Supplementary Materials

Photochemical Rearrangement Reactions of Bicyclic Molecules That Contain a Cyclopropane

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Details of the present computational approach are as follows:

The geometries and energetics of the stationary points on the potential energy surface were calculated using the DFT (M06-L)[1] method in conjunction with the 6-311G(d,p) basis set.[2] We denote our M06-L calculations by M06-L/6-311G(d,p). The DFT calculations were excuted using the Gaussian 09 software package.[3] Vibrational frequency calculations at the M06-L/6-311G(d,p) level were used to characterize all stationary points as either minima (the number of imaginary frequencies (NIMAG) = 0) or transition states (NIMAG = 1). Time-dependent density functional theory (TD-DFT) computations[4,5] were also performed with the same density functional and basis sets. Vertical excitations with 30 singlet and 30 triplet states were computed using ground state geometries to simulate the UV-vis spectra. The minimum energy crossing points between the singlet and triplet potential energy surfaces are also computed using the GAUSSIAN 09 package[3] and the code that was developed by Harvey et al.[6].

The Cartesian coordinates and the energies are given in the Supporting Information.

References:

(1) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res*. **2008**, *41*, 157.

(2) (a) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys*.**1980**, *72*, 650. (b) McLean, A. D.; Chandler, G. S. *J. Chem. Phys.* **1980**, *72*, 5639. (c) Curtiss, L. A. M.; McGrath, P.; Blandeau, J-P.; Davis, N. E.; Binning, R. C.; Radom, Jr. L. *J. Chem. Phys.* **1995**, *103*, 6104.

(3) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.;

Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, Liashenko, G.; Piskorz, A.; Komaromi, P.; I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S. and Pople, J. A. Gaussian, Inc., Wallingford CT, 2013.

(4) Casida, M. E.; Jamorski, C.; Casida, K. C.; Salahub, D. R. *J. Chem. Phys*. **1998**, *109*, 8218.

(5) Stratmann, R. E.; Scuseria, G. E.; Frisch, M. J. *J. Chem. Phys*. **1998**, *108*, 4439.

(6) (a) Harvey, J. N.; Aschi, M.; Schwarz, H.; Koch, W. *Theor. Chem. Acc.* 1998, *99*, 95. (b) Harvey, J. N.; Aschi, M. *Phys. Chem. Chem. Phys.* **1999**, *1*, 5555.

Table S1. The vertical excitation energies and oscillator strengths for the thirty lowest energy triplet excited states of molecule bicyclo[3,1,0]hex-3-en-2-one at the TD-DFT/M06-L/6-311G(d,p).

[3,1,0]-TDDFT- Singlet

Excited State	1:	Singlet-?Sym	3.5603 eV	348.24 nm	f=0.0007	<S**2>=0.000
25 -> 26		0.70667				
Excited State	2:	Singlet-?Sym	4.9808 eV	248.92 nm	f=0.0343	<S**2>=0.000
22 -> 26		-0.11453				
23 -> 26		0.29392				
24 -> 26		0.62663				
Excited State	3:	Singlet-?Sym	5.9355 eV	208.89 nm	f=0.1135	<S**2>=0.000
22 -> 26		0.10232				
23 -> 26		0.62356				
24 -> 26		-0.26471				
Excited State	4:	Singlet-?Sym	6.3633 eV	194.84 nm	f=0.0049	<S**2>=0.000
25 -> 27		0.70004				
Excited State	5:	Singlet-?Sym	7.0262 eV	176.46 nm	f=0.0104	<S**2>=0.000
21 -> 26		-0.13752				
22 -> 26		-0.21322				
25 -> 28		0.65260				
Excited State	6:	Singlet-?Sym	7.0677 eV	175.42 nm	f=0.0785	<S**2>=0.000
22 -> 26		0.62377				
24 -> 26		0.11094				
25 -> 28		0.24559				
Excited State	7:	Singlet-?Sym	7.1420 eV	173.60 nm	f=0.0100	<S**2>=0.000
21 -> 26		0.68444				
25 -> 28		0.10671				
Excited State	8:	Singlet-?Sym	7.5445 eV	164.34 nm	f=0.0381	<S**2>=0.000
20 -> 26		0.24000				
24 -> 27		0.60684				
24 -> 28		-0.20968				

Excited State 9:	Singlet-?Sym	7.7636 eV	159.70 nm	f=0.0281	<S**2>=0.000
25 -> 29	0.69210				
Excited State 10:	Singlet-?Sym	7.8574 eV	157.79 nm	f=0.0091	<S**2>=0.000
25 -> 30	0.69623				
Excited State 11:	Singlet-?Sym	7.8679 eV	157.58 nm	f=0.0016	<S**2>=0.000
19 -> 26	-0.42739				
20 -> 26	0.47370				
24 -> 28	0.26936				
Excited State 12:	Singlet-?Sym	7.9834 eV	155.30 nm	f=0.0028	<S**2>=0.000
19 -> 26	0.42192				
23 -> 27	-0.11730				
24 -> 28	0.52376				
Excited State 13:	Singlet-?Sym	8.3146 eV	149.12 nm	f=0.0086	<S**2>=0.000
19 -> 26	-0.13695				
20 -> 26	-0.14741				
23 -> 27	0.22098				
24 -> 28	0.12430				
25 -> 31	0.60278				
Excited State 14:	Singlet-?Sym	8.3239 eV	148.95 nm	f=0.0040	<S**2>=0.000
18 -> 26	0.66341				
23 -> 27	-0.22368				
Excited State 15:	Singlet-?Sym	8.4021 eV	147.56 nm	f=0.0843	<S**2>=0.000
18 -> 26	0.16797				
19 -> 26	-0.13028				
20 -> 26	-0.13780				
23 -> 27	0.43688				
24 -> 27	0.16186				
24 -> 28	0.19154				
25 -> 31	-0.34733				
25 -> 32	-0.12888				
Excited State 16:	Singlet-?Sym	8.5535 eV	144.95 nm	f=0.0153	<S**2>=0.000
20 -> 26	0.10960				

23 -> 27 0.22940
24 -> 29 -0.28437
25 -> 32 0.55452

Excited State 17: Singlet-?Sym 8.5950 eV 144.25 nm f=0.0497 <S**2>=0.000
19 -> 26 -0.14396
20 -> 26 -0.15268
23 -> 27 -0.14013
24 -> 27 0.10148
24 -> 29 0.41748
24 -> 30 -0.18287
25 -> 32 0.40799
25 -> 33 0.10984

Excited State 18: Singlet-?Sym 8.5998 eV 144.17 nm f=0.0227 <S**2>=0.000
17 -> 26 -0.12518
19 -> 26 0.15162
20 -> 26 0.19759
23 -> 27 0.25426
23 -> 28 -0.13440
24 -> 28 -0.11897
24 -> 29 0.48899
24 -> 30 0.16409
25 -> 33 -0.12371

Excited State 19: Singlet-?Sym 8.7826 eV 141.17 nm f=0.0070 <S**2>=0.000
17 -> 26 0.39320
24 -> 30 0.56107

Excited State 20: Singlet-?Sym 8.9029 eV 139.26 nm f=0.0152 <S**2>=0.000
17 -> 26 -0.17633
24 -> 30 0.10378
25 -> 33 0.65337

Excited State 21: Singlet-?Sym 8.9118 eV 139.12 nm f=0.0089 <S**2>=0.000
17 -> 26 0.52477
19 -> 26 0.11040
20 -> 26 0.14280
22 -> 27 0.17772
23 -> 28 -0.13118

24 -> 27 -0.11341
24 -> 30 -0.28093
25 -> 33 0.13717

Excited State 22: Singlet-?Sym 9.0430 eV 137.11 nm f=0.0446 <S**2>=0.000
23 -> 27 0.10407
23 -> 28 0.62509
25 -> 34 -0.26187

Excited State 23: Singlet-?Sym 9.2263 eV 134.38 nm f=0.0101 <S**2>=0.000
24 -> 31 0.69504

Excited State 24: Singlet-?Sym 9.3407 eV 132.74 nm f=0.0544 <S**2>=0.000
23 -> 27 0.10429
23 -> 28 0.19385
24 -> 33 -0.10951
25 -> 34 0.62807

Excited State 25: Singlet-?Sym 9.4806 eV 130.78 nm f=0.0223 <S**2>=0.000
22 -> 27 -0.35126
24 -> 32 0.58552
24 -> 33 -0.10035

Excited State 26: Singlet-?Sym 9.4941 eV 130.59 nm f=0.0077 <S**2>=0.000
16 -> 26 0.47798
22 -> 27 0.38817
24 -> 32 0.31332

Excited State 27: Singlet-?Sym 9.6995 eV 127.83 nm f=0.0186 <S**2>=0.000
23 -> 29 0.69173

Excited State 28: Singlet-?Sym 9.7430 eV 127.25 nm f=0.0344 <S**2>=0.000
16 -> 26 0.45787
20 -> 26 0.11059
22 -> 27 -0.34111
22 -> 28 0.23295
23 -> 29 -0.10753
24 -> 32 -0.16115

Excited State 29: Singlet-?Sym 9.8150 eV 126.32 nm f=0.0134 <S**2>=0.000

23 -> 30 0.68775

Excited State 30: Singlet-?Sym 9.9895 eV 124.11 nm f=0.0526 <S**2>=0.000
21 -> 27 -0.27501
22 -> 28 -0.26657
24 -> 33 0.53485
25 -> 35 0.13048

[3,1,0]-TDDFT- Triplet

Excitation energies and oscillator strengths:

Excited State 1: 3.010-?Sym 0.5198 eV 2385.34 nm f=0.0018 <S**2>=2.015
26A -> 27A 0.12264
24B -> 25B 0.99609

Excited State 2: 3.010-?Sym 1.9230 eV 644.74 nm f=0.0010 <S**2>=2.016
23B -> 25B 0.99405

Excited State 3: 3.011-?Sym 2.7710 eV 447.44 nm f=0.0116 <S**2>=2.016
22B -> 25B 0.98295

Excited State 4: 3.004-?Sym 3.2578 eV 380.58 nm f=0.0174 <S**2>=2.006
26A -> 27A 0.91959
18B -> 25B 0.12718
19B -> 25B -0.12081
21B -> 25B -0.18956
22B -> 25B -0.11719
24B -> 26B 0.24089

Excited State 5: 3.011-?Sym 3.4135 eV 346.92 nm f=0.1050 <S**2>=2.017
26A -> 27A 0.16369
20B -> 25B 0.11840
21B -> 25B 0.96626

Excited State 6: 3.011-?Sym 3.9902 eV 310.72 nm f=0.0002 <S**2>=2.017
18B -> 25B -0.12993
19B -> 25B -0.33791
20B -> 25B 0.90719
21B -> 25B -0.11536

24B -> 26B	-0.13870				
Excited State 7:	3.010-?Sym	4.1518 eV	298.63 nm	f=0.0010	<S**2>=2.015
26A -> 28A	0.96141				
19B -> 25B	-0.11898				
24B -> 26B	0.21726				
Excited State 8:	3.012-?Sym	4.3399 eV	285.68 nm	f=0.0046	<S**2>=2.018
19B -> 25B	0.89287				
20B -> 25B	0.36976				
24B -> 26B	0.19807				
Excited State 9:	3.035-?Sym	4.6031 eV	269.35 nm	f=0.0024	<S**2>=2.053
25A -> 27A	0.13591				
26A -> 27A	-0.12348				
26A -> 28A	-0.15863				
26A -> 29A	0.10166				
26A -> 30A	-0.10420				
18B -> 25B	-0.61368				
19B -> 25B	-0.13805				
24B -> 26B	0.71480				
Excited State 10:	3.012-?Sym	4.9611 eV	249.91 nm	f=0.0071	<S**2>=2.018
26A -> 29A	0.89118				
26A -> 30A	-0.19862				
18B -> 25B	0.34208				
Excited State 11:	3.015-?Sym	5.0692 eV	244.58 nm	f=0.0167	<S**2>=2.023
26A -> 27A	0.11488				
26A -> 29A	0.39811				
26A -> 30A	0.74496				
26A -> 31A	0.12489				
17B -> 25B	-0.19269				
18B -> 25B	-0.37065				
23B -> 26B	-0.11071				
24B -> 26B	-0.20923				
Excited State 12:	3.016-?Sym	5.2129 eV	237.84 nm	f=0.0283	<S**2>=2.024
26A -> 27A	-0.14591				
26A -> 28A	-0.11462				

