	M062X (49,434)[‡]	6-311+G(d,p)	16.0	-1.72	0.53
BMK (99,590)[‡]	6-31+G(d,p)	18.4	-1.32	0.22	M062X (99.302)[‡]	6-311+G(d,p)	16.0	-1.86	0.57
M062X	6-31+G(d,p)	16.2	-1.97	0.91	M062X (99.302)[‡]	6-311+G(d,p)	15.9	-1.92	0.42
M062X (49,434)[‡]	6-31+G(d,p)	16.5	-1.78	0.43	M062X (250.590)[‡]	6-311+G(d,p)	16.0	-1.91	0.26
M062X (99.302)[‡]	6-31+G(d,p)	16.4	-1.90	0.62	M062X (300,974)[‡]	6-311+G(d,p)	16.0	-1.89	-.32
M062X (99.590)[‡]	6-31+G(d,p)	16.5	-1.90	0.39	CAM-B3LYP	6-311+G(d,p)	14.6	-1.94	0.31

M062X (250.590) ‡	6-31+G(d,p)	16.6	-1.88	0.24	B2PLYP	6-311+G(d,p)	14.2	-1.25	0.32
M062X (300,974) ‡	6-31+G(d,p)	16.6	-1.87	0.30	B2PLYP-D	6-311+G(d,p)	14.2	-1.20	0.57
CAM-B3LYP	6-31+G(d,p)	15.3	-1.94	0.36	BHandHLYP	6-311+G(d,p)	15.1	-1.97	0.22
B2PLYP	6-31+G(d,p)	14.7	-1.25	0.38	BLYP	6-311+G(d,p)	8.5	-1.76	0.40
B2PLYP-D	6-31+G(d,p)	14.7	-1.20	0.55					
BHandHLYP	6-31+G(d,p)	15.7	-1.98	0.25					
BLYP	6-31+G(d,p)	9.2	-1.76	0.45					

Table S15. E_0, ΔE_{therm} and $Q^{\ddagger}/Q$ (energies in kcal/mol) for ring-opening of cis-CBEC.

Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$	Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$
B3LYP	6-31+G(d,p)	13.0	-1.94	0.87	B3LYP	6-311+G(d,p)	12.4	-1.93	0.92
B3LYP	6-31+G(d,p)-DCP †	14.4	-1.91	0.93	B971	6-311+G(d,p)	13.8	-1.90	0.76
B971	6-31+G(d,p)	14.3	-1.93	0.93	PBE	6-311+G(d,p)	12.3	-1.88	0.86
B971	6-31+G(d,p)-DCP †	12.4	-1.86	0.49	MPW1K	6-311+G(d,p)	17.1	-1.39	0.57
PBE	6-31+G(d,p)	12.9	-1.90	1.01	BMK	6-311+G(d,p)	18.6	-1.90	0.88
MPW1K	6-31+G(d,p)	17.6	-1.41	0.58	M062X	6-311+G(d,p)	16.7	-2.19	1.66
BMK	6-31+G(d,p)	19.3	-1.91	0.93	M062X (49,434) ‡	6-311+G(d,p)	16.7	-2.14	1.46
BMK (99,590) ‡	6-31+G(d,p)	19.1	-1.48	0.96	M062X (300,974) ‡	6-311+G(d,p)	16.8	-2.12	2.96
M062X	6-31+G(d,p)	17.0	-2.23	2.50	CAM-B3LYP	6-311+G(d,p)	15.5	-2.01	0.81
M062X (49,434) ‡	6-31+G(d,p)	17.2	-2.08	1.68	B2PLYP	6-311+G(d,p)	15.3	-1.12	0.72
M062X (300,974) ‡	6-31+G(d,p)	17.2	-2.10	2.22	B2PLYP-D	6-311+G(d,p)	14.9	-1.10	0.99
CAM-B3LYP	6-31+G(d,p)	16.1	-2.02	0.85	BHandHLYP	6-311+G(d,p)	15.7	-2.07	0.77
B2PLYP	6-31+G(d,p)	15.1	-1.93	0.95	BLYP	6-311+G(d,p)	9.1	-1.83	0.50
B2PLYP-D	6-31+G(d,p)	15.3	-1.12	0.72					
BHandHLYP	6-31+G(d,p)	16.3	-2.08	0.80					
BLYP	6-31+G(d,p)	9.7	-1.83	0.70					

Table S16. E_0, ΔE_{therm} and $Q^{\ddagger}/Q$ (energies in kcal/mol) for ring-opening of trans-CBEC.

Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$	Functional	Basis set	E_0	ΔE_{therm}	$Q^{\ddagger}/Q$
B3LYP	6-31+G(d,p)	13.1	-0.72	0.57	B3LYP	6-311+G(d,p)	12.5	-0.70	0.56
B3LYP	6-31+G(d,p)-DCP †	14.4	-0.70	0.56	B971	6-311+G(d,p)	13.7	-0.69	0.59
B971	6-31+G(d,p)	14.3	-0.71	0.61	PBE	6-311+G(d,p)	12.4	-0.63	0.56
B971	6-31+G(d,p)-DCP †	10.4	-0.65	0.26	BMK	6-311+G(d,p)	18.2	-0.90	0.59
PBE	6-31+G(d,p)	13.0	-0.67	0.60	M062X	6-311+G(d,p)	16.6	-0.95	0.59
BMK	6-31+G(d,p)	19.0	-0.95	0.72	M062X (49,434) ‡	6-311+G(d,p)	16.5	-0.95	0.48
BMK (99,590) ‡	6-31+G(d,p)	19.0	-1.54	0.75	M062X (300,974) ‡	6-311+G(d,p)	16.8	-0.84	0.55
M062X	6-31+G(d,p)	17.1	-0.90	0.62	CAM-B3LYP	6-311+G(d,p)	15.5	-0.79	0.58
M062X (49,434) ‡	6-31+G(d,p)	17.0	-0.94	0.67	B2PLYP	6-311+G(d,p)	14.6	-0.76	0.57
M062X (300,974) ‡	6-31+G(d,p)	17.2	-0.84	0.55	B2PLYP-D	6-311+G(d,p)	14.7	-0.69	0.54
CAM-B3LYP	6-31+G(d,p)	16.2	-0.81	0.59	BHandHLYP	6-311+G(d,p)	15.8	-0.88	0.64
B2PLYP	6-31+G(d,p)	15.1	-0.80	0.60	BLYP	6-311+G(d,p)	7.4	-0.60	0.25
B2PLYP-D	6-31+G(d,p)	15.2	-0.72	0.54					
BHandHLYP	6-31+G(d,p)	16.4	-0.90	0.64					
BLYP	6-31+G(d,p)	7.9	-0.61	0.24					

Table S17. Ring strain enthalpy(kcal/mol) within cyclopropane and cyclobutane calculated by DFT/6-31+G(d,p).

Functional	cyclopropane	cyclobutane
B3LYP	19.72	19.13
B3LYP-DCP	20.50	19.91
B971	22.14	21.55
B971-DCP	21.86	21.27
MPW1K	21.39	20.80
M062X	19.28	18.03
M062X (49,434) ‡	18.18	16.41

M062X (99.302) ‡	19.23	17.77
M062X (99.590) ‡	18.82	17.15
M062X (250.590) ‡	18.84	17.14
M062X (300,974) ‡	18.80	17.10
B2PLYP	20.02	16.71
B2PLYP-D	20.80	16.72
CAM-B3LYP	20.84	17.39
BHandHLYP	21.66	18.49
BLYP	18.06	15.42

Table S18. B971/6-31+G(d,p)-optimized Cartesian coordinates for CPC

6	-0.917087000	0.751358000	-0.134535000
6	0.279543000	-0.000063000	0.488234000
6	-0.917095000	-0.751349000	-0.134894000
1	-1.584549000	1.274435000	0.547183000
1	-0.733415000	1.267729000	-1.074209000
1	0.302048000	-0.000390000	1.576947000
1	-0.733421000	-1.267312000	-1.074788000
1	-1.584490000	-1.274734000	0.546654000
6	1.583492000	0.000113000	-0.166160000
1	1.659541000	0.000877000	-1.251323000
1	2.501164000	-0.000957000	0.413662000

