Phys. Chem. Chem. Phys.

Supporting Information for

Atmospheric Oxidation Mechanism of Gas-Phase Ozonolysis of Limonene in the Atmosphere.

Lingyu Wang[a] and Liming Wang[a,b]

[(a)] School of Chemistry & Chemical Engineering, South China University of Technology, Guangzhou, China 510640. E-mail: wanglm@scut.edu.cn.
[(b)] Guangdong Provincial Key Laboratory of Atmospheric Environment and Pollution Control, South China University of Technology, Guangzhou 510006, China

Figure S1. Time profiles of yields for Criegee intermediates in the reaction of Limonene and O_3 at 298 K and 760 Torr from RRKM-ME calculation.
Figure S2. Fractional yields of the Criegee intermediates and from 238 K to 328 K at 760 Torr from RRKM-ME calculation.
Figure S3. (A) The potential energy profiles of internal rotations for Syn-2a at M06-2X level. (B) The potential energy profiles of internal rotations for Syn-2b at M06-2X level. (C) The potential energy profiles of internal rotations for Anti-2b at M06-2X level.
Figure S4. The formation of CIs* and their decay curve (molar fraction relative to limonene consumed) in the ozonolysis of limonene in the processes of limonene + O_3 → POZs → CI* → P, in which CI is Anti-2b, Syn-2b, Syn-2a or Anti-2c, and P is SOZ, VHP, or Dioxirane. Five, one and zero of the internal rotations are treated as hindered rotors for isomerizations to SOZs, VHPs, and Dioxiranes, respectively.
Figure S5. The microcanonical rates of Criegee intermediates from RRKM theory. Five, one and zero of the internal rotations are treated as hindered rotors for isomerizations to SOZs, VHPs, and Dioxiranes, respectively.
Figure S6. **(A)**. The normalized internal energy distributions in Syn-2a* formed in the reaction of limonene + O_3 → POZs → Syn-2a* when subject to isomerization to SOZ, VHP, or Dioxirane at different reaction time (from RRKM-ME calculations). **(B)**. The normalized internal energy distributions in Syn-2b* formed in the reaction of limonene + O_3 → POZs → Syn-2b* when subject to isomerization to SOZ, VHP, or Dioxirane at different reaction time (from RRKM-ME calculations). **(C)**. The normalized internal energy distributions in Anti-2b* formed in the reaction of limonene + O_3 → POZs → Syn-2b* when subject to isomerization to SOZ, VHP, or Dioxirane at different reaction time (from RRKM-ME calculations).
Figure S7. Prior distributions and unimolecular rates of Anti-2c at reaction time of 10^{-8} s.
Figure S8. Decay of Anti-2c starting from the energy distributions, all at 298 K and 760 Torr. Initial fractions are 1.
Figure S9. Normalized energy distributions of SOZs from (A) Anti-2b, (B) Syn-2b and (C) Syn-2a (in the timescale of 10^{-8} s^{-1}) and *k(E)* of the decomposition of SOZs. Available energies are 445 kJ/mol (37200 cm^{-1}).
Table S1. Geometries and harmonic vibrational frequencies of important species and transition states in reaction of limonene with O_3 at M06-2X/6-311++G(2df,2p) level.

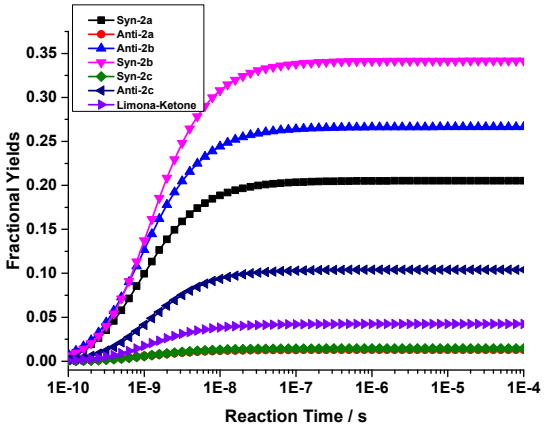


Figure S1. Time profiles of yields for Criegee intermediates in the reaction of Limonene and O_3 at 298 K and 760 Torr from RRKM-ME calculation.

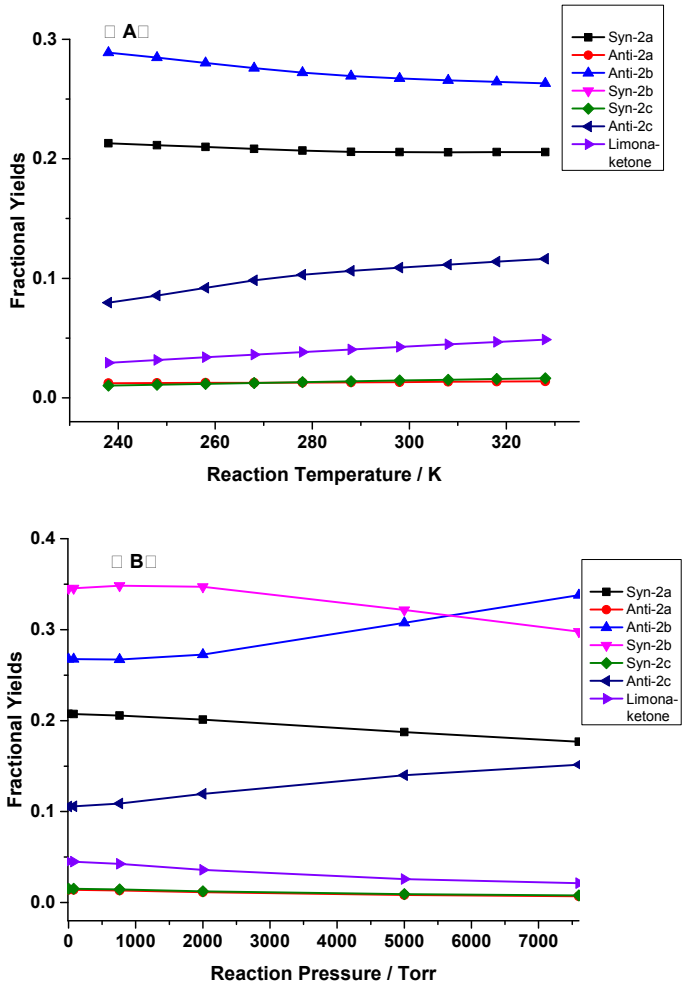


Figure S2. Fractional yields of the Criegee intermediates from (A) 238 K to 328 K at 760 Torr, (B) 0.76 Torr to 7600 Torr at 298 K from RRKM-ME calculation.

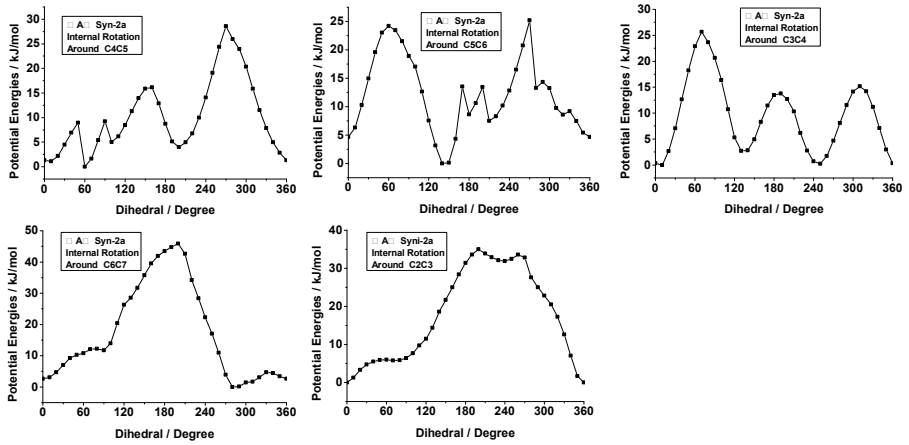


Figure S3(A) The potential energy profiles of internal rotations for Syn-2a at M06-2X level.

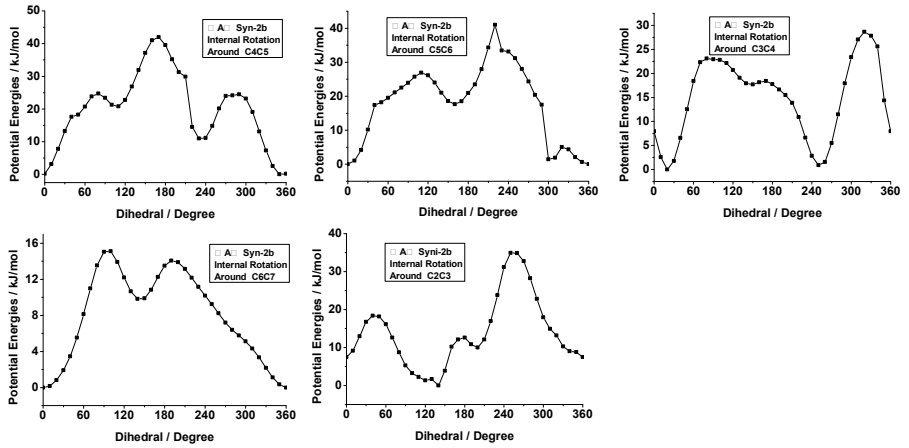


Figure S3(B) The potential energy profiles of internal rotations for Syn-2b at M06-2X level.