26A -> 29A -0.15528
26A -> 30A 0.59963
26A -> 31A -0.25615
17B -> 25B 0.46643
18B -> 25B 0.35905
22B -> 26B -0.10257
24B -> 26B 0.33395

Excited State 13: 3.013-?Sym 5.3175 eV 233.16 nm f=0.0256 <S**2>=2.020
26A -> 30A -0.12406
26A -> 31A 0.32179
26A -> 33A 0.11164
17B -> 25B 0.83463
18B -> 25B -0.26189
19B -> 25B 0.12129
23B -> 26B -0.12452
24B -> 26B -0.16727

Excited State 14: 3.020-?Sym 5.4443 eV 227.73 nm f=0.0260 <S**2>=2.030
26A -> 31A 0.88554
17B -> 25B -0.12922
18B -> 25B 0.21454
23B -> 26B 0.23695
24B -> 26B 0.20548

Excited State 15: 3.030-?Sym 5.7750 eV 214.69 nm f=0.0060 <S**2>=2.046
25A -> 27A 0.11059
26A -> 32A 0.92941
16B -> 25B 0.11189
22B -> 26B 0.12989
23B -> 26B 0.27355

Excited State 16: 3.024-?Sym 5.8575 eV 211.67 nm f=0.0053 <S**2>=2.036
26A -> 33A 0.89494
16B -> 25B -0.32890
23B -> 26B 0.26129

Excited State 17: 3.014-?Sym 5.9047 eV 209.97 nm f=0.0094 <S**2>=2.021
26A -> 32A -0.11719
26A -> 33A 0.30383

16B -> 25B 0.92327
23B -> 26B 0.10580

Excited State 18: 3.159-?Sym 6.3240 eV 196.05 nm f=0.0386 <S**2>=2.245
25A -> 27A -0.26490
26A -> 32A -0.15179
26A -> 33A -0.14979
26A -> 34A -0.58375
18B -> 25B -0.13748
22B -> 26B -0.11054
23B -> 26B 0.64267
24B -> 27B 0.18803
24B -> 28B 0.12181

Excited State 19: 3.667-?Sym 6.3635 eV 194.84 nm f=0.0081 <S**2>=3.112
25A -> 27A -0.52563
26A -> 32A 0.12227
26A -> 34A 0.55632
22B -> 26B -0.20228
24B -> 26B 0.10398
24B -> 27B 0.47799
24B -> 28B 0.26137

Excited State 20: 3.133-?Sym 6.4273 eV 192.90 nm f=0.0743 <S**2>=2.204
25A -> 27A 0.21602
26A -> 32A -0.24174
26A -> 33A -0.18999
26A -> 34A 0.57502
26A -> 35A -0.11403
18B -> 25B -0.13936
22B -> 26B 0.26297
23B -> 26B 0.53761
24B -> 26B -0.17173
24B -> 27B -0.21717

Excited State 21: 3.137-?Sym 6.9166 eV 179.26 nm f=0.0648 <S**2>=2.210
25A -> 27A -0.24351
26A -> 27A -0.11203
26A -> 34A -0.10152
22B -> 26B 0.88447

24B -> 27B 0.22474

Excited State 22: 3.027-?Sym 7.2735 eV 170.46 nm f=0.0006 <S**2>=2.041
25A -> 27A 0.17409
15B -> 25B 0.94157
24B -> 27B 0.22334

Excited State 23: 3.314-?Sym 7.3568 eV 168.53 nm f=0.0082 <S**2>=2.495
25A -> 27A 0.31057
26A -> 35A -0.53372
15B -> 25B -0.18547
24B -> 27B 0.60835
24B -> 28B -0.43245

Excited State 24: 3.104-?Sym 7.4074 eV 167.38 nm f=0.0257 <S**2>=2.158
25A -> 27A 0.14609
26A -> 35A 0.69612
15B -> 25B -0.15833
21B -> 26B -0.54048
24B -> 27B 0.28027
24B -> 28B -0.25339

Excited State 25: 3.063-?Sym 7.4308 eV 166.85 nm f=0.0390 <S**2>=2.096
26A -> 35A 0.42958
15B -> 25B -0.16058
21B -> 26B 0.82331
24B -> 27B 0.18688
24B -> 28B -0.17385

Excited State 26: 3.402-?Sym 7.7013 eV 160.99 nm f=0.0165 <S**2>=2.644
24A -> 27A 0.70693
25A -> 27A -0.36759
25A -> 28A 0.29799
26A -> 36A 0.10102
15B -> 25B 0.10413
24B -> 28B -0.45214

Excited State 27: 3.338-?Sym 7.8462 eV 158.02 nm f=0.0227 <S**2>=2.536
24A -> 27A 0.59274
25A -> 27A 0.25046

25A -> 28A -0.45194
26A -> 36A -0.27515
26A -> 37A 0.28730
20B -> 26B 0.19392
24B -> 27B 0.13589
24B -> 28B 0.35730

Excited State 28: 3.069-?Sym 7.9331 eV 156.29 nm f=0.0086 <S**2>=2.105
24A -> 27A 0.11811
25A -> 28A -0.26154
26A -> 36A 0.92763
24B -> 28B 0.10391

Excited State 29: 3.064-?Sym 7.9825 eV 155.32 nm f=0.0033 <S**2>=2.098
24A -> 27A -0.19940
25A -> 28A 0.25562
26A -> 36A 0.14512
26A -> 37A 0.90789

Excited State 30: 3.121-?Sym 8.0356 eV 154.29 nm f=0.0086 <S**2>=2.185
24A -> 27A 0.11951
25A -> 27A 0.14550
25A -> 28A 0.68318
26A -> 37A -0.19774
14B -> 25B 0.29390
19B -> 26B -0.12800
20B -> 26B 0.37638
24B -> 27B 0.11988
24B -> 28B 0.39174
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Table S2. The vertical excitation energies and oscillator strengths for the thirty lowest energy triplet excited states of molecule bicyclo[5,1,0]octa-3,5-dien-2-one at the TD-DFT/M06-L/6-311G(d,p).

[5,1,0]-TDDFT- Singlet

Excitation energies and oscillator strengths:

Excited State 1: Singlet-?Sym 2.6252 eV 472.28 nm f=0.0025 <S**2>=0.000

32 -> 33 0.69600

Excited State 2: Singlet-?Sym 3.1640 eV 391.86 nm f=0.0055 <S**2>=0.000
31 -> 33 0.68998
32 -> 34 0.10236

Excited State 3: Singlet-?Sym 3.7690 eV 328.96 nm f=0.0161 <S**2>=0.000
31 -> 34 0.59012
32 -> 34 0.36429

Excited State 4: Singlet-?Sym 4.2558 eV 291.33 nm f=0.1253 <S**2>=0.000
30 -> 33 -0.18613
31 -> 34 -0.33830
31 -> 35 0.15532
32 -> 34 0.51154
32 -> 35 -0.17929

Excited State 5: Singlet-?Sym 4.3516 eV 284.92 nm f=0.0025 <S**2>=0.000
29 -> 33 -0.12466
30 -> 33 0.65247
30 -> 34 0.11026
32 -> 34 0.14488
32 -> 35 -0.12908

Excited State 6: Singlet-?Sym 4.6648 eV 265.79 nm f=0.0284 <S**2>=0.000
29 -> 33 -0.19407
31 -> 34 -0.15307
31 -> 35 0.11865
32 -> 34 0.13586
32 -> 35 0.61937

Excited State 7: Singlet-?Sym 5.1366 eV 241.37 nm f=0.0308 <S**2>=0.000
28 -> 33 0.10841
31 -> 35 0.66679
32 -> 34 -0.14567

Excited State 8: Singlet-?Sym 5.3640 eV 231.14 nm f=0.0179 <S**2>=0.000
28 -> 33 0.56814
29 -> 33 -0.27563
30 -> 34 -0.27086

Excited State 9:	Singlet-?Sym	5.5068 eV	225.15 nm	f=0.0667	<S**2>=0.000
28 -> 33	0.17639				
29 -> 33	-0.24349				
30 -> 33	-0.10554				
30 -> 34	0.58315				
30 -> 35	0.14984				
Excited State 10:	Singlet-?Sym	5.5723 eV	222.50 nm	f=0.0420	<S**2>=0.000
28 -> 33	0.35832				
29 -> 33	0.52269				
29 -> 34	-0.10362				
30 -> 34	0.11760				
32 -> 35	0.15699				
Excited State 11:	Singlet-?Sym	6.0777 eV	204.00 nm	f=0.0108	<S**2>=0.000
28 -> 34	-0.12765				
29 -> 34	0.44730				
32 -> 36	0.51077				
Excited State 12:	Singlet-?Sym	6.1620 eV	201.21 nm	f=0.0038	<S**2>=0.000
28 -> 34	0.21264				
29 -> 34	0.48922				
30 -> 35	0.15521				
32 -> 36	-0.40839				
Excited State 13:	Singlet-?Sym	6.2373 eV	198.78 nm	f=0.0142	<S**2>=0.000
28 -> 34	0.63955				
29 -> 34	-0.11202				
32 -> 36	0.23063				
Excited State 14:	Singlet-?Sym	6.3115 eV	196.44 nm	f=0.0938	<S**2>=0.000
28 -> 34	-0.11848				
29 -> 33	0.10277				
29 -> 34	-0.10902				
30 -> 34	-0.11226				
30 -> 35	0.63922				
Excited State 15:	Singlet-?Sym	6.6125 eV	187.50 nm	f=0.0052	<S**2>=0.000
27 -> 33	0.28192				

32 -> 37 0.63923

Excited State 16: Singlet-?Sym 6.6366 eV 186.82 nm f=0.0101 <S**2>=0.000
27 -> 33 0.61546
29 -> 35 0.13515
32 -> 37 -0.28783

Excited State 17: Singlet-?Sym 6.8010 eV 182.30 nm f=0.0060 <S**2>=0.000
31 -> 36 0.70129

Excited State 18: Singlet-?Sym 6.8829 eV 180.13 nm f=0.0350 <S**2>=0.000
25 -> 33 0.12499
26 -> 33 0.67797

Excited State 19: Singlet-?Sym 7.2700 eV 170.54 nm f=0.0021 <S**2>=0.000
25 -> 33 -0.31835
27 -> 34 0.19238
28 -> 35 -0.30191
29 -> 35 0.45164
31 -> 37 -0.10324
32 -> 38 0.17608

Excited State 20: Singlet-?Sym 7.3173 eV 169.44 nm f=0.0040 <S**2>=0.000
28 -> 35 -0.19148
31 -> 37 0.66591
32 -> 38 0.10029

Excited State 21: Singlet-?Sym 7.3308 eV 169.13 nm f=0.0054 <S**2>=0.000
27 -> 34 0.21007
28 -> 35 0.29343
29 -> 35 -0.10729
32 -> 38 0.59132

Excited State 22: Singlet-?Sym 7.3419 eV 168.87 nm f=0.0071 <S**2>=0.000
25 -> 33 -0.12217
27 -> 34 0.59080
28 -> 35 0.16124
32 -> 38 -0.30142

Excited State 23: Singlet-?Sym 7.4456 eV 166.52 nm f=0.0284 <S**2>=0.000

25 -> 33 -0.28508
27 -> 34 -0.19726
28 -> 35 0.47869
29 -> 35 0.23340
31 -> 37 0.18220