Table S19. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state of CPC

6	1.201391000	-0.699790000	-0.108980000
6	-0.428564000	0.154507000	0.485190000
6	0.801792000	0.732603000	-0.150286000
1	1.755247000	-1.102854000	0.732867000
1	1.003207000	-1.347094000	-0.955731000
1	-0.397211000	0.032784000	1.566308000
1	0.640169000	1.148940000	-1.147455000
1	1.380296000	1.413136000	0.478312000
6	-1.611264000	-0.123505000	-0.184399000
1	-2.447511000	-0.590016000	0.328252000
1	-1.714322000	0.062211000	-1.251697000

Table S20. B971/6-31+G(d,p)-optimized Cartesian coordinates for cis-SCPC

6	3.142278000	0.377458000	-0.799808000
6	2.487028000	-0.681629000	0.114828000
6	3.027316000	0.627195000	0.685311000
1	4.118881000	0.145583000	-1.219388000
1	2.471621000	0.928434000	-1.454300000
1	3.085673000	-1.571382000	0.303568000
1	2.288681000	1.354895000	1.012972000
1	3.928004000	0.578079000	1.293442000
6	1.044491000	-0.954203000	0.064286000
1	0.688887000	-1.940683000	-0.241371000
8	0.221065000	0.109510000	-0.190146000
14	-1.467796000	0.076298000	-0.002047000
6	-2.179923000	-1.385049000	-0.958260000
1	-1.843951000	-2.346652000	-0.549248000
1	-3.277335000	-1.375419000	-0.911459000
1	-1.889834000	-1.346780000	-2.016055000
6	-2.042407000	1.713833000	-0.719502000
1	-3.129977000	1.827686000	-0.621065000
1	-1.567012000	2.555643000	-0.200588000
1	-1.789258000	1.788722000	-1.784369000
6	-1.880299000	-0.070356000	1.829503000
1	-1.471473000	0.777136000	2.394080000
1	-2.966226000	-0.093050000	1.991972000
1	-1.456951000	-0.989954000	2.253506000

Table S21. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state of cis-SCPC

6	-3.372814000	0.679382000	0.691708000

6	-2.405122000	-0.827699000	-0.030443000
6	-3.062612000	0.324363000	-0.720612000
1	-4.300129000	0.366054000	1.155051000
1	-2.698137000	1.316866000	1.247660000
1	-3.011900000	-1.697212000	0.195912000
1	-2.369418000	0.991893000	-1.230565000
1	-3.913828000	0.065879000	-1.350872000
6	-1.045341000	-0.930945000	0.219779000
1	-0.637770000	-1.757444000	0.798897000
8	-0.204463000	0.096722000	-0.090672000
14	1.489036000	0.035230000	-0.093915000
6	2.095985000	-0.572216000	1.579543000
1	1.772166000	-1.598426000	1.788036000
1	3.192168000	-0.562597000	1.616816000
1	1.727942000	0.067479000	2.389554000
6	2.012993000	1.803220000	-0.416404000
1	1.655532000	2.469643000	0.376149000
1	3.105121000	1.888818000	-0.462328000
1	1.607019000	2.163982000	-1.367798000
6	2.057371000	-1.123410000	-1.459590000
1	1.701158000	-0.781723000	-2.437876000
1	3.151979000	-1.178960000	-1.500049000
1	1.678496000	-2.140038000	-1.302877000

Table S22. B971/6-31+G(d,p)-optimized Cartesian coordinates for trans-SCPC

6	3.649474000	0.630212000	0.040544000
6	2.382637000	0.006979000	-0.518329000
6	3.433084000	-0.854700000	0.223357000
1	4.406203000	0.963592000	-0.665692000
1	3.545853000	1.268843000	0.916378000
1	2.346673000	-0.147097000	-1.596786000
1	3.168623000	-1.215377000	1.214825000
1	4.027161000	-1.545299000	-0.372066000
6	1.083830000	0.323960000	0.091109000
1	1.042567000	0.689484000	1.121721000
8	0.007785000	-0.393972000	-0.356788000
14	-1.610293000	-0.014690000	0.000968000
6	-1.828477000	0.128985000	1.869427000
1	-1.262630000	0.972195000	2.286134000
1	-2.885885000	0.290352000	2.119347000
1	-1.500288000	-0.785500000	2.379937000
6	-2.585555000	-1.459453000	-0.696480000
1	-3.664318000	-1.317222000	-0.549594000
1	-2.402436000	-1.568104000	-1.772813000
1	-2.297973000	-2.399979000	-0.210422000
6	-2.063621000	1.608400000	-0.839880000
1	-1.940205000	1.534485000	-1.927758000
1	-3.106766000	1.884684000	-0.635622000
1	-1.422986000	2.426086000	-0.485327000

