Radical Cations from Dicyclopropylidenemethane and Its Octamethyl Derivative

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SUPPORTING INFORMATION, PART 1 (ASCII)

B3LYP/6-31G(d) optimized geometries, energies, and thermal corrections of all the stationary points discussed in this work

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Dicyclopropylidenmethane
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2 (D2d), 1-A1
  Electronic energy=   -271.407869
  Zero-point correction=   0.124406
  Sum of electronic and zero-point Energies=   -271.283463
  Sum of electronic and thermal Energies=   -271.276363
  Sum of electronic and thermal Enthalpies=   -271.275419
  Sum of electronic and thermal Free Energies= -271.313328
  Frequencies --   115.9349   115.9351   199.1296
Charge = 0 Multiplicity = 1

6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.294081
6	0.000000	0.000000	-1.294081
6	0.000000	0.764113	2.561096
6	0.000000	-0.764113	2.561096
6	-0.764113	0.000000	-2.561096
6	0.764113	0.000000	-2.561096
1	-0.914024	1.277659	2.856838
1	0.914024	1.277659	2.856838
1	-0.914024	-1.277659	2.856838
1	0.914024	-1.277659	2.856838
1	-1.277659	0.914024	-2.856838
1	-1.277659	-0.914024	-2.856838
1	1.277659	0.914024	-2.856838
1	1.277659	-0.914024	-2.856838

2.+ (D2), 2-B2
 Electronic energy= -271.125264
 Zero-point correction= 0.122360
 Sum of electronic and zero-point Energies= -271.002904
 Sum of electronic and thermal Energies= -270.995438
 Sum of electronic and thermal Enthalpies= -270.994494
 Sum of electronic and thermal Free Energies= -271.033913
Frequencies -- 93.3085 108.4662 176.5896
Charge = 1 Multiplicity = 2
6 0.000000 0.000000 0.000000
6 0.000000 0.000000 1.294337
6 0.000000 0.000000 -1.294337
6 -0.302567 0.683468 2.596633
6 0.302567 -0.683468 2.596633
6 -0.302567 -0.683468 -2.596633
6 0.302567 0.683468 -2.596633
1 -1.362681 0.797141 2.822766
1 0.320447 1.544296 2.831262
1 -0.320447 -1.544296 2.831262
1 1.362681 -0.797141 2.822766
1 -1.362681 -0.797141 -2.822766
1 0.320447 -1.544296 -2.831262
1 -0.320447 1.544296 -2.831262
1 1.362681 0.797141 -2.822766

TS1 (internal rotation in 2.+, D2h) 2-B2G
 Electronic energy= -271.114916
 Zero-point correction= 0.121467
 Sum of electronic and zero-point Energies= -270.993448
 Sum of electronic and thermal Energies= -270.985915
 Sum of electronic and thermal Enthalpies= -270.984971
 Sum of electronic and thermal Free Energies= -271.026949
Frequencies -- -283.0313 14.1855 60.5025
Charge = 1 Multiplicity = 2
6 0.000000 0.000000 0.000000
6 1.291250 0.000000 0.000000
6 -1.291250 0.000000 0.000000
6 2.616562 0.739587 0.000000
6 2.616562 -0.739587 0.000000
6 -2.616562 0.739587 0.000000
6 -2.616562 -0.739587 0.000000

1 2.836071 1.275906 0.921489
1 2.836071 1.275906 -0.921489
1 -2.836071 1.275906 0.921489
1 -2.836071 1.275906 -0.921489
1 2.836071 -1.275906 0.921489
1 2.836071 -1.275906 -0.921489
1 -2.836071 -1.275906 0.921489
1 -2.836071 -1.275906 -0.921489