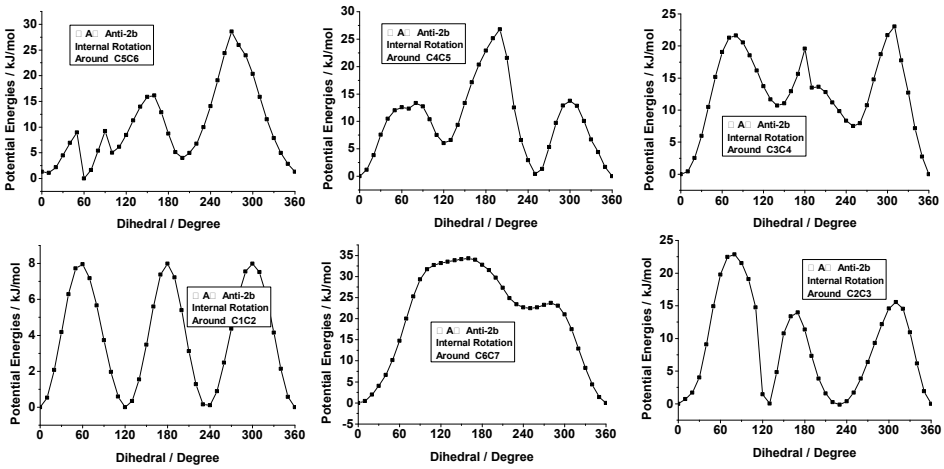


Figure S3(C) The potential energy profiles of internal rotations for Anti-2b at M06-2X level.

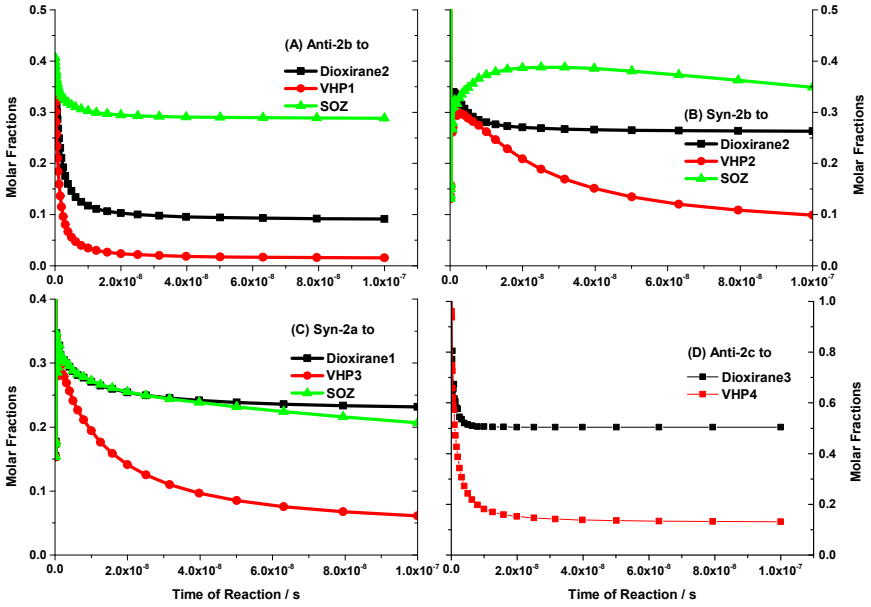


Figure S4. The formation of CIs* and their decay curve (molar fraction relative to limonene consumed) in the ozonolysis of limonene in the processes of limonene + O_3 → POZs → CI* → P, in which CI is Anti-2b, Syn-2b, Syn-2a or Anti-2c, and P is SOZ, VHP, or Dioxirane. Five, one and zero of the internal rotations are treated as hindered rotors for isomerizations to SOZs, VHPs, and Dioxiranes, respectively.

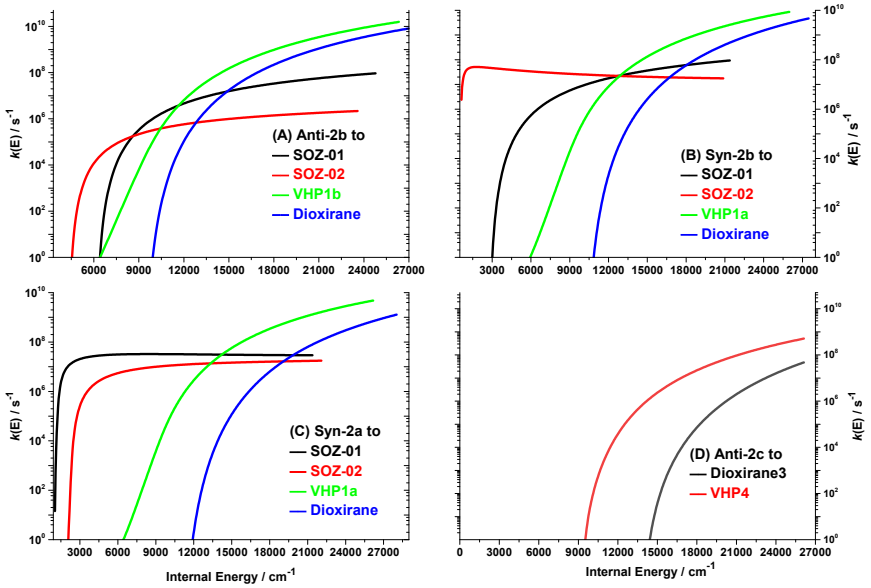


Figure S5. The microcanonical rates of Criegee intermediates from RRKM theory. Five, one and zero of the internal rotations are treated as hindered rotors for isomerizations to SOZs, VHPs, and Dioxiranes, respectively. Note that the rate coefficient for SOZ formation in Syn-2b decreases with increasing energy is an artifact of freezing some of the vibrational modes in the TS.

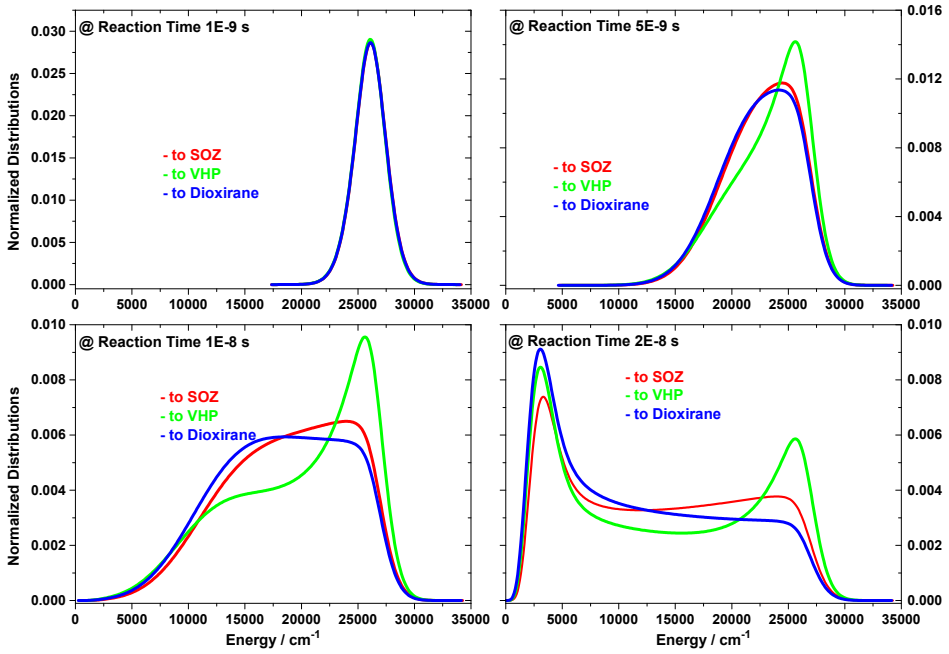


Figure S6(A). The normalized internal energy distributions in Syn-2a* formed in the reaction of limonene + O_3 → POZs → Syn-2a* when subject to isomerization to SOZ, VHP, or Dioxirane at different reaction time (from RRKM-ME calculations)

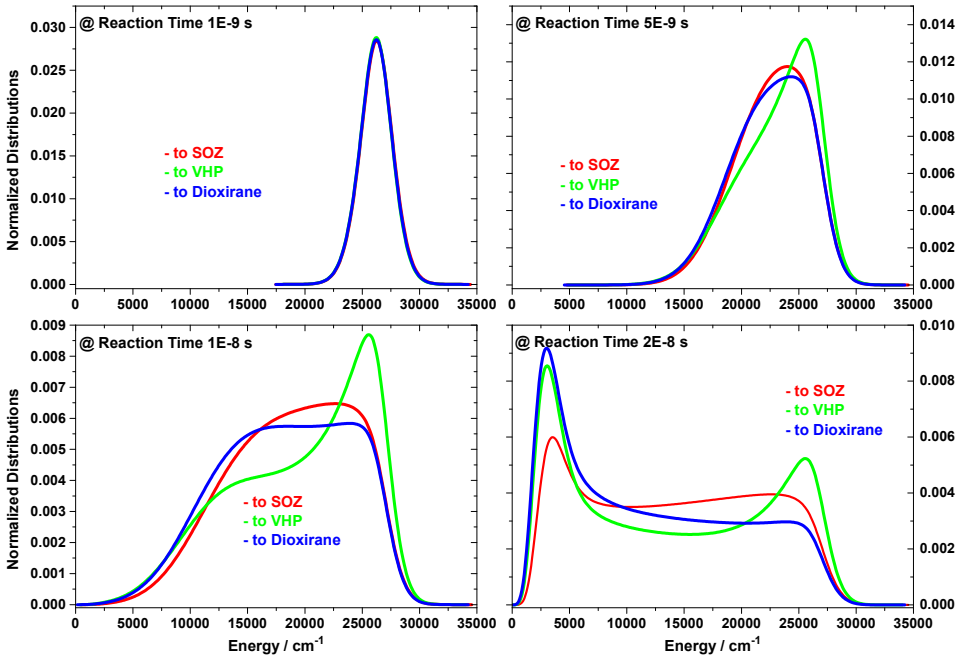


Figure S6(B). The normalized internal energy distributions in Syn-2b* formed in the reaction of limonene + O_3 → POZs → Syn-2b* when subject to isomerization to SOZ, VHP, or Dioxirane at different reaction time (from RRKM-ME calculations)