Excited State 24: Singlet-?Sym 7.4872 eV 165.60 nm f=0.0269 <S**2>=0.000
25 -> 33 0.48992
27 -> 34 0.11828
27 -> 35 -0.16267
28 -> 35 0.12015
29 -> 35 0.36983
32 -> 39 -0.10842

Excited State 25: Singlet-?Sym 7.5868 eV 163.42 nm f=0.0056 <S**2>=0.000
26 -> 34 0.69689

Excited State 26: Singlet-?Sym 7.6083 eV 162.96 nm f=0.0067 <S**2>=0.000
32 -> 39 0.68206
32 -> 40 -0.13768

Excited State 27: Singlet-?Sym 7.6628 eV 161.80 nm f=0.0041 <S**2>=0.000
32 -> 39 0.13961
32 -> 40 0.68415

Excited State 28: Singlet-?Sym 7.7993 eV 158.97 nm f=0.0026 <S**2>=0.000
24 -> 33 0.60984
25 -> 34 0.13227
30 -> 36 0.26937
32 -> 41 -0.15275

Excited State 29: Singlet-?Sym 7.8617 eV 157.71 nm f=0.0074 <S**2>=0.000
24 -> 33 -0.22682
25 -> 34 -0.13548
30 -> 36 0.64449

Excited State 30: Singlet-?Sym 7.8966 eV 157.01 nm f=0.0421 <S**2>=0.000
24 -> 33 0.15714
32 -> 41 0.65856

[5,1,0]-TDDFT- Triplet

Excitation energies and oscillator strengths:

Excited State 1:	3.055-?Sym	0.7058 eV	1756.75 nm	f=0.0016	<S**2>=2.083
33A -> 34A	0.99424				

Excited State 2:	3.040-?Sym	1.5700 eV	789.70 nm	f=0.0016	<S**2>=2.060
31A -> 34A	0.11917				
31B -> 32B	0.98517				

Excited State 3:	3.051-?Sym	2.1345 eV	580.87 nm	f=0.0052	<S**2>=2.077
31A -> 34A	-0.12465				
33A -> 35A	0.76695				
29B -> 32B	0.14256				
30B -> 32B	-0.59444				

Excited State 4:	3.055-?Sym	2.4296 eV	510.32 nm	f=0.0055	<S**2>=2.083
31A -> 34A	0.11625				
32A -> 34A	-0.17403				
33A -> 35A	0.60219				
29B -> 32B	0.10100				
30B -> 32B	0.74016				
31B -> 33B	-0.11884				

Excited State 5:	3.113-?Sym	3.1266 eV	396.55 nm	f=0.0070	<S**2>=2.173
30A -> 34A	-0.19679				
31A -> 34A	-0.16677				
32A -> 34A	0.42620				
33A -> 35A	-0.10065				
29B -> 32B	0.77515				
30B -> 32B	0.19022				
30B -> 33B	0.13998				
31B -> 33B	0.25168				

Excited State 6:	3.849-?Sym	3.4344 eV	361.00 nm	f=0.0021	<S**2>=3.454
30A -> 34A	0.14512				
31A -> 34A	0.45191				
32A -> 34A	0.75174				
29B -> 32B	-0.11599				

31B -> 33B -0.42276

Excited State 7: 3.412-?Sym 3.5503 eV 349.22 nm f=0.1353 <S**2>=2.661

29A -> 34A 0.12519
30A -> 34A 0.28113
32A -> 34A -0.32771
32A -> 35A 0.13666
33A -> 34A 0.11032
33A -> 35A -0.13089
29B -> 32B 0.53039
30B -> 32B -0.19100
30B -> 33B -0.38125
31B -> 33B -0.48433

Excited State 8: 3.243-?Sym 3.8730 eV 320.13 nm f=0.0016 <S**2>=2.379

30A -> 34A 0.30106
31A -> 34A -0.24880
32A -> 34A 0.14875
28B -> 32B 0.84428
29B -> 32B -0.10610
30B -> 33B -0.26211
31B -> 33B 0.12350

Excited State 9: 3.569-?Sym 3.9275 eV 315.68 nm f=0.0054 <S**2>=2.935

30A -> 34A -0.49124
31A -> 34A 0.24810
32A -> 34A -0.20749
28B -> 32B 0.51244
30B -> 33B 0.44650
30B -> 34B 0.10618
31B -> 33B -0.38494

Excited State 10: 3.048-?Sym 4.1025 eV 302.22 nm f=0.0306 <S**2>=2.073

31A -> 34A 0.72131
32A -> 34A -0.11067
27B -> 32B -0.14324
28B -> 32B 0.13014
29B -> 32B 0.11604
30B -> 32B -0.11575
30B -> 33B -0.17502

31B -> 33B 0.56324

Excited State 11: 3.045-?Sym 4.1955 eV 295.51 nm f=0.0031 <S**2>=2.068
33A -> 36A 0.99397

Excited State 12: 3.734-?Sym 4.5518 eV 272.39 nm f=0.0048 <S**2>=3.235
31A -> 35A -0.18352
32A -> 35A -0.34654
30B -> 33B -0.19450
31B -> 34B 0.87633
31B -> 35B 0.11262

Excited State 13: 3.166-?Sym 4.7415 eV 261.49 nm f=0.0049 <S**2>=2.256
30A -> 34A 0.18379
32A -> 35A -0.61204
33A -> 37A 0.63150
30B -> 33B 0.19272
30B -> 34B -0.16228
31B -> 34B -0.27225
31B -> 35B 0.14371

Excited State 14: 3.152-?Sym 4.7631 eV 260.30 nm f=0.0093 <S**2>=2.235
32A -> 35A 0.53470
33A -> 37A 0.75610
27B -> 32B -0.10583
30B -> 34B 0.15623
31B -> 34B 0.21925
31B -> 35B -0.11604

Excited State 15: 3.152-?Sym 4.9345 eV 251.26 nm f=0.0065 <S**2>=2.233
30A -> 34A -0.43041
30A -> 35A 0.16669
31A -> 35A 0.26093
32A -> 35A -0.13602
33A -> 37A 0.12626
27B -> 32B 0.61218
30B -> 33B -0.45672
30B -> 34B 0.16823
31B -> 34B -0.12943

Excited State 16:	3.135-?Sym	5.0542 eV	245.31 nm	f=0.0098	<S**2>=2.207
30A -> 34A	0.35605				
31A -> 34A	0.14964				
31A -> 35A	0.33173				
32A -> 35A	0.26344				
27B -> 32B	0.57046				
30B -> 33B	0.35726				
30B -> 34B	-0.34261				
31B -> 34B	0.20236				

Excited State 17:	3.311-?Sym	5.1378 eV	241.32 nm	f=0.0029	<S**2>=2.491
31A -> 35A	0.70221				
32A -> 35A	-0.11431				
25B -> 32B	0.18830				
26B -> 32B	0.34947				
27B -> 32B	-0.39426				
29B -> 33B	-0.26555				
31B -> 34B	0.13855				
31B -> 35B	-0.23950				

Excited State 18:	3.090-?Sym	5.2371 eV	236.74 nm	f=0.0033	<S**2>=2.137
31A -> 35A	-0.31488				
32A -> 35A	0.11305				
25B -> 32B	0.12581				
26B -> 32B	0.88565				
27B -> 32B	0.16721				
30B -> 34B	0.12055				
31B -> 35B	0.10756				

Excited State 19:	3.802-?Sym	5.3381 eV	232.26 nm	f=0.0007	<S**2>=3.364
29A -> 34A	0.41328				
30A -> 34A	-0.13081				
30A -> 35A	0.25401				
25B -> 32B	-0.22625				
26B -> 32B	0.22179				
29B -> 33B	0.55143				
30B -> 33B	0.12680				
30B -> 34B	-0.41665				
30B -> 35B	-0.10277				
31B -> 35B	-0.31638				

Excited State 20:	3.077-?Sym	5.3988 eV	229.65 nm	f=0.0070	<S**2>=2.117
29A -> 34A	0.13243				
33A -> 38A	0.88597				
25B -> 32B	-0.12480				
30B -> 34B	-0.19306				
31B -> 35B	0.29447				
Excited State 21:	3.164-?Sym	5.4637 eV	226.92 nm	f=0.0061	<S**2>=2.252
29A -> 34A	-0.15322				
30A -> 35A	0.19198				
31A -> 35A	-0.23775				
33A -> 38A	0.33836				
25B -> 32B	0.62410				
26B -> 32B	-0.13929				
31B -> 35B	-0.55680				
Excited State 22:	3.400-?Sym	5.4961 eV	225.59 nm	f=0.0085	<S**2>=2.641
29A -> 34A	0.24564				
30A -> 35A	-0.18500				
31A -> 34A	-0.11027				
31A -> 35A	0.23841				
25B -> 32B	0.55149				
29B -> 33B	0.52441				
30B -> 34B	0.18683				
31B -> 35B	0.44207				
Excited State 23:	3.454-?Sym	5.5606 eV	222.97 nm	f=0.0419	<S**2>=2.732
28A -> 34A	-0.15604				
29A -> 34A	0.32418				
30A -> 34A	0.24709				
30A -> 35A	-0.32737				
32A -> 35A	-0.17950				
33A -> 38A	0.22310				
33A -> 41A	0.14720				
23B -> 32B	0.11497				
24B -> 32B	0.11898				
25B -> 32B	-0.28254				
27B -> 32B	0.14682				
30B -> 33B	0.11702				
30B -> 34B	0.51646				

30B -> 35B 0.12832
31B -> 35B -0.32690

Excited State 24: 3.622-?Sym 5.6899 eV 217.90 nm f=0.0051 <S**2>=3.029
28A -> 34A 0.75269
29A -> 34A -0.36138
30A -> 35A -0.14356
31A -> 35A 0.10485
33A -> 38A 0.10700
33A -> 39A -0.35199
33A -> 41A 0.10234
28B -> 33B -0.12168
29B -> 33B 0.24806

Excited State 25: 3.235-?Sym 5.7129 eV 217.03 nm f=0.0014 <S**2>=2.366
28A -> 34A 0.42229
29A -> 34A 0.15242
30A -> 35A -0.19631
33A -> 39A 0.81821
33A -> 40A -0.10483
30B -> 35B 0.16041
31B -> 35B -0.10785

Excited State 26: 3.112-?Sym 5.7630 eV 215.14 nm f=0.0079 <S**2>=2.171
28A -> 34A 0.30171
29A -> 34A 0.50185
30A -> 35A -0.12206
33A -> 39A -0.33856
33A -> 40A 0.31559
33A -> 41A -0.46281
25B -> 32B 0.18505
29B -> 33B -0.35179

Excited State 27: 3.052-?Sym 5.8171 eV 213.14 nm f=0.0032 <S**2>=2.079
29A -> 34A -0.17850
33A -> 39A 0.20170
33A -> 40A 0.93332
33A -> 41A 0.14297
29B -> 33B 0.11208

Excited State 28:	3.145-?Sym	5.9109 eV	209.76 nm	f=0.0158	<S**2>=2.223
28A -> 34A	0.25267				
29A -> 34A	0.29613				
30A -> 35A	0.16282				
33A -> 41A	0.71245				
23B -> 32B	-0.13492				
24B -> 32B	-0.20111				
29B -> 33B	-0.24156				
29B -> 34B	0.11389				
30B -> 34B	0.13742				
30B -> 35B	-0.26670				
Excited State 29:	3.383-?Sym	5.9265 eV	209.20 nm	f=0.0634	<S**2>=2.611
28A -> 34A	-0.14680				
30A -> 34A	-0.18411				
30A -> 35A	-0.44665				
31A -> 35A	-0.10234				
33A -> 39A	-0.13968				
33A -> 41A	0.33869				
33A -> 42A	0.13019				
25B -> 32B	0.10852				
28B -> 33B	0.15265				
29B -> 34B	0.23277				
30B -> 33B	-0.18230				
30B -> 34B	-0.33393				
30B -> 35B	0.52496				
31B -> 35B	-0.13131				
Excited State 30:	3.132-?Sym	6.0243 eV	205.81 nm	f=0.0023	<S**2>=2.203
28A -> 34A	0.10621				
23B -> 32B	-0.17081				
24B -> 32B	0.85032				
28B -> 33B	0.32061				
29B -> 34B	0.17439				
30B -> 35B	-0.20969				

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Table S3. The vertical excitation energies and oscillator strengths for the thirty lowest energy triplet excited states of molecule bicyclo[2,1,0]pentan-2-one at the TD-DFT/M06-L/6-311G(d,p).