TS1 (internal rotation in 2.+, C2v) 2-B1
Electronic energy= -271.1141015
Zero-point correction= 0.121672
Sum of electronic and zero-point Energies= -270.992430
Sum of electronic and thermal Energies= -270.985248
Sum of electronic and thermal Enthalpies= -270.984304
Sum of electronic and thermal Free Energies= -271.024181
Frequencies -- -331.6910 54.2494 113.4322
Charge = 1 Multiplicity = 2
6 0.000000 0.000000 -0.012518
6 0.000000 0.000000 1.336068
6 0.000000 0.000000 -1.265259
6 0.000000 0.763202 2.586729
6 0.000000 -0.763202 2.586729
6 -0.733171 0.000000 -2.625616
6 0.733171 0.000000 -2.625616
1 -0.914418 1.295378 2.850233
1 0.914418 1.295378 2.850233
1 -0.914418 -1.295378 2.850233
1 0.914418 -1.295378 2.850233
1 -1.271065 0.925039 -2.821010
1 -1.271065 -0.925039 -2.821010
1 1.271065 0.925039 -2.821010
1 1.271065 -0.925039 -2.821010

TS (2.+ -> 2a.+)
Electronic energy= -271.094113
Zero-point correction= 0.120847
Sum of electronic and zero-point Energies= -270.973266
Sum of electronic and thermal Energies= -270.965862
Sum of electronic and thermal Enthalpies= -270.964918

Sum of electronic and thermal Free Energies= -271.005567
Frequencies -- -554.1573 107.0033 110.3867
Charge = 1 Multiplicity = 2

6	0.081429	0.009516	-0.067847
6	1.449654	0.012624	-0.174988
6	-1.182117	-0.000740	-0.021569
6	2.363435	-1.080454	0.022383
6	2.309509	1.083266	0.080656
6	-2.521908	0.033663	-0.726481
6	-2.475372	-0.054104	0.762139
1	2.128529	-1.866289	0.735969
1	3.318105	-1.119709	-0.491852
1	2.008952	1.921786	0.708570
1	3.327963	1.089367	-0.297061
1	-2.765593	-0.856080	-1.302659
1	-2.776781	0.982341	-1.193386
1	-2.688801	-1.006082	1.243121
1	-2.700154	0.832045	1.351546

2a.+ (C2v), 2-A2
Electronic energy= -271.130577
Zero-point correction= 0.121542
Sum of electronic and zero-point Energies= -271.009035
Sum of electronic and thermal Energies= -271.001112
Sum of electronic and thermal Enthalpies= -271.000168
Sum of electronic and thermal Free Energies= -271.041303
Frequencies -- 84.0174 91.5647 111.8302
Charge = 1 Multiplicity = 2

6	0.000000	0.000000	0.151585
6	0.000000	0.000000	1.556910
6	0.000000	0.000000	-1.095371
6	0.000000	1.254671	2.199823
6	0.000000	-1.254671	2.199823
6	-0.734651	0.000000	-2.444209
6	0.734651	0.000000	-2.444209
1	0.000000	2.176716	1.631238
1	0.000000	1.317865	3.283108
1	0.000000	-2.176716	1.631238
1	0.000000	-1.317865	3.283108
1	-1.271774	0.924467	-2.643700
1	-1.271774	-0.924467	-2.643700

1 1.271774 0.924467 -2.643700
1 1.271774 -0.924467 -2.643700

TS (2a.+ -> 3.+)
Electronic energy= -271.041990
Zero-point correction= 0.115847
Sum of electronic and zero-point Energies= -270.926143
Sum of electronic and thermal Energies= -270.917718
Sum of electronic and thermal Enthalpies= -270.916774
Sum of electronic and thermal Free Energies= -270.959771
Frequencies -- -489.2011 59.0241 79.7079
Charge = 1 Multiplicity = 2
6 0.054724 -0.076952 -0.128025
6 -1.274149 -0.088355 -0.114769
6 1.429018 0.001885 -0.016187
6 -2.051176 -0.754296 0.895947
6 -2.235970 0.742327 -0.780293
6 2.206691 -1.089894 -0.488140
6 1.965722 1.202357 0.526003
1 -1.723262 -0.792370 1.930388
1 -2.968640 -1.261779 0.615336
1 -2.050984 1.796463 -0.962810
1 -3.190891 0.317159 -1.069076
1 1.741068 -1.922544 -1.001481
1 3.275059 -1.126258 -0.299781
1 1.323993 1.942522 0.989052
1 3.024496 1.424376 0.431163