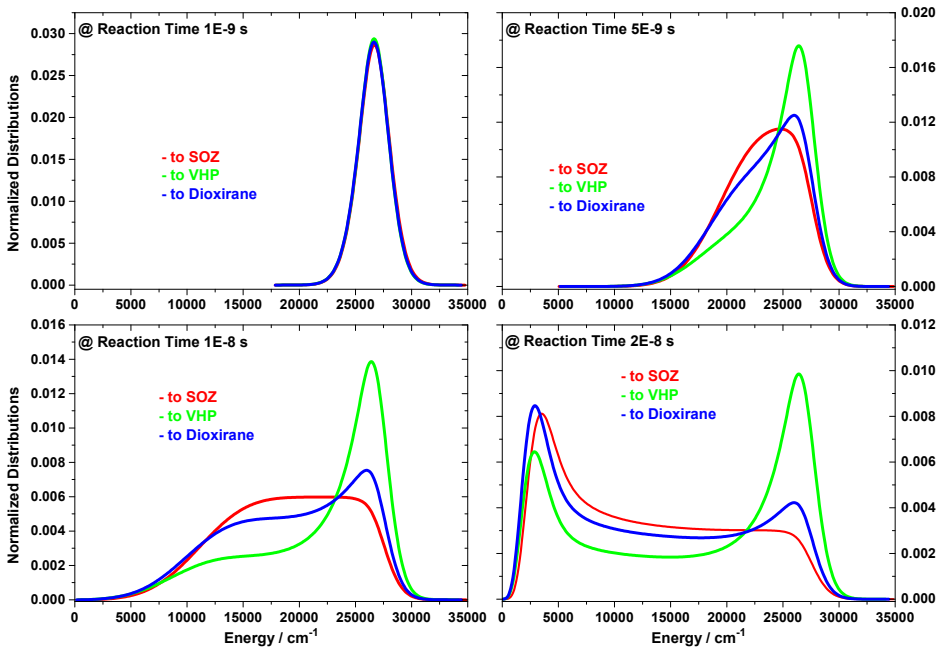


Figure S6(C). The normalized internal energy distributions in Anti-2b* formed in the reaction of limonene + O_3 → POZs → Syn-2b* when subject to isomerization to SOZ, VHP, or Dioxirane at different reaction time (from RRKM-ME calculations)

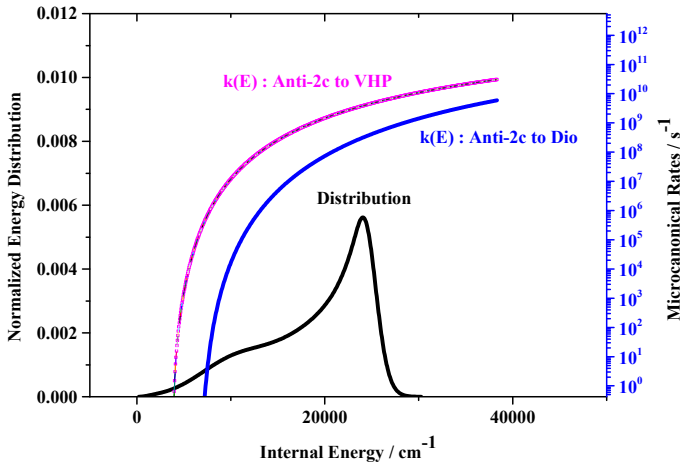


Figure S7. Prior distributions and unimolecular rates of Anti-2c at reaction time of 10^{-8} s.

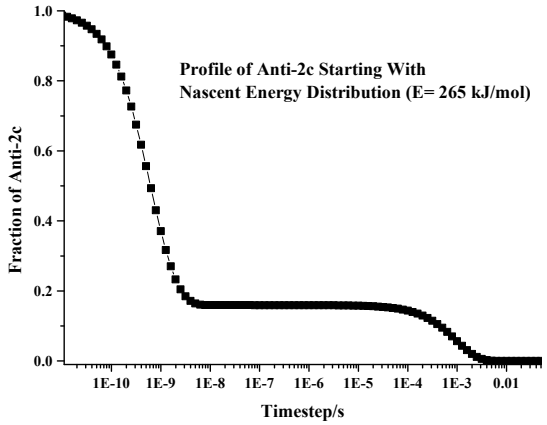
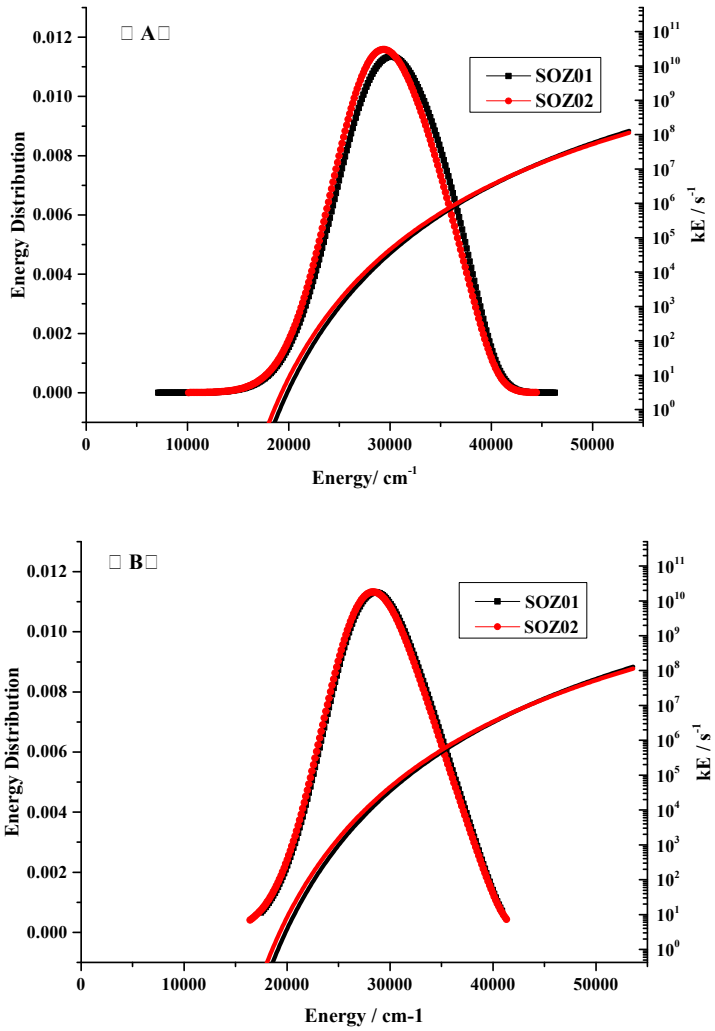


Figure S8. Decay of Anti-2c starting from the energy distributions, all at 298 K and 760 Torr. Initial fractions are 1.



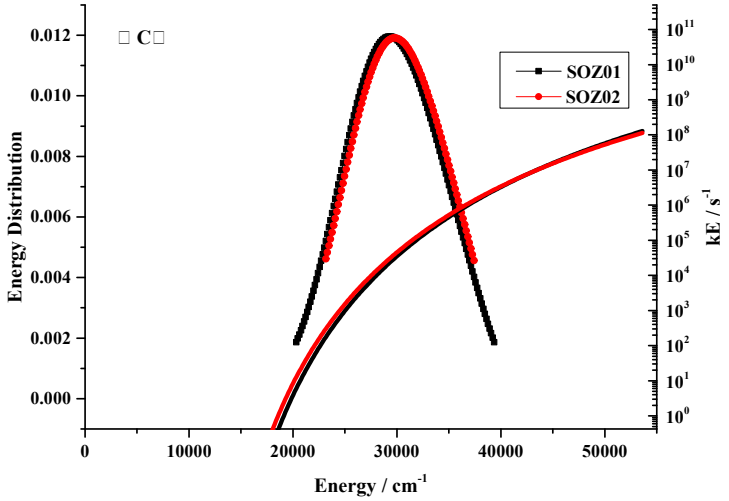


Figure S9. Normalized energy distributions of SOZs from (A) Anti-2b, (B) Syn-2b and (C) Syn-2a (in the timescale of 10^{-8} s^{-1}) and *k(E)* of the decomposition of SOZs. Available energies are 445 kJ/mol (37200 cm^{-1}).

Table S1. Geometries and harmonic vibrational frequencies of important species and transition states in reaction of limonene with O_3 at M06-2X/6-311++G(2df,2p) level.