[2,1,0]-TDDFT- Singlet

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-?Sym	4.8172 eV	257.38 nm	f=0.0006	<S**2>=0.000
22 -> 23		0.70671				
Excited State	2:	Singlet-?Sym	6.4329 eV	192.74 nm	f=0.0390	<S**2>=0.000
20 -> 23		-0.19860				
21 -> 23		0.67155				
Excited State	3:	Singlet-?Sym	7.0585 eV	175.65 nm	f=0.0120	<S**2>=0.000
22 -> 24		0.70636				
Excited State	4:	Singlet-?Sym	7.2836 eV	170.22 nm	f=0.0545	<S**2>=0.000
19 -> 23		-0.15090				
20 -> 23		0.64849				
21 -> 23		0.16778				
Excited State	5:	Singlet-?Sym	7.5446 eV	164.34 nm	f=0.0082	<S**2>=0.000
22 -> 25		0.70571				
Excited State	6:	Singlet-?Sym	7.7287 eV	160.42 nm	f=0.0047	<S**2>=0.000
19 -> 23		-0.10220				
22 -> 26		0.69704				
Excited State	7:	Singlet-?Sym	8.1116 eV	152.85 nm	f=0.0075	<S**2>=0.000
19 -> 23		-0.17698				
22 -> 27		0.68078				
Excited State	8:	Singlet-?Sym	8.2223 eV	150.79 nm	f=0.0152	<S**2>=0.000
18 -> 23		0.27247				
19 -> 23		0.59564				
21 -> 24		0.10591				
22 -> 27		0.16071				
Excited State	9:	Singlet-?Sym	8.3299 eV	148.84 nm	f=0.432	<S**2>=0.000
22 -> 28		0.70078				

Excited State 10:	Singlet-?Sym	8.4613 eV	146.53 nm	f=0.0140	<S**2>=0.000
21 -> 24	0.68071				
Excited State 11:	Singlet-?Sym	8.7527 eV	141.65 nm	f=0.0334	<S**2>=0.000
18 -> 23	-0.10297				
22 -> 29	0.68099				
Excited State 12:	Singlet-?Sym	8.9718 eV	138.19 nm	f=0.0410	<S**2>=0.000
17 -> 23	-0.30670				
21 -> 25	0.62942				
Excited State 13:	Singlet-?Sym	9.0045 eV	137.69 nm	f=0.0119	<S**2>=0.000
17 -> 23	0.57942				
18 -> 23	-0.19254				
21 -> 25	0.29792				
22 -> 30	-0.13678				
Excited State 14:	Singlet-?Sym	9.1227 eV	135.91 nm	f=0.0221	<S**2>=0.000
16 -> 23	-0.28764				
17 -> 23	0.21307				
18 -> 23	0.42516				
19 -> 23	-0.12990				
22 -> 30	0.37069				
Excited State 15:	Singlet-?Sym	9.1844 eV	134.99 nm	f=0.0101	<S**2>=0.000
20 -> 24	0.68011				
22 -> 30	0.10022				
Excited State 16:	Singlet-?Sym	9.2889 eV	133.48 nm	f=0.0055	<S**2>=0.000
16 -> 23	0.47656				
21 -> 26	0.22669				
22 -> 30	0.44728				
Excited State 17:	Singlet-?Sym	9.4211 eV	131.60 nm	f=0.0394	<S**2>=0.000
16 -> 23	-0.10659				
20 -> 25	0.10266				
21 -> 26	0.31439				
21 -> 27	0.56761				
21 -> 28	0.15853				

22 -> 30 -0.12709

Excited State 18: Singlet-?Sym 9.5476 eV 129.86 nm f=0.0556 <S**2>=0.000
20 -> 25 -0.29123
20 -> 26 -0.11295
21 -> 26 -0.34780
21 -> 27 0.39482
21 -> 28 -0.30652

Excited State 19: Singlet-?Sym 9.6608 eV 128.34 nm f=0.0160 <S**2>=0.000
20 -> 25 0.60842
21 -> 26 -0.11476
21 -> 28 -0.32084

Excited State 20: Singlet-?Sym 9.7983 eV 126.54 nm f=0.1467 <S**2>=0.000
15 -> 23 0.14819
16 -> 23 0.34294
18 -> 23 0.29958
19 -> 23 -0.15289
20 -> 23 -0.10622
20 -> 24 0.10342
20 -> 26 0.19409
21 -> 29 0.10020
22 -> 30 -0.28010
22 -> 32 -0.13707

Excited State 21: Singlet-?Sym 9.8429 eV 125.96 nm f=0.0182 <S**2>=0.000
16 -> 23 0.10573
20 -> 25 0.16395
20 -> 26 -0.12452
21 -> 26 -0.33245
21 -> 28 0.50139
21 -> 30 0.10968
22 -> 31 -0.14072

Excited State 22: Singlet-?Sym 9.9827 eV 124.20 nm f=0.0405 <S**2>=0.000
18 -> 23 -0.13406
20 -> 26 0.59599
20 -> 27 0.21737
21 -> 26 -0.12674

Excited State 23:	Singlet-?Sym	10.1119 eV	122.61 nm	f=0.0059	<S**2>=0.000
21 -> 29	0.67545				
22 -> 31	-0.13612				
Excited State 24:	Singlet-?Sym	10.1947 eV	121.62 nm	f=0.0058	<S**2>=0.000
20 -> 27	0.24190				
21 -> 29	0.10049				
22 -> 31	0.63188				
Excited State 25:	Singlet-?Sym	10.2542 eV	120.91 nm	f=0.0228	<S**2>=0.000
19 -> 24	-0.10805				
20 -> 26	-0.14324				
20 -> 27	0.59637				
20 -> 28	-0.16077				
21 -> 26	0.12484				
21 -> 30	-0.11989				
22 -> 31	-0.19322				
Excited State 26:	Singlet-?Sym	10.3860 eV	119.38 nm	f=0.0221	<S**2>=0.000
19 -> 24	0.63091				
22 -> 32	-0.27357				
Excited State 27:	Singlet-?Sym	10.5102 eV	117.97 nm	f=0.0778	<S**2>=0.000
15 -> 23	0.16559				
19 -> 24	0.20666				
20 -> 28	0.15343				
21 -> 30	-0.18434				
22 -> 32	0.56892				
Excited State 28:	Singlet-?Sym	10.6160 eV	116.79 nm	f=0.0961	<S**2>=0.000
20 -> 26	-0.12523				
20 -> 27	0.11163				
20 -> 28	0.62242				
20 -> 29	-0.11558				
21 -> 30	0.10121				
22 -> 32	-0.13431				
Excited State 29:	Singlet-?Sym	10.6932 eV	115.95 nm	f=0.0475	<S**2>=0.000
15 -> 23	-0.17435				

19 -> 24 0.10442

21 -> 30 0.60257

22 -> 32 0.16793

Excited State 30: Singlet-?Sym 10.7714 eV 115.10 nm f=0.0214 <S**2>=0.000

15 -> 23 0.49307

18 -> 23 -0.10102

18 -> 24 -0.20178

20 -> 29 -0.32164

21 -> 30 0.18871

[2,1,0]-TDDFT- Triplet

Excitation energies and oscillator strengths:

Excited State 1: 3.009-?Sym 1.5236 eV 813.74 nm f=0.0005 <S**2>=2.013

20B -> 22B 0.12096

21B -> 22B 0.99039

Excited State 2: 3.008-?Sym 2.2126 eV 560.35 nm f=0.0008 <S**2>=2.012

19B -> 22B -0.11110

20B -> 22B 0.98118

21B -> 22B -0.12926

Excited State 3: 3.009-?Sym 3.3141 eV 374.12 nm f=0.0016 <S**2>=2.014

23A -> 24A 0.99140

Excited State 4: 3.007-?Sym 3.3318 eV 372.12 nm f=0.0002 <S**2>=2.011

18B -> 22B 0.25262

19B -> 22B 0.95076

20B -> 22B 0.13573

Excited State 5: 3.008-?Sym 3.6922 eV 335.80 nm f=0.0021 <S**2>=2.012

23A -> 25A 0.98327

23A -> 26A 0.15600

Excited State 6: 3.012-?Sym 3.7777 eV 328.20 nm f=0.0087 <S**2>=2.018

23A -> 25A -0.12792

23A -> 26A 0.89901

18B -> 22B -0.36378
19B -> 22B 0.14836

Excited State 7: 3.009-?Sym 3.8634 eV 320.92 nm f=0.0152 <S**2>=2.013
23A -> 26A 0.36634
17B -> 22B 0.15635
18B -> 22B 0.87734
19B -> 22B -0.22790

Excited State 8: 3.009-?Sym 4.3804 eV 283.04 nm f=0.0019 <S**2>=2.013
23A -> 27A 0.93498
23A -> 28A -0.12501
16B -> 22B -0.12818
17B -> 22B -0.29399

Excited State 9: 3.010-?Sym 4.4688 eV 277.45 nm f=0.0016 <S**2>=2.016
23A -> 27A 0.19560
23A -> 28A 0.94855
16B -> 22B 0.15602
17B -> 22B 0.14979

Excited State 10: 3.009-?Sym 4.5445 eV 272.82 nm f=0.0431 <S**2>=2.014
23A -> 26A -0.10828
23A -> 27A 0.26632
23A -> 28A -0.25268
23A -> 29A 0.11261
16B -> 22B 0.51040
17B -> 22B 0.73584
18B -> 22B -0.14290

Excited State 11: 3.007-?Sym 4.7455 eV 261.27 nm f=0.0353 <S**2>=2.011
23A -> 30A 0.15779
16B -> 22B 0.80715
17B -> 22B -0.51837

Excited State 12: 3.009-?Sym 4.8344 eV 256.46 nm f=0.0056 <S**2>=2.013
23A -> 28A 0.12075
23A -> 29A 0.98380
16B -> 22B -0.10113