3.+
Electronic energy= -271.124515
Zero-point correction= 0.120766
Sum of electronic and zero-point Energies= -271.003749
Sum of electronic and thermal Energies= -270.995887
Sum of electronic and thermal Enthalpies= -270.994943
Sum of electronic and thermal Free Energies= -271.036121
Frequencies -- 76.2804 147.6186 156.9199
Charge = 1 Multiplicity = 2
6 -0.100536 -0.283544 -0.000336
6 2.243499 -0.811786 -0.000247
6 -0.988208 -1.471607 0.000159

6 1.239480 0.176295 -0.000004
6 -1.464270 -0.050347 0.000041
6 -2.471023 0.844469 -0.000054
6 1.461190 1.572184 0.000407
1 3.294501 -0.541907 -0.000041
1 -1.057381 -2.067399 0.915328
1 1.986948 -1.864772 -0.000451
1 -1.058461 -2.067257 -0.915030
1 -3.509136 0.522378 0.000667
1 2.466406 1.980176 0.000596
1 -2.276680 1.914062 -0.001239
1 0.633010 2.270737 0.000373

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both rings open (Doublet, C2), 2-B
Electronic energy= -271.054429
Zero-point correction= 0.117065
Sum of electronic and zero-point Energies= -270.937364
Sum of electronic and thermal Energies= -270.928707
Sum of electronic and thermal Enthalpies= -270.927763
Sum of electronic and thermal Free Energies= -270.970094
Frequencies -- 57.4140 111.8743 143.0735
Charge = 1 Multiplicity = 2
Full point group C2 NOp 2
6 0.000000 0.000000 0.468923
6 0.000000 1.351228 0.064466
6 0.000000 -1.351228 0.064466
6 -0.312787 2.259691 1.091924
6 0.247620 1.709673 -1.286392
6 0.312787 -2.259691 1.091924
6 -0.247620 -1.709673 -1.286392
1 -0.442388 1.924317 2.114458
1 -0.463316 3.313678 0.876952
1 0.565809 0.981586 -2.021102
1 0.168267 2.746748 -1.597064
1 0.442388 -1.924317 2.114458
1 0.463316 -3.313678 0.876952
1 -0.565809 -0.981586 -2.021102
1 -0.168267 -2.746748 -1.597064

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both rings open (Quartet, C2), 4-B
Electronic energy= -271.062196

Zero-point correction= 0.116137
Sum of electronic and zero-point Energies= -270.946058
Sum of electronic and thermal Energies= -270.937012
Sum of electronic and thermal Enthalpies= -270.936067
Sum of electronic and thermal Free Energies= -270.982243
Frequencies -- 12.0665 31.3161 89.5369
Charge = 1 Multiplicity = 4

6	0.000000	0.000000	0.256516
6	0.000000	1.356797	0.044916
6	0.000000	-1.356797	0.044916
6	-1.002351	2.029834	0.796916
6	1.002351	-2.029834	0.796916
6	0.864760	1.966395	-0.904884
6	-0.864760	-1.966395	-0.904884
1	-1.493173	1.554123	1.638316
1	1.493173	-1.554123	1.638316
1	1.539513	1.375980	-1.512884
1	-1.539513	-1.375980	-1.512884
1	0.892623	3.047514	-0.990384
1	-0.892623	-3.047514	-0.990384
1	-1.357364	3.004511	0.473716
1	1.357364	-3.004511	0.473716

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Octamethyl-dicyclopropylidenemethane