Table S23. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state of trans-SCPC

6	-3.737691000	-0.874397000	0.146472000
6	-2.304136000	0.240191000	-0.550950000
6	-3.593225000	0.607484000	0.115582000
1	-4.248972000	-1.403526000	-0.651368000
1	-3.400935000	-1.436751000	1.010139000
1	-2.321042000	0.045663000	-1.620373000
1	-3.478691000	1.090213000	1.090253000
1	-4.305160000	1.154634000	-0.506650000
6	-1.072726000	0.263178000	0.088416000
1	-0.979920000	0.542921000	1.139849000
8	0.036388000	-0.241856000	-0.528076000
14	1.633647000	-0.027728000	0.005300000
6	2.084149000	1.799396000	-0.091247000
1	1.432376000	2.405888000	0.550975000
1	3.120356000	1.967646000	0.231583000

1	1.984766000	2.175163000	-1.117467000
6	2.656113000	-1.062523000	-1.180248000
1	3.725297000	-0.999422000	-0.938901000
1	2.359762000	-2.117810000	-1.135455000
1	2.521498000	-0.719133000	-2.213475000
6	1.790485000	-0.647624000	1.780404000
1	1.477325000	-1.696354000	1.860576000
1	2.832521000	-0.580904000	2.121452000
1	1.180851000	-0.059419000	2.478701000

Table S24. B971/6-31+G(d,p)-optimized Cartesian coordinates for cis-MSCPC

6	-3.014988000	-0.667852000	-0.838316000
6	-2.455175000	0.263139000	0.262706000
6	-2.759318000	-1.200003000	0.552573000
1	-4.042143000	-0.510550000	-1.160361000
1	-2.319256000	-0.960188000	-1.620627000
1	-3.165906000	0.985712000	0.660963000
1	-1.904041000	-1.858404000	0.683840000
1	-3.613061000	-1.419979000	1.189900000
6	-1.067716000	0.769064000	0.208915000
8	-0.151442000	-0.144827000	-0.257886000
14	1.521146000	-0.227449000	-0.003711000
6	2.427265000	0.925294000	-1.191459000
1	2.204050000	1.981317000	-0.996058000
1	3.514279000	0.792267000	-1.102168000
1	2.148933000	0.710188000	-2.231187000
6	1.951706000	-2.016565000	-0.389079000
1	3.032189000	-2.192001000	-0.302794000
1	1.440868000	-2.703017000	0.297700000
1	1.648902000	-2.277397000	-1.411121000
6	1.915794000	0.211128000	1.786528000
1	1.377823000	-0.448724000	2.478853000
1	2.990895000	0.104468000	1.984189000
1	1.633810000	1.244678000	2.024034000
6	-0.802080000	2.224265000	-0.057203000
1	0.164566000	2.549531000	0.351069000
1	-0.788439000	2.450120000	-1.140386000
1	-1.580900000	2.844060000	0.401210000

Table S25. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state 1 of cis-MSCPC