Excited State 13: 3.010-?Sym 5.3503 eV 231.73 nm f=0.0230 <S**2>=2.015

23A -> 30A	0.97445
16B -> 22B	-0.10655

Excited State 14: 3.008-?Sym 5.8016 eV 213.71 nm f=0.0003 <S**2>=2.012

14B -> 22B	0.10951
15B -> 22B	0.98760

Excited State 15: 3.010-?Sym 6.2928 eV 197.02 nm f=0.0074 <S**2>=2.016

23A -> 31A	0.88213
23A -> 32A	-0.18116
14B -> 22B	0.41097

Excited State 16: 3.013-?Sym 6.4140 eV 193.30 nm f=0.0272 <S**2>=2.019

23A -> 31A	-0.39921
14B -> 22B	0.85440
20B -> 23B	-0.13448
21B -> 23B	-0.22110

Excited State 17: 3.011-?Sym 6.5025 eV 190.67 nm f=0.0017 <S**2>=2.017

23A -> 31A	0.16728
23A -> 32A	0.95655
14B -> 22B	0.10065
21B -> 23B	-0.16866

Excited State 18: 3.048-?Sym 6.9034 eV 179.60 nm f=0.0411 <S**2>=2.073

23A -> 32A	0.13004
13B -> 22B	-0.23446
14B -> 22B	0.13720
20B -> 23B	-0.18831
21B -> 23B	0.90462

Excited State 19: 3.011-?Sym 7.0009 eV 177.10 nm f=0.0195 <S**2>=2.017

13B -> 22B	0.96119
20B -> 23B	-0.10814
21B -> 23B	0.19394

Excited State 20: 3.011-?Sym 7.2146 eV 171.85 nm f=0.0109 <S**2>=2.017

23A -> 33A	0.97997
20B -> 23B	-0.15193

Excited State 21:	3.058-?Sym	7.6793 eV	161.45 nm	f=0.0665	<S**2>=2.088
23A -> 33A	0.12404				
14B -> 22B	0.11571				
19B -> 23B	0.14279				
20B -> 23B	0.92339				
21B -> 23B	0.14646				
Excited State 22:	3.187-?Sym	7.8723 eV	157.50 nm	f=0.0014	<S**2>=2.290
22A -> 24A	0.10707				
22A -> 26A	-0.14340				
23A -> 34A	0.91516				
21B -> 24B	-0.21406				
21B -> 26B	-0.20480				
Excited State 23:	3.931-?Sym	7.9987 eV	155.00 nm	f=0.0018	<S**2>=3.613
21A -> 24A	0.10320				
21A -> 26A	-0.13951				
22A -> 24A	-0.32457				
22A -> 25A	-0.18271				
22A -> 26A	0.36015				
23A -> 34A	0.38026				
21B -> 24B	0.58462				
21B -> 26B	0.38499				
21B -> 28B	-0.10584				
Excited State 24:	3.019-?Sym	8.2980 eV	149.42 nm	f=0.0159	<S**2>=2.029
12B -> 22B	0.98617				
Excited State 25:	3.774-?Sym	8.4029 eV	147.55 nm	f=0.0088	<S**2>=3.311
21A -> 26A	0.10169				
22A -> 25A	0.21284				
22A -> 26A	-0.32788				
23A -> 35A	0.10041				
21B -> 24B	0.72988				
21B -> 26B	-0.48402				
21B -> 28B	0.11928				
Excited State 26:	3.375-?Sym	8.5751 eV	144.59 nm	f=0.0047	<S**2>=2.598
22A -> 24A	0.91802				

22A -> 25A -0.13403
22A -> 26A 0.20544
19B -> 23B -0.11145
21B -> 24B 0.19801
21B -> 26B 0.13685

Excited State 27: 3.049-?Sym 8.6605 eV 143.16 nm f=0.0037 <S**2>=2.074
22A -> 26A 0.10562
23A -> 35A 0.95522
19B -> 23B -0.16509

Excited State 28: 3.427-?Sym 8.7613 eV 141.51 nm f=0.0048 <S**2>=2.686
20A -> 24A 0.12979
21A -> 24A 0.79501
22A -> 26A -0.14120
23A -> 35A 0.18121
19B -> 23B 0.22829
20B -> 24B -0.37574
21B -> 25B 0.18745

Excited State 29: 3.671-?Sym 8.7925 eV 141.01 nm f=0.0196 <S**2>=3.119
21A -> 24A -0.20812
22A -> 25A -0.14180
18B -> 23B 0.10915
19B -> 23B -0.23190
21B -> 25B 0.91137

Excited State 30: 3.070-?Sym 8.8601 eV 139.94 nm f=0.0342 <S**2>=2.106
21A -> 24A -0.36552
21A -> 25A 0.11689
21A -> 26A -0.12645
23A -> 35A 0.14632
18B -> 23B -0.21578
19B -> 23B 0.82191
21B -> 25B 0.15671

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[4,1,0]-TDDFT- Singlet

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-?Sym	4.4165 eV	280.73 nm	f=0.0018	<S**2>=0.000
29 -> 30		0.70504				
Excited State	2:	Singlet-?Sym	5.0346 eV	246.26 nm	f=0.0039	<S**2>=0.000
28 -> 30		-0.18257				
28 -> 31		0.14529				
29 -> 31		0.66494				
Excited State	3:	Singlet-?Sym	5.2730 eV	235.13 nm	f=0.0088	<S**2>=0.000
28 -> 30		0.66407				
28 -> 31		0.18228				
29 -> 31		0.14607				
Excited State	4:	Singlet-?Sym	6.4504 eV	192.21 nm	f=0.0041	<S**2>=0.000
29 -> 32		0.70131				
Excited State	5:	Singlet-?Sym	6.4973 eV	190.82 nm	f=0.0502	<S**2>=0.000
27 -> 30		0.36571				
27 -> 31		-0.19770				
28 -> 30		-0.12691				
28 -> 31		0.51355				
29 -> 31		-0.11388				
Excited State	6:	Singlet-?Sym	6.8742 eV	180.36 nm	f=0.0063	<S**2>=0.000
29 -> 33		0.70051				
Excited State	7:	Singlet-?Sym	7.0496 eV	175.87 nm	f=0.0887	<S**2>=0.000
26 -> 31		-0.10468				
27 -> 30		-0.23543				
27 -> 31		0.55209				
28 -> 31		0.29875				
Excited State	8:	Singlet-?Sym	7.1823 eV	172.62 nm	f=0.2105	<S**2>=0.000
23 -> 30		0.10657				
24 -> 30		-0.10453				
27 -> 30		0.49389				
27 -> 31		0.36244				
28 -> 31		-0.19628				
28 -> 32		-0.10654				

Excited State 9:	Singlet-?Sym	7.3064 eV	169.69 nm	f=0.0024	<S**2>=0.000
28 -> 32	0.69330				
Excited State 10:	Singlet-?Sym	7.4588 eV	166.23 nm	f=0.0144	<S**2>=0.000
29 -> 34	0.69798				
Excited State 11:	Singlet-?Sym	7.5795 eV	163.58 nm	f=0.0069	<S**2>=0.000
26 -> 30	0.66722				
26 -> 31	0.11435				
Excited State 12:	Singlet-?Sym	7.7173 eV	160.66 nm	f=0.0140	<S**2>=0.000
28 -> 33	0.69177				
Excited State 13:	Singlet-?Sym	7.8830 eV	157.28 nm	f=0.0157	<S**2>=0.000
23 -> 30	0.15337				
25 -> 30	0.68333				
Excited State 14:	Singlet-?Sym	8.0948 eV	153.17 nm	f=0.0237	<S**2>=0.000
29 -> 35	0.69425				
Excited State 15:	Singlet-?Sym	8.2287 eV	150.67 nm	f=0.0125	<S**2>=0.000
23 -> 30	0.15895				
24 -> 30	0.64104				
26 -> 31	0.19254				
Excited State 16:	Singlet-?Sym	8.2473 eV	150.33 nm	f=0.0180	<S**2>=0.000
26 -> 31	-0.35600				
28 -> 34	0.57669				
Excited State 17:	Singlet-?Sym	8.3524 eV	148.44 nm	f=0.0263	<S**2>=0.000
23 -> 30	-0.14092				
24 -> 31	-0.11974				
25 -> 31	-0.18247				
26 -> 31	0.39600				
27 -> 32	0.15165				
28 -> 34	0.36312				
29 -> 36	-0.25763				
Excited State 18:	Singlet-?Sym	8.4561 eV	146.62 nm	f=0.0170	<S**2>=0.000
25 -> 31	-0.10934				

26 -> 31 0.10299
27 -> 32 0.30861
29 -> 36 0.60492

Excited State 19: Singlet-?Sym 8.4834 eV 146.15 nm f=0.0094 <S**2>=0.000
25 -> 31 0.17976
26 -> 31 -0.17534
27 -> 32 0.59878
29 -> 36 -0.21382

Excited State 20: Singlet-?Sym 8.5258 eV 145.42 nm f=0.0356 <S**2>=0.000
23 -> 31 0.12073
25 -> 31 0.61251
26 -> 31 0.16295
28 -> 34 0.11628
29 -> 37 -0.11087

Excited State 21: Singlet-?Sym 8.6010 eV 144.15 nm f=0.0061 <S**2>=0.000
23 -> 30 0.12602
25 -> 31 0.13504
29 -> 37 0.67196

Excited State 22: Singlet-?Sym 8.7264 eV 142.08 nm f=0.0031 <S**2>=0.000
22 -> 30 0.51551
23 -> 31 0.13925
24 -> 31 0.29390
29 -> 38 0.33743

Excited State 23: Singlet-?Sym 8.7325 eV 141.98 nm f=0.0053 <S**2>=0.000
22 -> 30 0.42358
23 -> 30 -0.20130
23 -> 31 0.10319
24 -> 31 -0.35176
29 -> 38 -0.35404

Excited State 24: Singlet-?Sym 8.8179 eV 140.61 nm f=0.0053 <S**2>=0.000
22 -> 30 -0.17188
23 -> 30 -0.27415
23 -> 31 0.48276
24 -> 31 0.31206

29 -> 38 -0.18400

Excited State 25: Singlet-?Sym 8.8836 eV 139.57 nm f=0.0061 <S**2>=0.000
27 -> 33 0.68514

Excited State 26: Singlet-?Sym 8.9006 eV 139.30 nm f=0.0140 <S**2>=0.000
23 -> 30 0.11709
24 -> 31 0.25737
28 -> 35 0.58158
29 -> 38 -0.19951

Excited State 27: Singlet-?Sym 8.9591 eV 138.39 nm f=0.0864 <S**2>=0.000
23 -> 30 -0.14732
23 -> 31 0.16039
24 -> 31 -0.22232
26 -> 31 -0.16511
27 -> 33 0.15729
28 -> 35 0.36690
28 -> 36 -0.11986
29 -> 38 0.36096
29 -> 40 0.10423

Excited State 28: Singlet-?Sym 9.1145 eV 136.03 nm f=0.0152 <S**2>=0.000
23 -> 30 -0.15324
23 -> 31 -0.18493
29 -> 39 0.63603

Excited State 29: Singlet-?Sym 9.2783 eV 133.63 nm f=0.0308 <S**2>=0.000
22 -> 31 -0.15173
23 -> 30 0.18403
23 -> 31 0.20966
28 -> 36 0.52741
28 -> 37 0.13450
28 -> 38 0.10984
29 -> 39 0.19509

Excited State 30: Singlet-?Sym 9.3475 eV 132.64 nm f=0.0685 <S**2>=0.000
20 -> 30 0.13658
22 -> 31 0.40612
23 -> 30 -0.23105

23 -> 31 -0.17110

28 -> 36 0.38753

29 -> 39 -0.11022

Table S4. The vertical excitation energies and oscillator strengths for the thirty lowest energy triplet excited states of molecule bicyclo[4,1,0]hept-4-en-2-one at the TD-DFT/M06-L/6-311G(d,p).