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2-Me8 (D2d), 1-A1
Electronic energy= -585.932613
Zero-point correction= 0.349292
Sum of electronic and zero-point Energies= -585.583321
Sum of electronic and thermal Energies= -585.564015
Sum of electronic and thermal Enthalpies= -585.563071
Sum of electronic and thermal Free Energies= -585.628264
Frequencies -- 45.3586 45.3588 52.7873
Charge = 0 Multiplicity = 1

6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.295799
6	0.000000	0.000000	-1.295799
6	0.000000	0.776554	2.567047
6	0.000000	-0.776554	2.567047

6	-0.776554	0.000000	-2.567047
6	0.776554	0.000000	-2.567047
6	-1.262932	1.539439	2.956924
6	1.262932	1.539439	2.956924
6	-1.262932	-1.539439	2.956924
6	1.262932	-1.539439	2.956924
6	-1.539439	1.262932	-2.956924
6	-1.539439	-1.262932	-2.956924
6	1.539439	1.262932	-2.956924
6	1.539439	-1.262932	-2.956924
1	2.177093	1.049505	2.615136
1	1.243757	2.541903	2.511841
1	1.325116	1.662276	4.046525
1	-2.177093	1.049505	2.615136
1	-1.243757	2.541903	2.511841
1	-1.325116	1.662276	4.046525
1	2.177093	-1.049505	2.615136
1	1.243757	-2.541903	2.511841
1	1.325116	-1.662276	4.046525
1	-2.177093	-1.049505	2.615136
1	-1.243757	-2.541903	2.511841
1	-1.325116	-1.662276	4.046525
1	1.049505	2.177093	-2.615136
1	2.541903	1.243757	-2.511841
1	1.662276	1.325116	-4.046525
1	1.049505	-2.177093	-2.615136
1	2.541903	-1.243757	-2.511841
1	1.662276	-1.325116	-4.046525
1	-1.049505	2.177093	-2.615136
1	-2.541903	1.243757	-2.511841
1	-1.662276	1.325116	-4.046525
1	-1.049505	-2.177093	-2.615136
1	-2.541903	-1.243757	-2.511841
1	-1.662276	-1.325116	-4.046525

2-Me8.+ (D2), 2-B2

Electronic energy= -585.679593

Zero-point correction= 0.347533

Sum of electronic and zero-point Energies= -585.332060

Sum of electronic and thermal Energies= -585.312312

Sum of electronic and thermal Enthalpies= -585.311367

Sum of electronic and thermal Free Energies= -585.378392
Frequencies -- 42.1441 43.8187 44.7053
Charge = 1 Multiplicity = 2

6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.292927
6	0.000000	0.000000	-1.292927
6	-0.315313	0.689751	2.613313
6	0.315313	-0.689751	2.613313
6	-0.315313	-0.689751	-2.613313
6	0.315313	0.689751	-2.613313
6	-1.803477	0.860498	2.916912
6	0.502477	1.929138	2.960797
6	-0.502477	-1.929138	2.960797
6	1.803477	-0.860498	2.916912
6	-1.803477	-0.860498	-2.916912
6	0.502477	-1.929138	-2.960797
6	-0.502477	1.929138	-2.960797
6	1.803477	0.860498	-2.916912
1	1.548327	1.860736	2.658598
1	0.066397	2.811444	2.482566
1	0.470240	2.084116	4.045515
1	-2.423529	0.045116	2.541507
1	-2.167291	1.794448	2.478546
1	-1.938517	0.920912	4.003630
1	2.423529	-0.045116	2.541507
1	2.167291	-1.794448	2.478546
1	1.938517	-0.920912	4.003630
1	-1.548327	-1.860736	2.658598
1	-0.066397	-2.811444	2.482566
1	-0.470240	-2.084116	4.045515
1	-1.548327	1.860736	-2.658598
1	-0.066397	2.811444	-2.482566
1	-0.470240	2.084116	-4.045515
1	2.423529	0.045116	-2.541507
1	2.167291	1.794448	-2.478546
1	1.938517	0.920912	-4.003630
1	-2.423529	-0.045116	-2.541507
1	-2.167291	-1.794448	-2.478546
1	-1.938517	-0.920912	-4.003630
1	1.548327	-1.860736	-2.658598