6	-3.303730000	-0.767431000	-0.818689000
6	-2.327239000	0.335547000	0.447480000
6	-2.741703000	-1.100686000	0.520744000
1	-4.329162000	-0.429742000	-0.927763000
1	-2.704180000	-0.922208000	-1.708593000
1	-3.043289000	1.080787000	0.782045000
1	-1.909749000	-1.806884000	0.516066000
1	-3.466992000	-1.336395000	1.303028000
6	-1.055820000	0.788349000	0.098567000
8	-0.131846000	-0.142920000	-0.307502000
14	1.531488000	-0.247407000	-0.006664000
6	2.487507000	0.937301000	-1.121201000
1	2.276302000	1.987937000	-0.887413000
1	3.569127000	0.781741000	-1.006900000
1	2.236128000	0.769982000	-2.176435000
6	1.954594000	-2.027037000	-0.437358000
1	3.030005000	-2.217718000	-0.324943000
1	1.416076000	-2.728928000	0.211530000
1	1.679116000	-2.251167000	-1.475654000
6	1.871815000	0.129027000	1.809521000
1	1.313311000	-0.552057000	2.464069000
1	2.940331000	0.014388000	2.036276000
1	1.584956000	1.155209000	2.072605000
6	-0.727577000	2.237439000	-0.125745000
1	0.161733000	2.554709000	0.438734000
1	-0.523777000	2.440041000	-1.190054000

1	-1.563061000	2.872317000	0.186804000

Table S26. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state 2 of cis-MSCPC

6	-2.816184000	-1.175419000	-0.328614000
6	-2.431072000	0.266942000	-0.224885000
6	-2.750165000	-1.051003000	1.155553000
1	-3.804623000	-1.364703000	-0.753416000
1	-2.054384000	-1.809434000	-0.784676000
1	-3.234061000	0.990352000	-0.114465000
1	-1.830146000	-1.284867000	1.679880000
1	-3.633660000	-0.811082000	1.738154000
6	-1.143782000	0.771402000	-0.407826000
8	-0.140480000	-0.112542000	-0.714066000
14	1.459449000	-0.243894000	-0.175997000
6	2.532576000	1.138029000	-0.882200000
1	2.276971000	2.119072000	-0.464058000
1	3.591088000	0.947068000	-0.657713000
1	2.429101000	1.197337000	-1.973280000
6	2.013919000	-1.907755000	-0.850045000
1	3.054831000	-2.119909000	-0.572460000
1	1.386707000	-2.718656000	-0.459232000
1	1.945319000	-1.927992000	-1.944977000
6	1.510059000	-0.215211000	1.709767000
1	0.900462000	-1.022939000	2.134569000
1	2.539227000	-0.346776000	2.070810000
1	1.136496000	0.734128000	2.114270000
6	-0.784791000	2.217468000	-0.223624000
1	-0.125341000	2.379554000	0.646000000
1	-0.260731000	2.615430000	-1.104561000
1	-1.687031000	2.816847000	-0.063770000

Table S27. B971/6-31+G(d,p)-optimized Cartesian coordinates for trans-MSCPC

6	-3.563517000	-0.278259000	0.678675000
6	-2.221150000	-0.681307000	0.085528000
6	-3.437666000	-0.392693000	-0.823693000
1	-4.122407000	-1.044009000	1.212039000
1	-3.656743000	0.716643000	1.109416000
1	-1.964308000	-1.735264000	0.178127000
1	-3.420639000	0.527965000	-1.402886000
1	-3.905342000	-1.236444000	-1.326691000
6	-1.028625000	0.193540000	0.128313000
8	0.105402000	-0.434919000	-0.338419000
14	1.734690000	-0.126418000	0.004671000
6	1.943112000	0.254936000	1.839644000
1	1.562836000	-0.569537000	2.456005000
1	3.003510000	0.399791000	2.086898000
1	1.405674000	1.165632000	2.132991000
6	2.379365000	1.300698000	-1.049218000
1	3.462885000	1.420110000	-0.911053000
1	2.197938000	1.111339000	-2.115047000
1	1.904501000	2.255453000	-0.792040000
6	2.611015000	-1.720793000	-0.467708000
1	2.431162000	-1.967036000	-1.521805000
1	3.695858000	-1.634539000	-0.321361000
1	2.251784000	-2.561289000	0.139048000
6	-1.112084000	1.682203000	-0.053553000
1	-0.284381000	2.201181000	0.448715000
1	-1.070283000	1.968456000	-1.121115000
1	-2.043611000	2.080787000	0.362781000

Table S28. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state 1 of trans-MSCPC

6	3.708734000	-0.524762000	-0.803145000
6	2.091687000	-0.602506000	0.277817000
6	3.490057000	-0.200861000	0.633942000
1	4.020759000	-1.516640000	-1.112666000
1	3.627707000	0.251376000	-1.556247000