[4,1.0]-TDDFT- Triplet

Excitation energies and oscillator strengths:

Excited State 1: 3.007-?Sym 1.0687 eV 1160.09 nm f=0.0006 <S**2>=2.011

30A -> 31A 0.89338

28B -> 29B -0.45040

Excited State 2: 3.008-?Sym 1.4790 eV 838.31 nm f=0.0076 <S**2>=2.011

30A -> 31A 0.44229

27B -> 29B -0.21672

28B -> 29B 0.86958

Excited State 3: 3.007-?Sym 2.0528 eV 603.99 nm f=0.0051 <S**2>=2.011

24B -> 29B -0.10985

27B -> 29B 0.96781

28B -> 29B 0.19891

Excited State 4: 3.008-?Sym 2.8508 eV 434.92 nm f=0.0008 <S**2>=2.012

30A -> 32A 0.99880

Excited State 5: 3.011-?Sym 3.3320 eV 372.10 nm f=0.0045 <S**2>=2.017

30A -> 33A 0.42205

24B -> 29B 0.19415

25B -> 29B 0.23378

26B -> 29B 0.84265

Excited State 6: 3.008-?Sym 3.3973 eV 364.95 nm f=0.0040 <S**2>=2.012

30A -> 33A 0.90453

25B -> 29B -0.16273

26B -> 29B -0.37428

Excited State 7:	3.008-?Sym	3.6161 eV	342.87 nm	f=0.0562	<S**2>=2.012
24B -> 29B	0.41139				
25B -> 29B	0.82934				
26B -> 29B	-0.34747				
Excited State 8:	3.008-?Sym	3.8645 eV	320.83 nm	f=0.0044	<S**2>=2.012
30A -> 34A	0.99524				
Excited State 9:	3.011-?Sym	3.9957 eV	310.29 nm	f=0.0039	<S**2>=2.017
23B -> 29B	-0.51095				
24B -> 29B	0.74465				
25B -> 29B	-0.40361				
Excited State 10:	3.596-?Sym	4.1611 eV	297.96 nm	f=0.0087	<S**2>=2.982
29A -> 31A	0.53417				
23B -> 29B	0.53816				
24B -> 29B	0.30731				
25B -> 29B	-0.16240				
28B -> 30B	0.49481				
Excited State 11:	3.475-?Sym	4.2012 eV	295.12 nm	f=0.0033	<S**2>=2.769
29A -> 31A	-0.45344				
22B -> 29B	-0.12034				
23B -> 29B	0.64693				
24B -> 29B	0.30483				
25B -> 29B	-0.14833				
28B -> 30B	-0.43515				
28B -> 31B	-0.11964				
Excited State 12:	3.009-?Sym	4.4415 eV	279.15 nm	f=0.0134	<S**2>=2.013
30A -> 35A	0.99094				
Excited State 13:	3.009-?Sym	4.7282 eV	262.23 nm	f=0.0117	<S**2>=2.013
30A -> 36A	0.16270				
22B -> 29B	0.96529				
23B -> 29B	0.10934				
Excited State 14:	3.008-?Sym	4.8512 eV	255.57 nm	f=0.0107	<S**2>=2.012
30A -> 36A	0.98191				

22B -> 29B -0.14455

Excited State 15: 3.009-?Sym 4.9363 eV 251.17 nm f=0.0086 <S**2>=2.013
30A -> 37A 0.98574
30A -> 38A 0.13446

Excited State 16: 3.010-?Sym 5.0827 eV 243.94 nm f=0.0163 <S**2>=2.015
30A -> 37A -0.11842
30A -> 38A 0.96632
21B -> 29B -0.15899

Excited State 17: 3.007-?Sym 5.2012 eV 238.38 nm f=0.0009 <S**2>=2.011
30A -> 38A 0.14263
21B -> 29B 0.97696

Excited State 18: 3.010-?Sym 5.4676 eV 226.76 nm f=0.0091 <S**2>=2.015
30A -> 39A 0.98189

Excited State 19: 3.010-?Sym 5.7881 eV 214.21 nm f=0.0007 <S**2>=2.016
30A -> 40A 0.15006
20B -> 29B 0.98510

Excited State 20: 3.015-?Sym 5.9458 eV 208.52 nm f=0.0092 <S**2>=2.023
30A -> 40A 0.94777
20B -> 29B -0.13319
27B -> 30B -0.10294
28B -> 31B -0.21858

Excited State 21: 3.033-?Sym 6.1173 eV 202.68 nm f=0.0338 <S**2>=2.050
28A -> 31A -0.15925
29A -> 31A 0.34930
30A -> 40A 0.19372
18B -> 29B -0.13696
27B -> 30B 0.11375
28B -> 30B -0.51657
28B -> 31B 0.69110

Excited State 22: 3.262-?Sym 6.3246 eV 196.04 nm f=0.0164 <S**2>=2.411
28A -> 31A 0.55120

29A -> 31A -0.38092
18B -> 29B 0.11611
19B -> 29B 0.22766
27B -> 30B -0.32553
28B -> 30B 0.19515
28B -> 31B 0.55528

Excited State 23: 3.060-?Sym 6.5136 eV 190.35 nm f=0.0048 <S**2>=2.092
28A -> 31A -0.26705
19B -> 29B 0.94205
27B -> 30B 0.16670

Excited State 24: 3.426-?Sym 6.5752 eV 188.56 nm f=0.0035 <S**2>=2.684
27A -> 31A 0.17524
28A -> 31A 0.54703
27B -> 30B 0.77684
28B -> 30B -0.12902
28B -> 31B -0.10744

Excited State 25: 3.012-?Sym 6.7126 eV 184.70 nm f=0.0042 <S**2>=2.018
30A -> 41A 0.96052
30A -> 42A 0.19573
18B -> 29B -0.12681

Excited State 26: 3.478-?Sym 6.7639 eV 183.30 nm f=0.0481 <S**2>=2.773
27A -> 31A -0.40045
28A -> 31A 0.46788
29A -> 31A 0.29520
17B -> 29B 0.12299
18B -> 29B -0.37062
19B -> 29B 0.19675
27B -> 30B -0.30591
27B -> 31B -0.24050
28B -> 30B -0.26697
28B -> 31B -0.26747

Excited State 27: 3.128-?Sym 6.8904 eV 179.94 nm f=0.0155 <S**2>=2.196
27A -> 31A -0.51389
30A -> 42A 0.59075
18B -> 29B 0.58139

27B -> 30B 0.10972

Excited State 28: 3.048-?Sym 6.9125 eV 179.36 nm f=0.0100 <S**2>=2.072

27A -> 31A 0.39569

30A -> 41A -0.19328

30A -> 42A 0.76898

18B -> 29B -0.40288

27B -> 30B -0.13250

27B -> 31B -0.11538

Excited State 29: 3.160-?Sym 7.0603 eV 175.61 nm f=0.1031 <S**2>=2.246

27A -> 31A 0.58102

28A -> 31A 0.15550

29A -> 31A 0.21475

17B -> 29B 0.22362

18B -> 29B 0.46517

26B -> 30B 0.22603

27B -> 30B -0.26674

28B -> 30B -0.28905

28B -> 31B -0.15441

28B -> 32B 0.15018

Excited State 30: 3.693-?Sym 7.1014 eV 174.59 nm f=0.0002 <S**2>=3.159

29A -> 32A 0.74428

17B -> 29B 0.43367

27B -> 31B 0.17195

28B -> 32B -0.46377

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(All were calculated at the M06-L/6-311G(d,p) level of theory)

1. [2.1.0]-Rea-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.062254	1.728094	1.083829
6	0.161597	1.242023	0.108664
6	0.881459	-0.115814	0.036502
6	-0.344999	-0.834721	-0.395490
6	-1.492238	-0.502530	0.536245
6	-1.073214	0.530232	-0.428228
1	0.628889	1.941831	-0.588492
1	-0.401576	-1.680277	-1.071300
1	-1.303993	-0.364836	1.597873
1	-2.402550	-1.046996	0.312783
1	-1.705884	0.883826	-1.231870
8	2.040905	-0.422097	0.093878

M06L/6-311G**=-269.3424228

2. [2.1.0]-Min-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.404225	1.476075	1.224908
6	0.157721	1.264171	0.179857
6	0.936353	0.016914	-0.437500
6	-0.435182	-0.622715	-0.688091
6	-1.204716	-0.750949	0.590784
6	-1.150666	0.570795	-0.105252
1	0.361893	2.135860	-0.446452
1	-0.650503	-1.189891	-1.588155
1	-0.672442	-0.903480	1.525617
1	-2.144199	-1.288269	0.509310

1	-2.035955	1.061147	-0.492817
8	1.864491	-0.520092	0.253600

M06L/6-311G**=-269.2186183

3. [2.1.0]-TS1-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.135389	1.647081	1.154366
6	0.069286	1.311548	0.111267
6	0.878716	0.093590	-0.256813
6	-0.202979	-0.881627	-0.462114
6	-1.338427	-0.717851	0.477631
6	-1.217943	0.590980	-0.209286
1	0.261224	2.171589	-0.535518
1	-0.067409	-1.782207	-1.068145
1	-1.119051	-0.738522	1.551269
1	-2.233199	-1.288134	0.235226
1	-1.911138	0.888153	-0.989062
8	1.975284	-0.409724	0.210970

M06L/6-311G**=-269.2087198

4. [2.1.0]-T_1/S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.2668176	1.4694264	1.2193941
6	0.0405242	1.2649508	0.1615781
6	0.8508264	-0.0099529	-0.2533808
6	-0.0554368	-1.1082314	-0.1847237
6	-1.4015880	-0.6743360	0.3250196
6	-1.3176383	0.7628839	-0.0717725
1	0.3340924	2.1399063	-0.4201569
1	0.2125592	-2.1234334	-0.4603893

1	-1.4979768	-0.8145246	1.4172355
1	-2.2330755	-1.2191000	-0.1324541
1	-1.9962194	1.1980349	-0.7980319
8	2.0268680	-0.0007479	-0.5825273

Difference Gradient:

-1	-0.00298545	0.00078381	0.00118264
-2	0.03568009	-0.04733247	-0.04149544
-3	0.03601199	0.09802474	0.01019743
-4	-0.02167526	-0.08749204	0.04307891
-5	0.03076184	0.00665262	-0.08791323
-6	-0.10440334	0.06606497	0.05833341
-7	0.00294934	-0.00241112	0.00136648
-8	0.00822724	-0.00284590	0.00871035
-9	0.01123299	-0.00158419	-0.00234907
-10	0.00200323	-0.00169255	0.00315180
-11	-0.00255486	-0.00013213	0.00927861
-12	0.00475218	-0.02803574	-0.00354188

M06L/6-311G**=-269.2787403670

5. [2.1.0]-Int1-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.236290	1.437508	1.165194
6	-0.021125	1.204107	0.103818
6	0.890790	-0.109843	-0.019957
6	-0.008839	-1.184879	0.108485
6	-1.391125	-0.712303	-0.020862
6	-1.384000	0.757100	-0.015683
1	0.241107	2.107317	-0.479911
1	0.282536	-2.228183	0.094232
1	-2.114996	-1.208733	0.661548
1	-1.866772	-0.918613	-1.016711
1	-2.184602	1.341539	-0.466948
8	2.111529	-0.031990	-0.111526

M06L/6-311G**=-269.2695437

6. [2.1.0]-TS2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.227106	1.993868	0.638523
6	-0.053963	1.186816	-0.042863
6	0.886665	-0.058376	-0.009404
6	0.016088	-1.192591	-0.137586
6	-1.375400	-0.720505	-0.017060
6	-1.439686	0.695550	0.020283
1	0.101396	1.589229	-1.059433
1	0.302905	-2.227683	-0.016540
1	-1.089295	-0.768872	1.091166
1	-2.241063	-1.358077	-0.170365
1	-2.343826	1.280662	0.108261
8	2.105070	0.003188	0.066020

M06L/6-311G**=-269.2685487

7. [2.1.0]-Int2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.179843	-1.862466	-0.870957
6	-0.045290	-1.235296	0.000255
6	0.854064	-0.000185	-0.000181
6	-0.045188	1.235341	0.000126
6	-1.426922	0.667511	0.000274
6	-1.426902	-0.667406	-0.000412
1	0.178789	-1.860146	0.873596
1	-2.319062	1.284007	-0.000208
1	-2.318951	-1.283818	-0.001039
8	2.057652	-0.000000	-0.000199
1	0.180208	1.861516	0.872096
1	0.179379	1.861114	-0.872269

M06L/6-311G**=-269.3741087

8. [2.1.0]-TS3-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.233956	-1.762333	1.094491
6	0.237781	-1.240933	0.127092
6	-0.749776	-0.120382	0.129923
6	-0.121147	1.149693	0.122919
6	1.302005	0.851770	-0.100053
6	1.519131	-0.477439	-0.106787
1	-0.003470	-1.992793	-0.630280
1	2.072989	1.603077	-0.226376
1	2.473943	-0.967623	-0.246345
8	-1.997586	-0.104241	-0.170000
1	-0.452047	1.917561	0.820220
1	-1.472641	1.059787	-0.490275

M06L/6-311G**=-269.2575784

9. [2.1.0]-Pro-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.054665	-1.794181	-0.875336
6	-0.148991	-1.165078	-0.000056
6	0.717608	0.049466	-0.000096
6	-0.041381	1.167897	-0.000054
6	-1.439470	0.752257	-0.000050
6	-1.531036	-0.591024	-0.000024
1	0.053918	-1.793721	0.875729
1	-2.272977	1.445065	0.000577
1	-2.433559	-1.185521	-0.000068
8	2.059535	-0.112771	0.000148