Cartesian Coordinates (in Angstrom)	Vibrational Frequencies
Elements	(in cm^{-1})
limonene 0,1 C,0,-0.0088230586,-1.1865075526,-0.3162787206 C,0,1.4827320972,-1.1100334064,-0.6231341116 C,0,2.1634034674,0.0453618914,0.0642718339 C,0,1.4656934497,1.0411176037,0.6015793516 C,0,-0.0326819544,1.1520614107,0.5524119296 C,0,-0.6621163764,0.1833298915,-0.4616320301 H,0,1.9753447787,-2.0402863113,-0.3269731233 H,0,1.6429057884,-1.022410969,-1.7039469774 H,0,-0.4162865409,0.5641763956,-1.462030558 H,0,-0.1498843549,-1.5398824474,0.7094991056 H,0,1.9975932333,1.8420680244,1.1055384051 H,0,-0.3055983105,2.1804373688,0.3072959139 H,0,-0.4570021889,0.9546089973,1.5440560887 H,0,-0.4895943015,-1.9095176342,-0.9764147063 C,0,3.6620532667,-0.0027347337,0.0982961427 H,0,4.0670037165,-0.0800537581,-0.9137824218 H,0,4.0829011402,0.8833538685,0.5702020642 H,0,4.0076274543,-0.8838353467,0.6439968186 C,0,-2.1685917755,0.1861309403,-0.3416680491 C,0,-2.835669924,1.5084232105,-0.6082888598 H,0,-3.91819015,1.4042137985,-0.6414473853 H,0,-2.5894109887,2.2360774095,0.1673288472 H,0,-2.4965970285,1.9284358083,-1.5580286794 C,0,-2.878929813,-0.8865833423,-0.0114846939 H,0,-2.4218684257,-1.8446885335,0.1918624345 H,0,-3.9572109009,-0.834518934,0.0667712207	63.0211 79.5179 167.1485 183.9152 191.6462 224.8378 267.5967 314.7646 334.3557 358.6328 437.4452 450.7528 494.8709 532.1807 559.5492 654.8884 723.5392 785.7399 823.47 825.0301 914.5445 937.7686 939.456 950.5773 983.3544 1009.0931 1022.1575 1044.6067 1053.4856 1063.5269 1086.2192 1113.445 1151.238 1176.5688 1187.5311 1229.5816 1274.2144 1284.1046 1320.9798 1335.4399 1344.6121 1366.8686 1406.2924 1412.9218 1418.283 1420.2808 1459.192 1478.6145 1484.5564 1484.951 1491.725 1497.1625 1501.761 1508.8411 1737.7254 1768.9032 3004.0374 3023.546 3027.0188 3036.582 3040.7038 3051.6328 3060.9073 3084.7335 3090.6415 3095.2572 3111.4401 3128.1505 3137.0385 3142.3943 3155.4926 3235.2026
UM06-2X/6-311++G(2df,2p): E = -390.381391 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -389.8616086 Hartree	

O_3 0,1 O,0,-1.0370035806,2.3522674055,-0.02985346 O,0,0.1893212393,2.2570652672,-0.02985346 O,0,-1.5361006987,3.4764729374,-0.02985346	796.6021 1376.8923 1384.4189
UM06-2X/6-311++G(2df,2p): E = -390.381391 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -389.8616086 Hartree	
PRC1 0,1 C,0,-0.9690472608,-1.5994351792,-0.6217680281 C,0,0.5196832247,-1.7862383163,-0.8972975958 C,0,1.3976303127,-1.1740727089,0.164243023 C,0,0.913825762,-0.2950537692,1.0411658146 C,0,-0.5147042654,0.1751392247,1.0726132104 C,0,-1.2695569744,-0.1587718759,-0.2232182571 H,0,0.7569814385,-2.8499196973,-0.9856044529 H,0,0.7821844874,-1.3467803914,-1.8675895719 H,0,-0.8675990774,0.4951130995,-1.0097059909 H,0,-1.2740114423,-2.262567981,0.1930603792 H,0,1.5786233428,0.1100933132,1.7974001593 H,0,-0.5348149033,1.2508998636,1.2538805727 H,0,-1.0398810859,-0.2876618009,1.9165875396 H,0,-1.5488795401,-1.8799461469,-1.5019741906 C,0,2.8254721207,-1.6352761423,0.183905676 H,0,3.2718321215,-1.5584095537,-0.809615963 H,0,3.4267562438,-1.0499759559,0.8773572944 H,0,2.880223148,-2.6866632701,0.4764976192 C,0,-2.7376014243,0.1749542456,-0.0914886886 C,0,-3.0462332265,1.6217905827,0.1842973307 H,0,-4.1127343486,1.8202542837,0.1008204786 H,0,-2.7270383948,1.9055560697,1.1888044622 H,0,-2.513376759,2.2720974687,-0.5131324609 C,0,-3.7064545177,-0.7280016784,-0.1943172961 H,0,-3.5079545833,-1.77416281,-0.3802105807 H,0,-4.7447754704,-0.440483425,-0.0898097191 O,0,1.580043065,1.6005162922,-1.4648987035 O,0,1.3079006645,2.2208084802,-0.4356423061 O,0,2.6066274125,0.9219396385,-1.4734752645	30.896 46.6747 51.8744 68.3412 97.4068 112.9331 127.3 172.8725 186.4739 202.5265 213.7056 235.2516 277.7793 314.2992 339.195 360.4218 443.6598 451.4593 491.909 535.969 555.6255 654.3684 726.4415 784.9969 794.9196 824.1336 831.9194 914.7948 938.0461 941.7176 951.6726 980.7966 1009.5699 1021.4429 1051.0209 1055.1949 1062.9417 1084.9632 1114.9228 1149.1554 1176.2153 1189.0726 1234.9344 1278.9511 1286.9386 1316.8745 1337.9772 1344.2834 1359.8429 1363.9073 1380.6551 1406.0636 1410.4455 1421.7485 1424.3619 1455.7049 1481.1733 1484.6589 1485.954 1491.7769 1500.3139 1502.3118 1509.9323 1730.1475 1740.6565 2998.2954 3020.2469 3020.896 3040.6344 3041.4862 3045.7632 3064.1403 3080.3437 3094.1427 3100.1599 3103.0413 3139.3705 3147.7666 3155.6601 3158.6521 3239.7253
UM06-2X/6-311++G(2df,2p): E = -615.7746242 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0734527 Hartree	
TS1 0,1 C,0,-0.9566696843,-1.5848758278,-0.6429914201 C,0,0.5235987518,-1.7581070567,-0.9766859121 C,0,1.4398635667,-0.9885341568,-0.0530805717 C,0,0.9425873157,-0.1880234912,0.9429091112 C,0,-0.4931927328,0.2395683846,0.9807023001 C,0,-1.2646959749,-0.1329460493,-0.297355535 H,0,0.8014647746,-2.8131717977,-0.8968671992 H,0,0.7232180099,-1.4745519922,-2.011036991 H,0,-0.8815575689,0.4944184449,-1.1116775959 H,0,-1.2178311644,-2.2150115815,0.2124378164 H,0,1.5509114075,0.0107168013,1.8162596445 H,0,-0.5280916234,1.3174573087,1.1519753047 H,0,-0.989548281,-0.2240666033,1.8412632465 H,0,-1.5649602054,-1.9175380293,-1.4840648114 C,0,2.8787647215,-1.3922070645,-0.0531653929	-343.8054 49.1825 57.3681 92.2096 135.0734 155.7432 182.2718 197.325 203.1317 217.9537 232.7686 278.9878 312.4538 342.7231 371.4544 444.5864 475.5644 486.4824 503.077 553.642 567.573 658.2469 729.7364 779.9842 794.4707 816.1725 865.9931 911.1193 929.8017 934.1499 955.9881 966.5885 1003.0454 1019.8073 1041.8025 1051.4002 1058.6265 1077.6416 1114.6441 1146.9448 1162.5908 1182.9021 1215.2667 1230.5717 1270.934