1	1.863534000	-1.664164000	0.327504000
1	3.629887000	0.845754000	0.913307000
1	3.982629000	-0.856993000	1.355422000
6	1.017526000	0.241215000	-0.001555000
8	-0.126855000	-0.358024000	-0.478436000
14	-1.736361000	-0.141537000	-0.000796000
6	-1.824117000	0.039872000	1.874421000
1	-1.290858000	0.933815000	2.222944000
1	-2.867578000	0.125094000	2.206615000
1	-1.380627000	-0.829345000	2.376373000
6	-2.603966000	-1.701018000	-0.589123000
1	-3.679446000	-1.663324000	-0.370914000
1	-2.483442000	-1.826642000	-1.672551000
1	-2.188202000	-2.590818000	-0.100387000
6	-2.486872000	1.370688000	-0.845483000
1	-2.372048000	1.306203000	-1.935209000
1	-3.561531000	1.437003000	-0.626535000
1	-2.022444000	2.307460000	-0.513467000
6	1.073784000	1.739139000	-0.096298000
1	0.934172000	2.069308000	-1.138121000
1	0.280118000	2.214646000	0.498443000
1	2.030264000	2.132378000	0.260680000

Table S29. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state 2 of trans-MSCPC

6	-3.528627000	-0.185716000	0.583811000
6	-2.127226000	-0.579195000	0.230553000
6	-3.742630000	-0.511242000	-0.853631000
1	-4.018799000	-0.844489000	1.304521000
1	-3.675097000	0.860171000	0.862522000
1	-1.892881000	-1.639479000	0.280765000
1	-3.664618000	0.265134000	-1.606805000
1	-4.048093000	-1.505040000	-1.163534000
6	-1.057552000	0.270921000	-0.046797000
8	0.091173000	-0.321499000	-0.521708000
14	1.698890000	-0.094708000	-0.042917000
6	2.440827000	1.421138000	-0.888611000
1	1.971357000	2.355538000	-0.557053000
1	3.515168000	1.493475000	-0.670015000
1	2.326055000	1.355353000	-1.978263000
6	2.576706000	-1.649323000	-0.628998000
1	3.651492000	-1.605156000	-0.408598000
1	2.165248000	-2.541392000	-0.140759000
1	2.459172000	-1.776052000	-1.712624000
6	1.784178000	0.088916000	1.832213000
1	1.347798000	-0.783616000	2.334646000
1	2.826743000	0.183164000	2.164779000
1	1.243251000	0.978589000	2.179845000
6	-1.122654000	1.768495000	-0.141470000
1	-0.331507000	2.248536000	0.452961000
1	-0.985515000	2.099664000	-1.183319000
1	-2.081261000	2.156024000	0.216029000

Table S30. B971/6-31+G(d,p)-optimized Cartesian coordinates for CBC

6	-0.585018000	-0.000332000	-0.403719000
6	0.451807000	1.082116000	0.088401000
6	1.565084000	0.000693000	0.030192000
6	0.452516000	-1.081717000	0.083768000
1	0.232609000	1.381560000	1.120954000
1	0.560491000	1.982800000	-0.526654000
1	2.316831000	-0.000578000	0.826941000
1	2.080399000	0.002980000	-0.937958000
1	0.233814000	-1.385486000	1.115256000
1	0.562759000	-1.980187000	-0.534275000
1	-0.611893000	0.003397000	-1.501355000
6	-1.955938000	-0.002182000	0.150025000
1	-2.106915000	-0.021097000	1.228664000

1	-2.838802000	0.025147000	-0.483570000

Table S31. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state of CBC

6	0.759254000	-0.088030000	0.436000000
6	-0.284324000	-1.072689000	-0.100580000
6	-1.533122000	-0.173605000	0.013269000
6	-0.823559000	1.161455000	-0.142889000
1	0.660968000	0.148629000	1.498293000
1	-0.325250000	-2.022482000	0.450979000
1	-0.063842000	-1.301462000	-1.151655000
1	-1.980733000	-0.257277000	1.011625000
1	-2.321784000	-0.373108000	-0.725334000
1	-1.002228000	1.980050000	0.553762000
1	-0.553108000	1.469999000	-1.152255000
6	1.988625000	0.140052000	-0.149365000
1	2.205650000	-0.208550000	-1.157875000
1	2.739085000	0.761107000	0.333852000