1 0.066397 -2.811444 -2.482566
1 0.470240 -2.084116 -4.045515

TS1 (internal rotation in 2-Me8.+, D2h) 2-B2G
Electronic energy= -585.672225
Zero-point correction= 0.346806
Sum of electronic and zero-point Energies= -585.325419
Sum of electronic and thermal Energies= -585.306186
Sum of electronic and thermal Enthalpies= -585.305242
Sum of electronic and thermal Free Energies= -585.371986
Frequencies -- -67.1801 20.6062 33.1898
Charge = 1 Multiplicity = 2
6 0.000000 0.000000 0.000000
6 0.000000 0.000000 -1.290811
6 0.000000 0.000000 1.290811
6 0.000000 0.751785 -2.635016
6 0.000000 -0.751785 -2.635016
6 0.000000 0.751785 2.635016
6 0.000000 -0.751785 2.635016
6 1.270080 1.533982 -2.954266
6 -1.270080 1.533982 -2.954266
6 1.270080 1.533982 2.954266
6 -1.270080 1.533982 2.954266
6 1.270080 -1.533982 -2.954266
6 -1.270080 -1.533982 -2.954266
6 1.270080 -1.533982 2.954266
6 -1.270080 -1.533982 2.954266
1 2.182701 1.042034 2.616084
1 2.182701 1.042034 -2.616084
1 -2.182701 1.042034 2.616084
1 -2.182701 1.042034 -2.616084
1 2.182701 -1.042034 2.616084
1 2.182701 -1.042034 -2.616084
1 -2.182701 -1.042034 2.616084
1 -2.182701 -1.042034 -2.616084
1 1.224760 2.525221 2.493647
1 1.224760 2.525221 -2.493647
1 -1.224760 2.525221 2.493647
1 -1.224760 2.525221 -2.493647
1 1.224760 -2.525221 2.493647
1 1.224760 -2.525221 -2.493647

1 -1.224760 -2.525221 2.493647
1 -1.224760 -2.525221 -2.493647
1 1.336905 1.670553 4.040407
1 -1.336905 1.670553 4.040407
1 -1.336905 1.670553 -4.040407
1 1.336905 1.670553 -4.040407

TS2 (internal rotation in 2-Me8.+, Cs) 2-A'
Electronic energy= -585.671364
Zero-point correction= 0.347147
Sum of electronic and zero-point Energies= -585.324217
Sum of electronic and thermal Energies= -585.304823
Sum of electronic and thermal Enthalpies= -585.303879
Sum of electronic and thermal Free Energies= -585.371256
Frequencies -- -40.4105 38.2906 47.1158
Charge = 1 Multiplicity = 2
6 0.270477 0.009387 0.000000
6 0.124893 -1.316977 0.000000
6 0.400400 1.254654 0.000000
6 0.028379 -2.575801 0.775737
6 0.028379 -2.575801 -0.775737
6 -0.807454 2.552835 0.000000
6 0.691245 2.702092 0.000000
6 -1.265394 -2.845268 1.546929
6 1.267491 -3.028608 1.550733
6 -1.265394 -2.845268 -1.546929
6 1.267491 -3.028608 -1.550733
6 -1.604828 2.629386 1.271821
6 -1.604828 2.629386 -1.271821
6 1.374832 3.231734 1.270206
6 1.374832 3.231734 -1.270206
1 2.205938 -2.762062 1.061315
1 1.267658 -2.576680 2.548054
1 1.242230 -4.117283 1.673396
1 -2.154781 -2.445662 1.056239
1 -1.201809 -2.400014 2.545316
1 -1.398858 -3.926171 1.667709
1 2.205938 -2.762062 -1.061315
1 1.267658 -2.576680 -2.548054
1 1.242230 -4.117283 -1.673396