H,0,3.253635504,-1.4469195652,-1.0757915624	1272.0776 1285.0459 1318.7163
H,0,3.4859063778,-0.6780242464,0.4992753613	1324.1789 1346.471 1367.9091
H,0,2.992633849,-2.3826622245,0.3946147293	1393.5903 1411.0593 1414.0059
C,0,-2.7326733073,0.1898251552,-0.137713318	1420.0026 1456.6288 1467.8687
C,0,-3.05581895,1.6482573396,0.0405300322	1477.8574 1483.1079 1491.3689
H,0,-4.1295943926,1.8208872626,0.008871358	1497.2327 1501.5755 1507.8406
H,0,-2.6821097149,2.0210677634,0.9959220643	1610.1391 1734.3923 3015.2091
H,0,-2.5822573383,2.2463267272,-0.7409768134	3027.37 3040.5764 3043.7483
C,0,-3.6871361692,-0.733746591,-0.1404803565	3046.7037 3050.2124 3090.8368
H,0,-3.4759206131,-1.7869572625,-0.2619763102	3091.2852 3105.5191 3108.1161
H,0,-4.7262945639,-0.4566583485,-0.0192645133	3114.3529 3138.0702 3158.2326
O,0,1.4333561932,1.7050410787,-0.8126610106	3158.3978 3182.7501 3238.7404
O,0,1.9475288852,1.6847724479,0.3423521941	
O,0,1.8073321975,0.7206036042,-1.518562869	
UM06-2X/6-311++G(2df,2p): E = -615.7671373 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0666574 Hartree	
POZ1 0,1	
C,0,-0.5618791836,-1.150950869,-1.1272568826	26.8902 63.8115 134.9323
C,0,0.8858653374,-0.98020298,-1.5812440745	145.3122 178.3016 187.0459
C,0,1.7903792898,-0.4308900535,-0.4777335718	209.2364 239.0469 262.7777
C,0,1.1741450344,0.7740336553,0.2423437413	294.994 354.7539 376.1027
C,0,-0.312052589,0.686480132,0.5374890865	392.7331 444.3745 450.6052
C,0,-1.1382434072,0.1797289242,-0.6519571352	488.1659 543.5282 550.8564
H,0,1.299860433,-1.9270015996,-1.930938183	623.442 659.9419 725.5851
H,0,0.9166084649,-0.281586513,-2.418049267	747.0094 763.4876 812.4989
H,0,-1.0174534846,0.9086302096,-1.4628561853	875.31 891.6109 915.0385
H,0,-0.6248247259,-1.8856106961,-0.3180255183	924.1791 944.0774 959.9384
H,0,1.7334231198,0.9507525745,1.1658694611	972.1876 995.7143 1010.9761
H,0,-0.6497297468,1.6687039458,0.8679122482	1021.2213 1043.6945 1051.2935
H,0,-0.4492920721,0.0031935209,1.381956833	1065.9009 1080.2394 1100.8634
H,0,-1.1549958034,-1.5433820257,-1.9539654485	1147.3823 1176.2025 1187.9717
C,0,2.2948912938,-1.4938886629,0.472520439	1212.4513 1263.057 1270.8523
H,0,2.8305046567,-2.2655737202,-0.0781323229	1291.005 1312.2829 1318.5472
H,0,2.9622951476,-1.0617997759,1.2161443	1343.8299 1364.0193 1374.7621
H,0,1.452633365,-1.9602436369,0.9834002567	1388.5849 1412.1445 1416.3501
C,0,-2.6089773697,0.145630165,-0.3009639256	1421.6236 1427.2836 1459.8118
C,0,-3.2354117926,1.4803434619,0.0025241333	1475.1715 1488.4184 1489.3965
H,0,-4.3184957504,1.3992501202,0.064798758	1493.125 1499.963 1509.1215
H,0,-2.8745240081,1.8817134753,0.9510241247	1510.8524 1735.6683 3020.5653
H,0,-2.9835823587,2.2107861051,-0.7690349536	3035.7309 3040.9267 3042.9647
C,0,-3.3226004063,-0.9736971342,-0.2566102422	3058.1716 3059.4091 3063.4896
H,0,-2.8963360626,-1.944203923,-0.4680065484	3090.3832 3093.3638 3104.9433
H,0,-4.3748342837,-0.9490485338,-0.0048577184	3111.6261 3136.9282 3139.3571
O,0,2.4001051974,1.371278222,-1.6073048773	3143.9817 3162.6385 3246.4899
O,0,1.4343483585,1.8516364664,-0.648682089	
O,0,2.9360018262,0.2113269156,-1.0371523582	
UM06-2X/6-311++G(2df,2p): E = -615.881057 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1608158 Hartree	
PRC2 0,1	
C,0,0.0686669753,1.5143225688,0.1061314488	27.701 39.3526 61.9771
C,0,-1.3664520358,1.6416888709,-0.3949703019	78.9067 94.9684 117.089
C,0,-2.1763118465,0.3918011406,-0.1625897559	125.4909 148.9167 180.7299
C,0,-1.5981584958,-0.7601287271,0.1838743763	185.2983 210.2682 251.2942
C,0,-0.1151939999,-0.9673631096,0.2823299233	285.5419 314.6764 334.5084
C,0,0.6804813465,0.1908364956,-0.3401062895	360.008 444.0495 456.8296

H,0,-1.8656026568,2.4783630118,0.1017331913 H,0,-1.3755517358,1.8815459578,-1.4630558504 H,0,0.5527929008,0.1146011966,-1.427639763 H,0,0.0777917515,1.5605588146,1.1993186072 H,0,-2.2266986877,-1.6166185342,0.4074335418 H,0,0.1373239925,-1.9062831876,-0.2144902559 H,0,0.1793361093,-1.0845790604,1.331990496 H,0,0.664901463,2.3516920665,-0.2580085748 C,0,-3.6621049855,0.5244164799,-0.3170357083 H,0,-3.9110912624,0.9068428744,-1.3105386301 H,0,-4.1692121901,-0.4291282573,-0.1743885962 H,0,-4.0650830371,1.2396590195,0.4036827021 C,0,2.1552569492,0.0410636652,-0.0489201947 C,0,2.796966114,-1.2065455024,-0.5936571287 H,0,3.879591843,-1.1695046234,-0.4916866792 H,0,2.4383593415,-2.0937319775,-0.0680546879 H,0,2.5491130591,-1.3406609189,-1.6487955881 C,0,2.8584920269,0.9254935121,0.6495530219 H,0,2.4182896404,1.8233465319,1.0596590862 H,0,3.9139260958,0.7714486376,0.8346348069 O,0,-2.4223483451,-1.3449890439,-2.7817333935 O,0,-1.8714581964,-2.2661066398,-2.1739871937 O,0,-1.7957775541,-0.2889325814,-2.90270279	490.3551 532.5031 557.17 655.2407 726.4436 783.8943 799.1978 821.8421 832.112 915.8002 937.2255 941.4554 950.0375 979.6127 1008.4743 1021.202 1047.2903 1051.29 1060.8801 1083.3638 1113.4008 1151.1097 1178.2901 1187.9694 1231.1164 1275.5116 1285.6087 1321.058 1335.9241 1339.6304 1346.3065 1367.7326 1373.0722 1405.859 1410.6123 1417.9704 1420.1512 1454.4715 1478.3333 1481.1977 1485.5522 1487.973 1496.1903 1498.5888 1505.2421 1734.9571 1736.6628 3009.6262 3021.546 3035.9948 3038.6647 3040.0526 3043.1799 3069.4553 3080.3389 3088.8235 3099.3139 3101.0771 3132.0877 3137.9475 3140.2968 3154.4372 3237.5531
UM06-2X/6-311++G(2df,2p): E = -615.7761686 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0746576 Hartree	
TS2 0,1 C,0,0.6554829902,1.1158502768,-0.9346830409 C,0,-0.8604647057,1.2515945051,-1.0701225672 C,0,-1.6235538597,0.6812646495,0.0991788488 C,0,-0.9849689567,0.0161616464,1.1090862619 C,0,0.4677548576,-0.3410945933,1.0630661918 C,0,1.032227497,-0.2463925311,-0.3615882392 H,0,-1.1359506112,2.3056135814,-1.1665345074 H,0,-1.2030352341,0.7675398703,-1.9879031674 H,0,0.524858054,-1.0175970814,-0.9542809246 H,0,1.0376252636,1.8961871026,-0.2697798444 H,0,-1.5032431591,-0.1166159082,2.0521234541 H,0,0.5897576533,-1.3479187881,1.4642105525 H,0,1.0353524602,0.329640562,1.7188919054 H,0,1.1239743395,1.2663353472,-1.9074756537 C,0,-3.0503632914,1.113411867,0.2644287118 H,0,-3.5430995678,1.2072398056,-0.7025077838 H,0,-3.6085531239,0.4000961253,0.8723577748 H,0,-3.0978604847,2.0854076677,0.7615895017 C,0,2.5111864008,-0.5554500785,-0.3734420566 C,0,2.8793785107,-1.9609931354,0.0166941126 H,0,3.9398543269,-2.1483741417,-0.1388465976 H,0,2.6529961437,-2.1513775075,1.0672057235 H,0,2.3065108872,-2.6844391383,-0.5671340835 C,0,3.4413848455,0.3369775161,-0.6946922711 H,0,3.1991810224,1.3525287831,-0.9750589009 H,0,4.4906654563,0.0715227446,-0.6861945175 O,0,-2.595124904,-1.8750534184,-0.0770792038 O,0,-1.6846251503,-2.1037652046,0.7627398657 O,0,-2.18803919,-1.2163578941,-1.071622355	- 302.8742 44.1324 52.2391 82.0218 126.616 140.7795 170.1913 186.3853 195.9562 212.5973 227.5978 269.4498 315.7612 342.6985 371.1701 448.0378 460.9712 465.7932 499.5621 556.483 559.3468 655.1975 733.6835 779.9487 795.632 818.9126 858.3521 912.4149 936.2541 937.8513 956.0124 966.5797 1004.6496 1018.854 1043.0977 1054.772 1060.954 1080.3152 1117.972 1145.6685 1166.354 1184.5631 1219.0987 1234.348 1275.5663 1286.8564 1290.4464 1320.7711 1332.4977 1349.7672 1370.8388 1401.4791 1413.7943 1414.6459 1423.428 1455.7886 1473.4999 1479.1095 1487.7116 1489.6452 1491.3264 1501.1705 1510.1558 1619.0171 1730.2683 3024.4343 3036.8243 3040.5878 3043.9634 3047.4844 3052.4686 3080.9441 3095.8083 3101.5208 3106.1537 3107.8373 3135.1872 3136.9163 3154.7483 3160.1275 3239.4393
UM06-2X/6-311++G(2df,2p): E = -615.7704613 Hartree	

RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0699531 Hartree

POZ2
0,1

C,0,-0.6395470177,-0.9572263026,-1.1793307158	29.0571	47.8638	123.946
C,0,0.6748501165,-1.5101323678,-0.6177030435	151.5975	163.86	194.6341
C,0,1.6682292114,-0.4385117813,-0.2022056415	234.949	268.4766	273.5202
C,0,1.0417813208,0.5915341396,0.7836224643	297.2227	336.7838	367.3011
C,0,-0.4658618067,0.4637949306,0.9148397412	391.5617	440.6566	496.9302
C,0,-1.1216551298,0.3230383804,-0.4668315559	506.5153	527.2378	570.446
H,0,0.4831294605,-2.1156077927,0.2713529801	628.4056	657.1555	724.8829
H,0,1.1502899195,-2.1720367107,-1.3429684276	735.6054	768.21	804.7797
H,0,-0.7687092356,1.1765611387,-1.0499011556	876.7808	903.7069	916.4355
H,0,-1.3921674662,-1.7404831252,-1.1138954497	929.9435	940.0503	945.1393
H,0,1.540833303,0.5364315236,1.7541883574	951.6853	1005.4186	1015.2496
H,0,-0.8506874615,1.3408313654,1.4377920092	1018.4468	1033.086	1040.6056
H,0,-0.7040363275,-0.4039059676,1.5352642407	1061.9412	1075.6514	1100.9668
H,0,-0.5165283937,-0.7354921503,-2.2385273578	1140.6768	1152.7556	1164.4299
C,0,2.9655864506,-1.0187729672,0.3317734146	1224.6164	1255.8826	1262.1125
H,0,3.4037936928,-1.6941025451,-0.4021183902	1277.2916	1301.5238	1321.7887
H,0,3.6738975192,-0.2194172051,0.5446392315	1347.2741	1362.8848	1370.3841
H,0,2.7814536711,-1.5741185688,1.2519836137	1385.3422	1406.9138	1409.1134
C,0,-2.6248238702,0.465371237,-0.3308914382	1412.9616	1420.6539	1455.1025
C,0,-3.1285316156,1.8773583927,-0.4325636405	1476.729	1486.4697	1488.9785
H,0,-4.1926536146,1.9441925422,-0.2158377856	1493.565	1496.0382	1499.9332
H,0,-2.5908213674,2.5324031301,0.2567768225	1508.4204	1744.9052	3036.8661
H,0,-2.9500840122,2.2686048413,-1.4363554191	3046.619	3052.6125	3055.2357
C,0,-3.4441068024,-0.5493106609,-0.0829949925	3063.7348	3073.3507	3080.9648
H,0,-3.0980149705,-1.5711628979,-0.002961721	3089.7295	3093.9056	3099.9635
H,0,-4.5048358168,-0.386145485,0.0550370588	3126.0086	3134.0732	3135.8492
O,0,2.3528976008,1.5835442766,-0.7536599122	3140.6198	3154.9352	3233.322
O,0,1.3190441782,1.8514673277,0.1757724495			
O,0,1.9239672641,0.3845722923,-1.341648617			

UM06-2X/6-311++G(2df,2p): E = -615.8787048 Hartree
RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1587739 Hartree

PRC3
0,1

C,0,0.0071725857,1.3310796338,-0.0065362114	39.4583	55.2977	62.9337
C,0,-1.4678998411,1.2047079603,-0.3763096959	83.3371	102.5923	111.3052
C,0,-2.0814591087,-0.1010108597,0.0592356766	133.063	170.2462	182.0195
C,0,-1.3273923168,-1.1430339592,0.4162287571	201.9976	223.6897	261.7763
C,0,0.1723897789,-1.1153898879,0.4655242098	293.0638	322.7618	335.772
C,0,0.7685389525,0.0522746865,-0.3366504794	357.8806	445.3681	449.6674
H,0,-2.0378337233,2.0291850295,0.0595073927	497.8805	535.9125	558.9143
H,0,-1.5939714766,1.2960594083,-1.4612862685	652.5908	726.3674	783.0626
H,0,0.5986294786,-0.1732036613,-1.3980904656	794.8928	821.8099	834.5223
H,0,0.0938343302,1.532680243,1.0649404411	914.147	936.4185	939.1489
H,0,-1.8129644582,-2.072260762,0.693888084	954.0729	983.4506	1008.7845
H,0,0.5614368414,-2.0663807732,0.0978764063	1022.1603	1045.0498	1051.8157
H,0,0.5103838393,-1.0371172209,1.5087852837	1066.0225	1088.0165	1114.0661
H,0,0.4492273879,2.1800629301,-0.5295171573	1150.4875	1172.1591	1193.9413
C,0,-3.5769844108,-0.1657335713,0.0376103788	1227.1282	1273.604	1283.395
H,0,-3.9615334393,0.1045437909,-0.9487935447	1318.6728	1331.9614	1338.9613
H,0,-3.9404421154,-1.1586243607,0.2955323471	1346.9426	1362.7741	1374.5683
H,0,-3.9911081794,0.5494696862,0.7521769114	1406.8527	1412.773	1417.993
C,0,2.264382877,0.1335739934,-0.1333580444	1420.6262	1460.1311	1478.0618
C,0,3.0439991843,-1.0779036313,-0.5687596385	1478.4947	1481.7494	1491.0415
H,0,4.1145591436,-0.8851296072,-0.5466490465	1492.7165	1500.6167	1507.5901

H,0,2.842262368,-1.930542059,0.0823951178	1730.5329 1735.8978 2994.7744
H,0,2.7646554378,-1.3763497667,-1.5815930324	3009.6459 3018.3795 3034.5482
C,0,2.8742799586,1.1854719694,0.4015290056	3047.3953 3048.1454 3068.9668
H,0,2.3367065838,2.0627790234,0.7325827595	3075.9711 3091.0984 3096.7577
H,0,3.9493149947,1.197119398,0.5275472463	3105.8708 3127.8248 3135.5652
O,0,-1.4638731352,0.0021205348,3.2276902173	3156.6121 3171.5011 3242.333 3209.2166
O,0,-2.0702322735,-1.0684476428,3.1398958048	3218.8043 3864.8131
O,0,-1.9503627041,0.9789694855,2.6481740645	
UM06-2X/6-311++G(2df,2p): E = -615.7763309 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E =-615.0743409 Hartree	
TS3 0,1	
C,0,-0.5525389184,-0.6617527761,1.3875815423	-318.025 41.9711 65.351
C,0,0.7587344046,-1.408039695,1.1775943288	102.3472 140.1665 159.5125
C,0,1.5474854438,-0.9028888425,-0.004392968	164.1031 182.2545 193.0057
C,0,0.9345984965,-0.2308768136,-1.0282376058	205.4782 243.0319 288.2029
C,0,-0.4782850087,0.2599892126,-0.9272367166	325.3402 353.8368 368.8058
C,0,-1.325196563,-0.5410365729,0.0790127946	446.4003 466.3198 493.1738
H,0,1.3775314247,-1.3614178079,2.0746775598	522.5424 534.877 564.663
H,0,0.5571952492,-2.4713881362,0.9999722512	642.3672 725.7052 772.3211
H,0,-1.4541031738,-1.5512843572,-0.3318355681	797.8521 826.7827 859.6245
H,0,-0.3389407825,0.3376608439,1.7756192956	905.1029 920.4246 948.0899
H,0,1.4270567821,-0.1806980519,-1.9900875848	952.4137 984.0064 1009.8045
H,0,-0.9347324478,0.2572481668,-1.9165636555	1018.5211 1028.135 1054.4461
H,0,-0.4679290496,1.3077352407,-0.5946623625	1067.1091 1093.2801 1112.3136
H,0,-1.155225587,-1.1786680272,2.1352683329	1141.4469 1160.4631 1192.8786
C,0,2.9302811524,-1.4452010678,-0.1695495398	1218.0453 1234.2341 1271.7815
H,0,2.8949550644,-2.5237134164,-0.3435346615	1277.4947 1290.5565 1326.552
H,0,3.4441659824,-0.9684486004,-1.0017009968	1337.7008 1345.7088 1359.9403
H,0,3.5108761879,-1.276172437,0.7376206543	1402.699 1413.5069 1417.4879
C,0,-2.7059480289,0.0607232857,0.2109776584	1423.2502 1452.4255 1476.9908
C,0,-3.5425646068,0.0458259623,-1.0397958202	1478.6815 1486.5309 1490.948
H,0,-4.5685064128,0.3408402409,-0.8297694876	1495.4433 1500.3061 1507.7764
H,0,-3.1438572588,0.7309416109,-1.7902703406	1611.219 1732.1279 2996.2053
H,0,-3.5520120515,-0.9496913314,-1.488941448	3015.0418 3021.9468 3042.2066
C,0,-3.1687015332,0.5812387246,1.3416347421	3052.4118 3053.6248 3092.7004
H,0,-2.5827563913,0.6118714649,2.2491455283	3096.386 3101.069 3107.7171
H,0,-4.1647325387,1.0019768163,1.3899084122	3115.5815 3133.5056 3152.9629
O,0,1.7534570218,1.8495061081,0.3829661612	3153.0287 3187.7986 3234.8012
O,0,2.0859367977,1.6925051144,-0.8234184931	
O,0,2.2139806053,0.9385517612,1.1325490073	
UM06-2X/6-311++G(2df,2p): E = -615.7696933 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.069057 Hartree	
POZ3 0,1	
C,0,0.4167374273,-0.9664609804,-0.9639022774	29.9471 72.9858 73.7414
C,0,-0.9296254062,-1.4939577199,-0.4873055719	169.1528 189.0897 218.7154
C,0,-1.8651017008,-0.4074962422,0.0300781921	226.9297 245.6741 266.6742
C,0,-1.1834072417,0.6597299926,0.8983391792	305.834 343.0591 368.8232
C,0,0.2289758181,1.0437000603,0.4785222572	389.1131 443.4679 460.442
C,0,1.1038587381,-0.1737985098,0.144151858	469.4141 516.2295 560.0648
H,0,-1.4461442504,-2.0319667969,-1.2841730278	610.9872 627.6821 724.8471
H,0,-0.7758680736,-2.2099471857,0.3245829034	751.7033 776.9699 837.1055
H,0,1.1557047168,-0.8140718393,1.0365123558	888.1388 899.8014 917.2244
H,0,0.2682994087,-0.3216750673,-1.8336301963	926.2142 948.3662 954.6967
H,0,-1.2464724357,0.3961141097,1.9545202269	966.9721 986.3356 1014.1108
H,0,0.6681964055,1.6486434444,1.270791282	1022.9245 1038.106 1053.8905