Table S32. B971/6-31+G(d,p)-optimized Cartesian coordinates for cis-CBEC

6	-0.765125000	0.100937000	-0.622526000
6	0.310086000	-0.192978000	-1.739653000
6	0.239311000	1.301968000	-2.156092000
6	-0.364955000	1.619323000	-0.760673000
1	-1.762146000	-0.039864000	-1.060622000
1	0.055151000	-0.956834000	-2.483206000
1	1.282187000	-0.441932000	-1.296421000
1	-0.490253000	1.464234000	-2.958824000
1	1.176679000	1.798688000	-2.430018000
1	-1.174881000	2.355351000	-0.695637000
1	0.415394000	1.887427000	-0.037801000
6	-0.696881000	-0.586987000	0.693693000
1	-1.572994000	-1.130374000	1.050951000
6	0.472681000	-0.471256000	1.626040000
1	1.398548000	-0.302128000	1.054591000
1	0.360409000	0.427111000	2.263878000
6	0.646703000	-1.698304000	2.540618000
1	0.831086000	-2.604254000	1.950396000
1	1.487888000	-1.562954000	3.231373000
1	-0.256616000	-1.868626000	3.140478000

Table S33. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state of cis-CBEC

6	0.462744000	-0.128277000	0.761096000
6	1.152144000	1.077202000	0.110681000
6	2.501902000	0.409200000	-0.224913000
6	1.978046000	-1.006014000	-0.405166000
1	0.915785000	-0.429026000	1.708649000
1	1.201914000	1.961201000	0.762559000
1	0.634930000	1.369072000	-0.810711000
1	3.182238000	0.459461000	0.634867000
1	3.028212000	0.830502000	-1.092995000
1	2.467719000	-1.853724000	0.073312000
1	1.481306000	-1.236973000	-1.347726000
6	-0.839539000	-0.557103000	0.558348000
1	-1.211344000	-1.347425000	1.214912000
6	-1.762381000	-0.163117000	-0.563654000
1	-1.321541000	0.639847000	-1.167166000
1	-1.897649000	-1.021879000	-1.244106000
6	-3.153248000	0.278448000	-0.059992000
1	-3.074357000	1.169256000	0.574816000
1	-3.820084000	0.511946000	-0.899421000
1	-3.625136000	-0.514289000	0.534601000

Table S34. B971/6-31+G(d,p)-optimized Cartesian coordinates for trans-CBEC

6	-0.599995000	-0.025789000	-0.628973000
6	-1.494939000	1.111743000	0.028680000
6	-2.377136000	0.007973000	0.674870000

6	-1.762615000	-1.025671000	-0.311516000
1	-0.405751000	0.142569000	-1.698395000
1	-2.034059000	1.684361000	-0.736200000
1	-0.984647000	1.811574000	0.700469000
1	-3.463073000	0.151727000	0.641221000
1	-2.087550000	-0.192115000	1.713178000
1	-2.401898000	-1.192645000	-1.186394000
1	-1.466656000	-1.999808000	0.095821000
6	0.681607000	-0.303627000	0.075685000
1	0.645180000	-0.841193000	1.026886000
6	1.951098000	0.410619000	-0.280660000
1	2.047971000	0.458338000	-1.377823000
1	1.895924000	1.468548000	0.046160000
6	3.211584000	-0.227781000	0.328058000
1	3.334683000	-1.260592000	-0.020335000
1	4.113040000	0.333743000	0.054791000
1	3.149204000	-0.249311000	1.423756000

Table S35. B971/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state of trans-CBEC