1	0.312551	2.191660	-0.000014
1	2.468750	0.757752	-0.000389

M06L/6-311G**=-269.3552506

10. [3.1.0]-Rea-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.208121	-0.915486	-0.401950
6	-1.343459	0.062417	-0.436285
6	-0.745748	1.370459	-0.067747
6	0.566181	1.268540	0.189300
6	1.025785	-0.121622	-0.050348
1	-0.122312	-1.746757	-1.089216
1	-2.139306	0.001340	-1.168943
1	-1.340706	2.273430	0.026059
1	1.226684	2.053518	0.534274
8	2.159725	-0.541915	0.005941
1	-1.032545	-0.623677	1.661534
6	-1.278663	-0.967146	0.661730
1	-1.965460	-1.805505	0.620562

M06L/6-311G**=-307.4613456

11. [3.1.0]-Min-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.171702	-0.892845	-0.438382
6	-1.391826	0.074856	-0.348246
6	-0.864757	1.374937	0.016254
6	0.567884	1.264704	0.214467
6	1.019840	-0.039944	-0.105286
1	-0.074162	-1.647808	-1.212867
1	-2.221665	-0.012685	-1.040917

1	-1.316883	2.296272	-0.335663
1	1.221007	2.036153	0.605296
8	2.170551	-0.513858	0.002194
1	-0.935445	-0.828653	1.650412
6	-1.187718	-1.083682	0.627491
1	-1.867581	-1.920571	0.518394

M06L/6-311G**=-307.3620635

12. [3.1.0]-TS1-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.043795	-0.997082	-0.374302
6	-1.511906	0.099106	-0.290257
6	-0.910618	1.344465	-0.067408
6	0.489084	1.239713	0.293483
6	1.044697	-0.050532	-0.048407
1	-2.333301	-0.005490	-0.993714
1	-1.279543	2.233923	-0.573204
1	1.112322	2.061306	0.632543
8	2.239806	-0.376405	-0.052270
1	-0.982421	-0.883473	1.612205
6	-1.184045	-1.085485	0.562284
1	-1.843840	-1.935764	0.420830
1	0.107830	-1.760374	-1.132861

M06L/6-311G**=-307.3561242

13. [3.1.0]-T_1/S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.1039655	-1.1767570	-0.2199149
6	-1.6284373	0.1712019	-0.2729193
6	-0.8481349	1.3413351	-0.1113604

6	0.4727571	1.2259968	0.2308854
6	1.0737323	-0.0981495	-0.0310443
1	-2.4858862	0.1471980	-0.9396488
1	-1.3045058	2.3101814	-0.3024225
1	1.1222204	2.0660553	0.4477604
8	2.2808615	-0.2704587	-0.1721451
1	-1.1268972	-0.8902423	1.5431197
6	-1.2107473	-1.0596133	0.4613617
1	-1.8635090	-1.9133424	0.2832330
1	0.3188507	-1.9694973	-0.9279830

Difference Gradient:

-1	0.07812556	-0.03106805	0.04185071
-2	-0.06184664	0.10680229	0.04551076
-3	-0.08876106	-0.03201168	-0.02126604
-4	0.03879369	-0.04887777	0.01261781
-5	-0.02284862	0.00299075	0.00980108
-6	-0.01703988	0.01141926	0.02017030
-7	0.00403556	-0.00215477	-0.01339830
-8	0.00212659	0.00222937	-0.00490843
-9	0.03887593	-0.00287987	-0.00801049
-10	0.00429792	0.00539612	-0.00704953
-11	0.01285784	0.00120994	-0.08915680
-12	-0.00147968	-0.00011963	-0.00000779
-13	0.01286278	-0.01293595	0.01384672

M06L/6-311G**=-307.3828399800

14. [3.1.0]-Int1-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.326915	-1.192373	0.026796
6	1.819725	0.117182	-0.027644
6	1.065108	1.262100	-0.000602
6	-0.331116	1.205255	0.029520
6	-1.142497	-0.012225	0.006641
1	-0.825449	-2.158178	0.041304
1	2.902868	0.137357	-0.055129

1	1.552524	2.233667	-0.000583
1	-0.894433	2.136228	0.048477
8	-2.377800	-0.007633	-0.034065
1	1.499062	-1.808735	-0.824954
6	1.130160	-1.169803	-0.002636
1	1.501034	-1.740091	0.870956

M06L/6-311G**=-307.416002

15. [3.1.0]-TS2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.325463	-1.193747	-0.047467
6	-1.828883	0.074329	-0.056691
6	-1.071530	1.238761	-0.004821
6	0.312112	1.221779	0.032868
6	1.124963	0.016416	0.000136
1	-2.911404	0.089665	-0.077566
1	-1.583213	2.197711	0.008954
1	0.859342	2.159324	0.074933
8	2.361435	-0.003842	-0.030648
6	-1.132731	-1.168997	-0.016893
1	-1.662255	-2.085923	-0.270774
1	0.830653	-2.154305	-0.018589
1	-0.800959	-1.306980	1.085438

M06L/6-311G**=-307.4107885

16. [3.1.0]-Int2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.279294	-1.265980	0.001931
6	-1.812551	0.046069	-0.001652
6	-1.037365	1.268815	-0.000007

6	0.313808	1.272703	0.002130
6	1.081738	0.029000	0.000321
1	-2.895159	0.114759	-0.002741
1	-1.575688	2.213769	-0.000543
1	0.884705	2.195483	0.002887
8	2.300614	0.006741	-0.002553
6	-1.202044	-1.148972	-0.000540
1	-1.784397	-2.066800	-0.001060
1	0.612502	-1.857809	0.864957
1	0.615849	-1.863152	-0.856175

M06L/6-311G**=-307.477154

17. [3.1.0]-TS3-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.380869	1.145572	-0.183930
6	1.773357	0.126549	0.158928
6	1.171472	-1.150038	0.000756
6	-0.181864	-1.334247	-0.190906
6	-0.975418	-0.171178	-0.103805
1	2.842202	0.185509	0.329548
1	1.809095	-2.027884	0.071810
1	-0.630930	-2.319977	-0.231651
8	-2.205938	-0.047498	0.252900
6	1.022204	1.268798	0.032159
1	1.495292	2.246555	0.038243
1	-0.819901	1.786998	-0.953214
1	-1.621543	1.196051	0.442854

M06L/6-311G**=-307.4175216

18. [3.1.0]-Pro-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	-0.261423	1.195314	0.000543
6	1.850373	0.026243	-0.000709
6	1.165263	-1.186282	0.000045
6	-0.221380	-1.219136	0.000525
6	-0.938927	-0.023594	0.000498
1	2.934447	0.044187	-0.000980
1	1.716782	-2.121136	-0.000053
1	-0.767697	-2.155715	0.000969
8	-2.297670	-0.109971	-0.000721
6	1.128512	1.213880	0.000053
1	1.647175	2.167412	0.000185
1	-0.824345	2.125779	0.000819
1	-2.659510	0.780684	-0.000898

M06L/6-311G**=-307.5042095

19. [4.1.0]-Rea-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.835747	1.234530	1.528083
6	0.755379	1.240814	0.429551
1	1.513911	1.955686	0.099743
6	-0.623445	1.656577	0.018312
1	-0.861605	2.715037	0.076036
6	-1.545733	0.790306	-0.401850
1	-2.529890	1.142827	-0.697452
6	-1.310762	-0.666638	-0.442264
1	-1.902991	-1.240822	-1.147173
6	-0.929905	-1.355405	0.829344
1	-0.874703	-0.743184	1.723269
1	-1.253337	-2.376059	0.993773
6	0.119155	-1.146405	-0.237650
1	0.442237	-2.027558	-0.779264
6	1.182702	-0.130749	-0.066039
8	2.343286	-0.373932	-0.321680

M06L/6-311G**=-346.782817

20. [4.1.0]-Min-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.750130	1.138664	1.482816
6	0.635840	1.305682	0.394739
1	1.288374	2.154287	0.163778
6	-0.779241	1.601320	0.039323
1	-1.091795	2.641791	0.022936
6	-1.653030	0.642381	-0.300404
1	-2.670611	0.910568	-0.571427
6	-1.281828	-0.773529	-0.372521
1	-1.903386	-1.401757	-1.002028
6	-0.654812	-1.446604	0.842824
1	-0.575598	-0.832549	1.733004
1	-0.903123	-2.486252	1.027002
6	0.201442	-1.107220	-0.335814
1	0.527857	-1.940825	-0.950630
6	1.121861	0.065152	-0.345667
8	2.379595	-0.238377	-0.180041

M06L/6-311G**=-346.6622779

21. [4.1.0]-TS1-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.927947	1.052462	1.692006
6	0.893363	1.113377	0.577912
1	1.750372	1.752805	0.311809
6	-0.353921	1.695667	0.028458
1	-0.374871	2.769857	-0.152853
6	-1.431462	0.953906	-0.429545
1	-2.233912	1.483646	-0.944922

6	-1.485030	-0.463301	-0.414541
1	-2.179961	-0.946758	-1.095984
6	-1.076003	-1.287532	0.795209
1	-1.016327	-0.744947	1.734097
1	-1.578665	-2.246745	0.866850
6	0.028221	-1.184988	-0.178277
1	0.236589	-2.063106	-0.786649
6	1.119550	-0.254757	-0.043995
8	2.287565	-0.561431	-0.454459

M06L/6-311G**=-346.6579847

22. [4.1.0]-T_1/S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.6285213	0.8448700	1.6424200
6	0.8341454	1.0419096	0.5776624
1	1.6946571	1.7119373	0.5493299
6	-0.3466661	1.6741943	-0.0766943
1	-0.2675557	2.7332602	-0.3043045
6	-1.4778374	1.0086018	-0.5123736
1	-2.1810606	1.5810573	-1.1138337
6	-1.8041297	-0.3199751	-0.2733720
1	-2.6515718	-0.7528653	-0.7968518
6	-1.0096701	-1.2124888	0.6383228
1	-0.9290149	-0.7601684	1.6363016
1	-1.5045996	-2.1761268	0.7639303
6	0.3253617	-1.3656177	-0.0029207
1	0.5600261	-2.2576759	-0.5773724
6	1.2676386	-0.2890280	-0.0611351
8	2.3752105	-0.3937294	-0.5839930

Difference Gradient:

-1	0.00335360	0.00843624	0.00358247
-2	0.00975039	-0.01731834	0.03384982
-3	0.00005750	-0.00134780	-0.00098101
-4	0.01444017	0.00926585	-0.01128894
-5	0.00381615	-0.00069756	-0.00425583

-6	-0.02412731	-0.04008922	-0.00352309
-7	-0.00055872	-0.00012831	-0.00052269
-8	-0.05978581	0.04633418	0.00035764
-9	-0.00775891	0.00352034	0.01453606
-10	0.01803974	-0.01047932	-0.05104621
-11	0.00668336	0.00421047	-0.00451827
-12	0.00087083	-0.00117458	-0.00132641
-13	0.01769404	-0.02417302	0.01193284
-14	0.00934286	-0.00837445	0.01088753
-15	0.01502308	0.04721419	0.00828209
-16	-0.00684096	-0.01519869	-0.00596600

M06L/6-311G**=-346.7129953550

23. [4.1.0]-Int1-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.590130	-0.995856	0.761426
6	0.344784	-1.474312	-0.224731
1	0.051284	-2.308912	-0.861315
6	1.635831	-0.936080	-0.345085
1	2.419533	-1.573866	-0.749805
6	1.946077	0.339519	0.017786
1	2.986485	0.641403	0.096832
6	0.938042	1.408401	0.188113
1	0.968531	1.691144	1.265551
1	1.343976	2.317012	-0.279040
6	-0.470460	1.280353	-0.240499
1	-0.971550	2.222975	-0.448935
6	-1.338174	0.199262	-0.027214
8	-2.514957	0.046752	-0.310907
1	-0.104795	-0.588968	1.651451
1	-1.369626	-1.702526	1.033730