H,0,0.1607493567,1.6689446634,-0.4136071133	1064.0984 1081.7263 1108.5039
H,0,1.0449693729,-1.8004160312,-1.2790984857	1125.9159 1164.7947 1181.3835
C,0,-3.0841683186,-0.995943062,0.7264147415	1200.1737 1240.8239 1264.2514
H,0,-2.7844601687,-1.6148122041,1.5727706245	1278.6699 1298.6615 1308.3235
H,0,-3.7372352217,-0.1997276819,1.0791728902	1343.1132 1353.051 1360.9725
H,0,-3.6411715207,-1.6162170039,0.0248296505	1378.322 1404.5997 1411.5575
C,0,2.5201872662,0.258065076,-0.1652842583	1414.0061 1420.9851 1458.2352
C,0,3.3005835112,0.8104592522,0.9965257478	1482.7315 1487.4631 1492.5958
H,0,4.3362824351,0.9963079839,0.7200498801	1496.6942 1501.5822 1504.5358
H,0,2.8746935909,1.749768447,1.352818349	1507.3921 1738.1147 2989.9368
H,0,3.2867116792,0.113381976,1.8373632592	3046.7884 3047.4432 3051.6406
C,0,3.0594766467,0.1677526383,-1.3753928546	3055.9824 3067.0189 3098.0064
H,0,2.5198937959,-0.2252209986,-2.2254620245	3101.9991 3107.6549 3110.9023
H,0,4.0760222446,0.4943665045,-1.5527727504	3122.4844 3130.547 3141.0098
O,0,-2.2446810909,1.7596792266,-0.6834681601	3148.4867 3156.1701 3236.8119
O,0,-2.0879588338,1.7373895199,0.7129781502	
O,0,-2.3072659911,0.3776214383,-1.0843931874	
UM06-2X/6-311++G(2df,2p): E = -615.879111 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1590818 Hartree	
PRC4 0,1	
C,0,-0.0095690493,1.3158385009,0.0445483739	40.6355 51.9496 61.2808
C,0,-1.4777725351,1.1930608275,-0.3515451789	83.8971 104.2879 114.8428
C,0,-2.0899792853,-0.1196388927,0.0665669227	131.1594 180.0138 192.8487
C,0,-1.3355754664,-1.1599916237,0.4250676208	206.5493 224.0246 260.8126
C,0,0.1638152729,-1.1364275248,0.4737788635	288.3275 319.8526 334.93
C,0,0.7582921837,0.0464486589,-0.3076501051	358.3978 445.4115 457.583
H,0,-2.0544684146,2.0135581098,0.0824998372	494.5327 533.7957 558.4249
H,0,-1.5859255362,1.293472536,-1.4377395797	653.6725 724.129 783.0539
H,0,0.5932724909,-0.1595784123,-1.3739244363	797.6681 822.045 841.1724
H,0,0.0598405447,1.4844084233,1.1223210275	913.5605 936.685 943.0128
H,0,-1.8212269846,-2.0925859233,0.6938861214	950.0556 983.2189 1006.7772
H,0,0.5502946148,-2.0801112359,0.08486481	1019.6435 1043.5372 1052.3474
H,0,0.4912860898,-1.0767499552,1.5189335984	1065.0953 1087.6397 1114.5293
H,0,0.4370626912,2.178970816,-0.4506146033	1148.6594 1174.6538 1190.4064
C,0,-3.5862374639,-0.1944424197,0.0426316475	1226.3546 1271.9879 1282.0222
H,0,-3.9731378237,0.0814195017,-0.9410845211	1320.3364 1332.5263 1338.2478
H,0,-3.9445120069,-1.19317146,0.2880155787	1348.1287 1363.2903 1372.3698
H,0,-4.0172258841,0.5155343688,0.755217397	1407.3363 1412.1742 1418.0238
C,0,2.2530091365,0.1303861131,-0.0998103788	1419.9106 1455.2815 1475.5218
C,0,3.0398729247,-1.0614579946,-0.5738900987	1482.7287 1486.2875 1491.032
H,0,4.109735837,-0.8672759125,-0.5349574768	1498.2275 1499.5543 1504.5415
H,0,2.8338886804,-1.9391413616,0.0417211468	1734.844 1738.283 2999.1746
H,0,2.7698774559,-1.3206931535,-1.6000654662	3017.6089 3021.048 3029.6043
C,0,2.8558749215,1.168073368,0.4693925183	3047.7594 3054.9417 3070.8631
H,0,2.3120275142,2.030150791,0.8288676927	3072.3507 3080.9563 3103.9058
H,0,3.930656749,1.1820450911,0.5973924766	3106.7716 3127.5532 3135.1558
O,0,-2.6717166534,-0.0383096059,3.0737299392	3155.438 3167.4175 3235.463
O,0,-1.9587671618,0.9004942158,2.7059956306	
O,0,-2.1445241621,-1.1495350563,3.1653425922	
UM06-2X/6-311++G(2df,2p): E = -615.7759304 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0741245 Hartree	
TS4 0,1	
C,0,-0.3831024243,-0.0690545329,1.2783488446	-299.8693 39.6473 60.2782
C,0,0.844143031,-0.9725467956,1.2986689261	74.7457 138.617 142.7635
C,0,1.5134228029,-1.0689103099,-0.0459329323	160.5258 183.6091 198.8007

C,0,0.8321760363,-0.7622152289,-1.1919863879	200.3 240.5398 274.8183
C,0,-0.5682397784,-0.2263986571,-1.2052006878	316.0147 344.9325 365.2451
C,0,-1.3094412453,-0.4413335294,0.1264640339	437.2312 453.7513 491.8274
H,0,1.5677068919,-0.6216586591,2.0364080632	514.4717 529.1094 557.8213
H,0,0.560257197,-1.9858777813,1.6064598383	648.2395 725.1094 774.6542
H,0,-1.5334905033,-1.5135118093,0.208388136	796.9308 820.6938 862.9767
H,0,-0.0608318033,0.9683597885,1.1613379219	911.8853 924.8315 949.1558
H,0,1.2523786124,-1.0779909592,-2.1395294969	951.2156 981.9951 1010.4664
H,0,-1.1156735698,-0.6868188309,-2.0287636904	1016.6147 1027.7221 1053.9413
H,0,-0.5327787228,0.8485522736,-1.4167130303	1065.6158 1091.7953 1114.1711
H,0,-0.9111349958,-0.1461496788,2.2293833333	1143.3107 1162.9048 1194.4021
C,0,2.8220270648,-1.798921623,-0.1226621635	1220.9567 1231.6373 1273.7692
H,0,2.6537857666,-2.878603472,-0.1324320444	1283.696 1286.912 1325.2142
H,0,3.3610274782,-1.5388914119,-1.0345790755	1338.8184 1350.9863 1363.47
H,0,3.4526653261,-1.5652527229,0.7336701124	1409.1852 1412.1759 1415.6166
C,0,-2.6351488219,0.2850451751,0.1170613563	1420.2488 1455.0936 1473.9363
C,0,-3.6103209735,-0.1614391498,-0.93828088	1481.5271 1489.4372 1490.0742
H,0,-4.5888526622,0.2888687958,-0.7851718509	1496.8537 1498.7203 1504.0872
H,0,-3.2649791806,0.1160194667,-1.9360748486	1622.4715 1734.0793 3002.5849
H,0,-3.7218917225,-1.2479582758,-0.9297874932	3024.655 3029.3378 3044.1319
C,0,-2.9376589994,1.2621265943,0.9639354856	3044.593 3050.2517 3082.2945
H,0,-2.2481892546,1.6077465025,1.7208021361	3091.4375 3100.8934 3105.9076
H,0,-3.8999464402,1.7554106067,0.9186722384	3110.419 3133.6925 3146.8469
O,0,2.8457762497,1.1128807507,-0.9501364607	3153.0198 3191.6794 3234.0675
O,0,2.4597801955,0.9591915295,0.2412859388	
O,0,1.8915268855,1.1822178143,-1.7687373025	
UM06-2X/6-311++G(2df,2p): E = -615.7701897 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0698216 Hartree	
POZ4 0,1	
C,0,0.6113370098,0.9695065667,1.1867536841	46.5799 927.8448 1415.1504
C,0,-0.7205921956,1.4872223568,0.6555026319	67.8604 948.736 1421.5676
C,0,-1.6262060292,0.4127783389,0.0726881823	130.0562 954.6569 1459.5223
C,0,-0.9059344085,-0.6458440761,-0.7719742552	166.3277 976.46 1480.3348
C,0,0.4578382224,-1.0558453907,-0.230104222	172.3472 988.7365 1487.4084
C,0,1.3363319909,0.1536263209,0.1200380215	180.796 1013.8719 1490.1035
H,0,-1.2784680811,2.0098025098,1.4346980505	207.9676 1020.3792 1493.1386
H,0,-0.5374516015,2.214742333,-0.1392797621	233.5076 1043.2608 1500.9462
H,0,1.4285874137,0.7788187188,-0.780105821	277.1965 1056.1264 1505.4114
H,0,0.4380752109,0.3434884955,2.0647613328	289.8413 1066.2036 1507.3645
H,0,-0.8556947377,-0.3410008737,-1.8195812214	346.1747 1090.7702 1742.5303
H,0,0.9354186296,-1.7063482755,-0.9619180202	357.4549 1108.8305 2990.7607
H,0,0.3004864681,-1.6455636,0.6754127941	391.6278 1123.1957 3048.5047
H,0,1.2260830006,1.8133870272,1.5026856451	427.2117 1163.2082 3050.5465
C,0,-2.8242808769,1.0057804546,-0.6511743352	466.8108 1183.9152 3055.63
H,0,-2.4917237876,1.6027601738,-1.4999977736	475.3722 1196.487 3059.1257
H,0,-3.4839533535,0.2192901611,-1.0115022721	515.3463 1249.9294 3075.2478
H,0,-3.3814315651,1.649177836,0.0290913825	563.7289 1269.1405 3088.3527
C,0,2.7352334201,-0.2825701115,0.4937645711	615.2378 1273.9537 3101.2256
C,0,3.5640710478,-0.8395432668,-0.6316021908	626.8918 1299.9703 3107.9426
H,0,4.5783877784,-1.0551002522,-0.3025469705	727.6505 1305.8049 3109.4765
H,0,3.1353720038,-1.7618694786,-1.0267179737	748.4407 1342.8575 3130.4678
H,0,3.6131884587,-0.1297469758,-1.4604277547	783.472 1353.6632 3131.7005
C,0,3.2221091561,-0.1878368873,1.7255325084	829.6357 1363.8169 3140.4965
H,0,2.6488129526,0.2150301852,2.5486093861	881.8386 1377.5669 3144.1509
H,0,4.2283526683,-0.5180333547,1.948733804	893.0446 1406.966 3159.0706
O,0,-2.6011095852,-1.5446594828,0.4881882088	914.8151 1410.2228 3240.4538