6	-0.443609000	-0.623585000	0.473843000
6	-1.836363000	-0.930554000	-0.109405000
6	-2.287913000	0.501480000	-0.471905000
6	-1.352637000	1.272453000	0.448666000
1	-0.329306000	-0.697918000	1.557563000
1	-2.478628000	-1.375334000	0.661248000
1	-1.801812000	-1.628497000	-0.955916000
1	-3.357844000	0.703614000	-0.319350000
1	-2.055151000	0.723341000	-1.520598000
1	-1.661861000	1.411532000	1.485518000
1	-0.723689000	2.068811000	0.053301000
6	0.712678000	-0.725515000	-0.277949000
1	0.624595000	-0.848878000	-1.361408000
6	2.101574000	-0.524027000	0.265465000
1	2.063525000	-0.478424000	1.362936000
1	2.727266000	-1.394345000	0.009313000
6	2.789871000	0.747466000	-0.280445000
1	2.230058000	1.646890000	0.003314000
1	3.811033000	0.841391000	0.110517000
1	2.850214000	0.721504000	-1.376061000

Table S36.M06-2X/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state 1 of trans-MSCPC

6	3.530529000	-0.618444000	-0.732313000
6	1.776521000	-0.560198000	0.124552000
6	3.154331000	-0.481381000	0.693687000
1	3.714740000	-1.590194000	-1.171268000
1	3.661101000	0.263270000	-1.345997000
1	1.369700000	-1.554595000	-0.031993000
1	3.413575000	0.466036000	1.164795000
1	3.422264000	-1.318605000	1.337021000
6	0.942138000	0.501904000	-0.157490000
8	-0.238353000	0.263079000	-0.825561000
14	-1.651197000	-0.148381000	-0.005332000
6	-1.443201000	-1.810736000	0.838577000
1	-0.670965000	-1.764474000	1.613309000
1	-2.379998000	-2.117262000	1.316498000
1	-1.161864000	-2.586595000	0.119268000
6	-2.965732000	-0.218054000	-1.329149000
1	-3.937223000	-0.492033000	-0.905300000
1	-3.070368000	0.752088000	-1.823773000
1	-2.705615000	-0.958955000	-2.091182000
6	-2.024176000	1.163938000	1.283260000
1	-2.175224000	2.144890000	0.821739000
1	-2.931310000	0.910798000	1.842205000
1	-1.202618000	1.245776000	2.003549000
6	1.290847000	1.951151000	-0.059541000
1	1.401476000	2.375766000	-1.066334000

1	0.489190000	2.509101000	0.437620000
1	2.219183000	2.118614000	0.489477000

Table S37. M06-2X/6-31+G(d,p)-optimized Cartesian coordinates for ring-opening transition state 2 of trans-MSCPC

6	-3.475569000	-0.160246000	0.620710000
6	-2.102950000	-0.599557000	0.234140000
6	-3.746931000	-0.427546000	-0.810619000
1	-3.972420000	-0.822512000	1.328700000
1	-3.566642000	0.877967000	0.938617000
1	-1.904127000	-1.666026000	0.253590000
1	-3.626989000	0.360982000	-1.541998000
1	-4.100284000	-1.394864000	-1.142342000
6	-1.034553000	0.213795000	-0.078125000
8	0.095654000	-0.394454000	-0.563366000
14	1.675578000	-0.112352000	-0.058075000
6	2.378648000	1.415266000	-0.893472000
1	1.906090000	2.337823000	-0.543905000
1	3.452895000	1.493856000	-0.693014000
1	2.244009000	1.355410000	-1.978291000
6	2.624583000	-1.625901000	-0.604762000
1	3.686633000	-1.536854000	-0.354505000
1	2.232653000	-2.526888000	-0.124051000
1	2.540785000	-1.758352000	-1.687856000
6	1.689376000	0.087701000	1.806773000
1	1.248964000	-0.788662000	2.292485000
1	2.713053000	0.204731000	2.177567000
1	1.116934000	0.966197000	2.121966000
6	-1.064067000	1.705843000	-0.175944000
1	-0.304460000	2.171299000	0.465661000
1	-0.851248000	2.018578000	-1.207147000
1	-2.034013000	2.112977000	0.114809000

† Method and Basis set-specific Dispersion-correcting potentials, as described in I. D. Mackie and G. A. DiLabio, *J. Phys. Chem. A*, 2008, **112**, 10968.

‡ Non-default (Gaussian-03 and Gaussian-09) integration grid size used, with radial and angular points indicated in parenthesis.