1 -2.154781 -2.445662 -1.056239
1 -1.201809 -2.400014 -2.545316
1 -1.398858 -3.926171 -1.667709
1 0.984896 2.792568 2.188900
1 2.443830 3.008412 1.218629
1 1.252691 4.318914 1.318958
1 0.984896 2.792568 -2.188900
1 2.443830 3.008412 -1.218629
1 1.252691 4.318914 -1.318958
1 -1.048656 2.331148 2.160338
1 -2.515158 2.027101 1.201563
1 -1.919539 3.675106 1.411633
1 -1.048656 2.331148 -2.160338
1 -2.515158 2.027101 -1.201563
1 -1.919539 3.675106 -1.411633

2-Me8.+ TS for opening of first ring
Electronic energy= -585.664455
Zero-point correction= 0.346014
Sum of electronic and zero-point Energies= -585.318441
Sum of electronic and thermal Energies= -585.298654
Sum of electronic and thermal Enthalpies= -585.297710
Sum of electronic and thermal Free Energies= -585.367325
Frequencies -- -220.8577 11.5230 39.6064
Charge = 1 Multiplicity = 2
6 0.040800 -0.002858 -0.138433
6 -1.218625 -0.016695 -0.093588
6 -2.589211 -0.139491 -0.804798
6 -2.551043 0.132961 0.673864
6 -2.908469 0.972561 -1.796300
6 -2.932934 -1.525908 -1.334084
6 -2.845852 1.525387 1.217829
6 -2.854437 -0.973662 1.677423
6 1.379464 -0.024952 -0.341109
6 2.463372 0.895188 -0.087165
6 2.445912 -0.897626 0.111749
6 2.322172 1.840445 1.085488
6 3.488837 1.327098 -1.117969
6 2.275527 -1.563156 1.459001
6 3.456234 -1.571968 -0.794314
1 3.308056 2.126774 1.469522

1 1.823270 2.761985 0.755999
1 1.735583 1.415178 1.903045
1 4.511300 1.235261 -0.736682
1 3.407612 0.799965 -2.067074
1 3.311854 2.392152 -1.316168
1 3.253359 -1.769114 1.910132
1 1.685128 -0.963951 2.155937
1 1.769752 -2.529825 1.331621
1 3.244783 -2.648742 -0.766187
1 4.480013 -1.435539 -0.429997
1 3.397661 -1.253459 -1.833627
1 -2.538781 1.951482 -1.488613
1 -2.476823 0.736951 -2.773544
1 -3.996855 1.040580 -1.916375
1 -2.588821 -2.336563 -0.690784
1 -4.022237 -1.608828 -1.433846
1 -2.493492 -1.667866 -2.325837
1 -2.513338 2.329474 0.560344
1 -3.928150 1.629172 1.362918
1 -2.363633 1.658294 2.191007
1 -2.514070 -1.959061 1.356850
1 -3.938655 -1.022282 1.837160
1 -2.384005 -0.745976 2.638624

2a-Me8.+ (C2), 2-A
Electronic energy= -585.699602
Zero-point correction= 0.346934
Sum of electronic and zero-point Energies= -585.352668
Sum of electronic and thermal Energies= -585.332487
Sum of electronic and thermal Enthalpies= -585.331542
Sum of electronic and thermal Free Energies= -585.400908
Frequencies -- 28.0677 37.0692 55.5383
Charge = 1 Multiplicity = 2
6 0.000000 0.000000 0.222276
6 0.000000 0.000000 1.613777
6 0.000000 0.000000 -1.028830
6 0.222223 1.265534 2.254303
6 -0.222223 -1.265534 2.254303
6 -0.748609 -0.017842 -2.389088
6 0.748609 0.017842 -2.389088