M06L/6-311G**=-346.7175593

24. [4.1.0]-TS2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.588350	-1.023050	0.716990
6	0.472103	-1.521004	-0.186246
1	0.303595	-2.461859	-0.702572
6	1.668438	-0.877987	-0.342295
1	2.487014	-1.420732	-0.811791
6	1.919950	0.450283	0.030411
1	2.946079	0.794652	0.106746
6	0.911524	1.440152	0.132569
1	0.277549	1.407008	1.117159
1	1.265326	2.469700	0.113543
6	-0.523699	1.298747	-0.201557
1	-1.062246	2.231746	-0.340104
6	-1.327922	0.122949	-0.009097
8	-2.491972	0.009419	-0.367207
1	-0.146690	-0.650297	1.651951
1	-1.327114	-1.786116	0.958069

M06L/6-311G**=-346.7046071

25. [4.1.0]-Int2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1.177137	2.054733	-0.556916
6	0.519070	1.188355	-0.484578
1	0.257578	0.889820	-1.513267
6	-0.742191	1.483761	0.254744
1	-0.811991	2.455665	0.735912
6	-1.807827	0.660948	0.285690
1	-2.731041	1.016395	0.738733
6	-1.803547	-0.666184	-0.291245
1	-2.722749	-1.025331	-0.749539
6	-0.735615	-1.485600	-0.252646

1	-0.798645	-2.457355	-0.735126
6	0.521322	-1.184166	0.492292
6	1.347785	0.001658	0.000776
8	2.550005	0.000626	-0.004703
1	1.181513	-2.048603	0.568739
1	0.254167	-0.882966	1.518884

M06L/6-311G**=-346.7873435

26. [4.1.0]-TS3-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1.019922	-1.643379	1.196943
6	0.636758	-1.198220	0.268667
1	2.063155	-1.242145	-0.051329
6	-0.702492	-1.601180	-0.131625
1	-0.844911	-2.660700	-0.340339
6	-1.778684	-0.789454	-0.230324
1	-2.721099	-1.242160	-0.529951
6	-1.846068	0.599731	0.181298
1	-2.827380	0.924497	0.528928
6	-0.868871	1.521445	0.219753
1	-1.107411	2.502616	0.622993
6	0.516237	1.355663	-0.331858
6	1.196794	0.089529	0.035389
8	2.476493	-0.006960	0.000986
1	1.187014	2.181805	-0.063536
1	0.496720	1.370058	-1.439408

M06L/6-311G**=-346.6841309

27. [4.1.0]-Pro-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z

1	1.276684	-1.831085	0.855843
6	0.520917	-1.059749	0.701001
1	0.115530	-0.775066	1.681695
6	-0.586138	-1.531383	-0.192984
1	-0.477721	-2.495535	-0.683102
6	-1.704216	-0.802606	-0.377801
1	-2.523051	-1.251619	-0.937424
6	-1.895110	0.550411	0.064233
1	-2.920149	0.891743	0.184084
6	-0.909113	1.488572	0.167919
1	-1.224418	2.511643	0.363118
6	0.487762	1.308420	-0.085784
6	1.152217	0.134900	0.067652
8	2.444759	-0.058808	-0.291195
1	1.055144	2.180817	-0.406895
1	2.741993	0.708171	-0.793162

M06L/6-311G**=-346.7765415

28. [5.1.0]-Rea-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.811759	-0.216780	-0.240282
1	-1.851636	0.191820	-1.247573
6	-1.198298	-1.492619	-0.055583
1	-1.192358	-1.893651	0.958234
6	-0.001286	-1.466501	-0.744890
1	-0.000802	-0.962290	-1.712864
6	1.115763	-1.110292	0.145411
1	1.394637	-1.807359	0.931094
6	-0.173627	1.237103	0.235640
6	-1.425561	0.620275	0.799713
1	-1.254532	0.127956	1.759301
6	0.973900	0.390754	0.737033
1	1.161945	0.434929	1.805433
6	2.076064	-0.020664	-0.186485
1	3.082705	-0.089265	0.211484

1	2.021931	0.410553	-1.182007
8	-0.086633	1.992456	-0.708305

M06L/6-311G**=-384.7299843

29. [5.1.0]-Min-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.108042	-1.302993	-0.358796
1	0.781746	-1.358814	-1.398529
6	2.172308	-0.359783	-0.047726
1	2.710351	-0.430831	0.898234
6	1.484944	0.883129	-0.439857
1	1.662405	1.290662	-1.436723
6	0.322147	1.430237	0.322462
1	0.607621	2.122409	1.116996
6	-1.091979	-0.815416	0.190584
6	0.169102	-1.478494	0.623169
1	0.485559	-1.263149	1.645682
6	-0.952761	0.635895	0.646761
1	-1.385021	0.830477	1.625697
6	-0.985509	1.738857	-0.356094
1	-1.503868	2.658752	-0.109742
1	-1.082723	1.435891	-1.394723
8	-1.954229	-1.209249	-0.553739

M06L/6-311G**=-384.7074885

30. [5.1.0]-TS1-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.315632	-1.601282	-0.071079
1	0.030470	-1.696620	-1.121308
6	1.703731	-1.245450	0.151504

1	2.160085	-1.323944	1.138778
6	1.838528	-0.022818	-0.669907
1	2.356732	-0.086830	-1.627571
6	1.077207	1.148255	-0.456347
1	1.176844	1.925162	-1.208380
6	-1.482898	-0.110698	0.046809
6	-0.627518	-1.111586	0.770960
1	-0.329511	-0.865151	1.789326
6	-0.760993	1.179533	-0.013346
1	-1.244740	1.950438	-0.605405
6	0.415651	1.574689	0.806422
1	0.640860	0.964259	1.675034
1	0.491667	2.635042	1.036936
8	-2.519805	-0.295776	-0.558438

M06L/6-311G**=-384.7020963

31. [5.1.0]-T_1/S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.2762282	-1.5290377	-0.2024954
1	-0.0306465	-1.5350209	-1.2463105
6	1.5753620	-1.1233715	0.1210070
1	1.8338928	-1.0842733	1.1796020
6	2.0151948	-0.0021508	-0.7277386
1	2.6171441	-0.1541151	-1.6215873
6	1.4672793	1.1943300	-0.4492841
1	1.7089435	2.0307391	-1.1005557
6	-1.6285798	-0.1185764	0.2383091
6	-0.6319391	-1.1287110	0.7530702
1	-0.2978794	-1.0789990	1.7897740
6	-0.9688740	1.1348384	0.0995064
1	-1.4386227	1.8359991	-0.5877113
6	0.4094539	1.4883930	0.6141275
1	0.6330264	0.9578799	1.5428819
1	0.4486095	2.5530799	0.8603775
8	-2.7466510	-0.4237807	-0.1789849

Difference Gradient:

-1	-0.01587459	0.04374211	0.03006026
-2	0.00062195	0.00131073	-0.00260142
-3	0.05191884	-0.03642801	-0.01482589
-4	0.00299295	-0.00011461	-0.00185964
-5	-0.01981855	0.00799902	0.01669606
-6	0.00985647	0.00694845	0.00606010
-7	0.00784114	0.00875181	-0.02562850
-8	0.00338929	0.00409654	0.00046336
-9	-0.00776617	-0.08780429	0.00311881
-10	-0.04278771	-0.04239656	0.01338692
-11	-0.00004083	0.00841424	-0.00373908
-12	0.00558981	0.05640427	-0.01331870
-13	-0.00678451	0.00985166	0.00808273
-14	0.00352939	-0.01203572	-0.01170942
-15	-0.00145061	-0.00349675	-0.00307355
-16	-0.00397275	0.00110084	-0.00366290
-17	0.01275586	0.03365629	0.00255087

M06L/6-311G**=-384.7251161560

32. [5.1.0]-Int1-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.025355	1.793292	0.289697
1	0.018997	2.837837	0.608085
6	1.202348	1.432875	-0.468427
1	1.655406	2.269916	-1.003605
6	2.041130	0.335558	-0.328146
1	3.074196	0.531464	-0.620311
6	1.848923	-0.932079	0.185504
1	2.739216	-1.450085	0.541616
6	-1.469372	-0.234675	-0.032348
6	-1.021259	1.031531	0.647540
1	-1.793984	1.463762	1.281495
6	-0.697154	-1.379814	-0.252624
1	-1.227625	-2.170529	-0.781274

6	0.615877	-1.722935	0.304216
1	0.875201	-2.760308	0.050839
1	0.519901	-1.792656	1.419306
8	-2.642048	-0.108989	-0.446078

M06L/6-311G**=-384.7760896

33. [5.1.0]-TS2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.541008	-1.313207	-0.511913
1	0.197961	-1.399799	-1.545543
6	1.957542	-1.005611	-0.271510
1	2.770700	-1.677935	-0.539385
6	2.214615	0.212150	0.272296
1	3.229112	0.478265	0.567758
6	1.085333	1.112986	0.531276
1	0.760416	1.254606	1.562094
6	-1.590583	-0.254414	0.169843
6	-0.339929	-1.041355	0.465815
1	0.045541	-0.989159	1.482444
6	-1.238021	1.121552	-0.267757
6	0.196705	1.491433	-0.473490
1	0.565350	1.677816	-1.486993
8	-2.740872	-0.647982	0.139050
1	-2.021258	1.661549	-0.793636
1	-0.580866	2.237312	0.153496

M06L/6-311G**=-384.7076543

34. [5.1.0]-Int2-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.466474	-1.425718	-0.179773

1	0.081805	-1.881103	-1.094870
6	1.889625	-1.064775	-0.139486
1	2.648619	-1.834010	-0.272579
6	2.282177	0.230474	-0.003990
1	3.346521	0.448636	0.072820
6	1.275119	1.278698	0.178204
1	1.294717	1.812312	1.131577
6	-1.612874	-0.230502	0.195878
6	-0.405307	-0.922038	0.718580
1	0.042607	-0.418317	1.575143
6	-1.224518	1.322239	0.014621
6	0.146502	1.283466	-0.555875
1	0.200804	0.769824	-1.518336
8	-2.657432	-0.659814	-0.205372
1	-2.005867	1.746578	-0.618699
1	-1.252939	1.803531	0.998970

M06L/6-311G**=-384.8072147

35. [5.1.0]-TS3-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.304798	-0.378956	-0.038486
6	-1.006140	0.907480	0.682474
1	-1.546988	1.034120	1.628695
6	0.013187	1.781778	0.332404
1	-0.131216	2.822799	0.631642
6	1.172840	1.504220	-0.412755
1	1.640554	2.362780	-0.891672
6	1.951759	0.357827	-0.371030
1	2.940820	0.503398	-0.824103
6	-0.620951	-1.564629	-0.121044
1	-1.149084	-2.412641	-0.550380
6	0.708685	-1.762722	0.299307
1	0.964139	-2.789624	0.575905
6	1.804676	-0.921106	0.213062
1	2.756168	-1.398604	0.443279

8	-2.464396	-0.100757	-0.551471
1	-2.074775	1.140464	-0.105200

M06L/6-311G**=-384.7016182

36. [5.1.0]-Pro-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.335641	0.180231	-0.035537
6	0.867035	-1.019038	0.673639
1	1.578680	-1.420863	1.397444
6	-0.271564	-1.687693	0.462423
1	-0.415509	-2.615257	1.017975
6	-1.341250	-1.346558	-0.474104
1	-1.701043	-2.168200	-1.092930
6	-1.993723	-0.178418	-0.543893
1	-2.846664	-0.128611	-1.221470
6	0.702804	1.358976	-0.146924
1	1.272330	2.167295	-0.601792
6	-0.605122	1.692565	0.397684
1	-0.654657	2.644046	0.929249
6	-1.762072	1.028345	0.245365
1	-2.657063	1.482048	0.669492
8	2.618858	0.088213	-0.510174
1	2.882561	-0.836629	-0.488489

M06L/6-311G**=-384.8494029