6	0.000000	2.569170	1.550450
6	0.735032	1.368074	3.658298
6	0.000000	-2.569170	1.550450
6	-0.735032	-1.368074	3.658298
6	-1.560894	1.234438	-2.695883
6	-1.503483	-1.304021	-2.700214
6	1.503483	1.304021	-2.700214
6	1.560894	-1.234438	-2.695883
1	-0.430404	2.460512	0.553606
1	-0.676743	3.199397	2.145259
1	0.939497	3.134013	1.468464
1	1.478271	2.173049	3.717733
1	1.197635	0.445725	4.014135
1	-0.062215	1.642678	4.365400
1	0.430404	-2.460512	0.553606
1	-0.939497	-3.134013	1.468464
1	0.676743	-3.199397	2.145259
1	-1.478271	-2.173049	3.717733
1	0.062215	-1.642678	4.365400
1	-1.197635	-0.445725	4.014135
1	0.990984	2.205323	-2.362743
1	2.493276	1.278552	-2.235446
1	1.642927	1.376386	-3.785514
1	1.087000	-2.157904	-2.361272
1	2.547007	-1.165536	-2.227703
1	1.707140	-1.300777	-3.780785
1	-1.087000	2.157904	-2.361272
1	-2.547007	1.165536	-2.227703
1	-1.707140	1.300777	-3.780785
1	-0.990984	-2.205323	-2.362743
1	-2.493276	-1.278552	-2.235446
1	-1.642927	-1.376386	-3.785514

TS (2-Me8.+ -> 3-Me8+.)

(not found)

3-Me8+.

Electronic energy= - 585.699373

Zero-point correction= 0.346367

Sum of electronic and zero-point Energies= -585.353006

Sum of electronic and thermal Energies= -585.332779
Sum of electronic and thermal Enthalpies= -585.331834
Sum of electronic and thermal Free Energies= -585.401262
Frequencies -- 41.9531 45.1133 71.4501
Charge = 1 Multiplicity = 2

6	0.129164	-0.246091	0.185467
6	-1.237493	0.138703	0.187032
6	1.456883	0.088824	0.007878
6	-2.002010	-0.925961	-0.429196
6	1.163229	-1.328888	0.412736
6	-0.821347	2.496455	1.050657
6	2.042257	2.277075	-1.063280
6	-2.895735	-0.654483	-1.598041
6	1.388013	-1.783302	1.856696
6	-1.938674	-2.340949	0.041195
6	1.409406	-2.416891	-0.634887
6	-1.712936	1.417366	0.513147
6	2.399904	0.961918	-0.441567
6	-3.175592	1.753922	0.456144
6	3.854235	0.612600	-0.363845
1	-2.617590	-1.313536	-2.433085
1	0.748308	-2.636664	2.107997
1	-2.857261	0.380087	-1.940771
1	1.191496	-0.980340	2.572995
1	-3.939039	-0.908003	-1.357765
1	2.428567	-2.104612	1.982668
1	-2.939865	-2.611312	0.413933
1	2.458119	-2.731213	-0.594435
1	-1.233399	-2.498559	0.856239
1	1.200153	-2.059880	-1.647724
1	-1.728282	-3.041182	-0.776978
1	0.794993	-3.301781	-0.439794
1	4.286022	0.558601	-1.373074
1	-3.466532	2.322966	1.346816
1	-3.819603	0.874137	0.391202
1	4.030647	-0.336543	0.145537
1	-3.400950	2.399468	-0.405776
1	4.406408	1.405086	0.159098
1	0.215010	2.183152	1.178179
1	0.967032	2.405121	-1.193284

1	-1.196361	2.837285	2.024693
1	2.529900	2.372171	-2.042267
1	-0.841371	3.379428	0.395708
1	2.427777	3.104336	-0.450926