O,0,-2.0493666959,-0.4303271332,1.141952903 O,0,-1.8073852742,-1.7395323494,-0.7100889136	
UM06-2X/6-311++G(2df,2p): E = -615.8792726 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1590783 Hartree	
TS-POZ1-Syn-2a 0,1 C,0,0.5747308099,1.9430319689,-0.3559764283 C,0,-0.8305389669,2.2670045318,0.146562266 C,0,-1.8092155638,1.0836757571,0.0657265812 C,0,-1.0988850652,0.0527612519,1.4291836852 C,0,0.4122715423,0.0816500821,1.3272149535 C,0,1.0124762132,0.5142795185,-0.0188197449 H,0,-0.8006590367,2.6232832653,1.1792803679 H,0,-1.2683828274,3.0768516666,-0.4409328378 H,0,0.5875169767,-0.155566957,-0.7665673413 H,0,1.2623633735,2.6590679518,0.096292265 H,0,-1.5318658095,0.4146254228,2.3577322014 H,0,0.7256484701,-0.9383568046,1.5618932681 H,0,0.7892349434,0.7341153453,2.1183645103 H,0,0.6298197987,2.0806022958,-1.4354687937 C,0,-3.229153256,1.4029827553,0.5210636927 H,0,-3.7093789571,2.0134250508,-0.2443252192 H,0,-3.799513518,0.4827900164,0.6295108466 H,0,-3.2448034725,1.9576249436,1.4595025564 C,0,2.5088440189,0.2865210488,-0.0541804687 C,0,2.959024464,-1.111854421,0.2818243601 H,0,3.9891831254,-1.2750593623,-0.0270944191 H,0,2.8998302921,-1.3018231633,1.3554579339 H,0,2.3241179469,-1.851774786,-0.2104037732 C,0,3.3913678854,1.2106557845,-0.4175166219 H,0,3.1106712233,2.2191848389,-0.6830826162 H,0,4.4449671623,0.970395638,-0.4763311049 O,0,-1.3194968148,-1.4509632172,-0.1009607652 O,0,-1.730301425,-1.0653416813,1.0705404587 O,0,-1.700836933,0.3053531585,-0.9446724528	-545.365 52.6422 96.7759 121.0173 175.86 187.7487 190.3891 214.2066 241.243 281.6173 293.0668 327.7821 340.8919 371.71 439.5125 445.3975 458.6776 500.8211 549.2757 581.9176 596.3336 626.1208 723.1163 750.0378 787.2456 822.5181 887.0962 917.0185 918.9764 954.0217 964.4122 991.0324 1003.0612 1009.0829 1022.264 1052.6499 1066.3883 1086.025 1114.9091 1139.065 1160.7094 1193.0094 1208.2743 1252.1932 1261.563 1290.0778 1297.2819 1316.9986 1345.9074 1353.9121 1380.7518 1399.1121 1409.9563 1415.5007 1432.3286 1456.2535 1458.9545 1469.96 1483.9243 1491.1038 1493.1353 1501.1763 1505.9822 1515.2326 1731.4789 3045.2677 3046.1779 3048.5652 3051.8738 3073.872 3086.0944 3093.0527 3103.3708 3107.8308 3119.4133 3124.9797 3141.8013 3148.9453 3158.6887 3161.1555 3242.8929
UM06-2X/6-311++G(2df,2p): E = -615.8372997 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1309965 Hartree	
TS-POZ1-Syn-2b 0,1 C,0,0.7331736548,1.1335611447,-0.626434181 C,0,-0.7383567288,0.8665983405,-0.9165517733 C,0,-1.5591940682,0.4905719266,0.2956903732 C,0,-0.7083043895,-1.0184975253,1.0308221477 C,0,0.7515550143,-0.56604855,1.1801623278 C,0,1.4219315963,-0.128458836,-0.1227569778 H,0,-1.2097381638,1.7624881884,-1.3336524758 H,0,-0.8307170484,0.0693277154,-1.649089175 H,0,1.2508376504,-0.9258158322,-0.8548559923 H,0,0.837938093,1.9339480265,0.1114897028 H,0,-1.2343342193,-1.0639710719,1.998390715 H,0,1.2721281575,-1.4153332371,1.6240528186 H,0,0.8056659674,0.2481206234,1.9074144371 H,0,1.2141548919,1.4827289923,-1.5406402435 C,0,-1.7807449489,1.5252229994,1.3594391545 H,0,-0.844174061,1.7525061717,1.8643802015 H,0,-2.1558604664,2.449475348,0.9175587976 H,0,-2.4984221288,1.1639642121,2.0930747314	- 561.2609 37.6861 65.2483 140.1868 160.8543 175.1782 194.1228 218.5476 227.7874 258.828 322.4745 338.8472 369.453 379.0227 420.32 450.9309 496.1442 510.8751 538.8419 565.8175 579.2018 655.9943 688.5616 726.9394 762.7306 816.0874 890.4936 904.8479 935.0845 950.7249 957.7006 992.7553 1006.6649 1015.2748 1021.3546 1064.7161 1072.0529 1076.6414 1126.313 1139.8055 1190.3176 1212.8156 1227.7823 1263.7847 1286.0916 1294.4157 1309.5816 1332.8688 1351.324 1362.5585 1379.2786 1400.9491 1415.8716 1424.3787

C,0,2.9167599607,0.0053484727,0.066942617	1426.6361 1457.9525 1474.3297
C,0,3.6729788038,-1.2916806717,0.1520842406	1481.1837 1489.0897 1491.8119
H,0,4.732812108,-1.1205890844,0.3280449093	1499.4554 1503.9164 1504.3644
H,0,3.2926011934,-1.9302115411,0.9505919629	1514.536 1735.6237 2982.3259
H,0,3.5618964342,-1.8521527118,-0.7785060739	3038.6136 3041.6919 3045.1991
C,0,3.5419148363,1.175237204,0.1400684865	3053.1578 3058.6927 3065.9957
H,0,3.0236722343,2.1198679137,0.0516468955	3094.866 3099.2649 3103.7388
H,0,4.6133493653,1.2219926517,0.2844611412	3136.6619 3142.6491 3151.1491
O,0,-2.5086121842,-1.1470715013,-0.806461113	3157.1485 3161.6028 3237.1383
O,0,-0.9765540954,-1.9310634817,0.1880415506	
O,0,-2.6880415086,-0.1910658169,0.0533414548	
UM06-2X/6-311++G(2df,2p): E = -615.8438707 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1374944 Hartree	
TS-POZ2-Anti-2a 0,1	
C,0,0.411254369,0.9701184524,-1.3942465274	- 572.897 54.2435 86.3458
C,0,-0.524353785,1.7844817777,-0.5112319189	116.775 153.7086 194.2151
C,0,-1.7943782359,1.0052302725,-0.1092234958	219.389 237.2946 253.7123
C,0,-1.0682987309,-0.7326367697,0.2610774491	286.6497 324.4978 358.6992
C,0,0.3834584659,-0.621270188,0.5895658476	387.0079 397.6872 429.0759
C,0,1.2146481908,-0.0711279709,-0.5981542569	442.2909 471.1804 515.0713
H,0,-0.0100113979,2.1208887632,0.3920376231	539.9431 580.4925 591.8704
H,0,-0.8684232065,2.6762631524,-1.0367551743	622.2321 713.3235 729.8469
H,0,1.4239785741,-0.914573228,-1.2622510066	764.2758 787.7657 887.0371
H,0,1.0958699921,1.6169685913,-1.9394254622	914.3827 938.5161 948.2559
H,0,-1.7899560746,-0.975487761,1.0349036702	959.2172 970.7117 992.9406
H,0,0.7640325387,-1.5896403922,0.9200140314	1000.8272 1028.5521 1043.7437
H,0,0.4676305254,0.0524431412,1.4458882136	1067.9592 1081.0809 1110.5343
H,0,-0.1987615272,0.4667905882,-2.1453689163	1146.3738 1170.4871 1180.108
C,0,-2.3852258107,1.3843387964,1.2451272291	1214.7962 1225.9231 1255.8937
H,0,-2.6502713226,2.4425601726,1.230147916	1275.7206 1296.9379 1334.337
H,0,-3.2885461605,0.8038734001,1.422914802	1341.8448 1360.6897 1383.2754
H,0,-1.6780384599,1.2273708675,2.0615983916	1389.359 1396.5801 1416.6744
C,0,2.5488879309,0.4097178886,-0.0621350013	1433.8425 1449.7403 1470.4051
C,0,3.4299413322,-0.6681223077,0.5101265748	1480.4369 1491.3408 1491.894
H,0,4.4085416284,-0.2759090684,0.7777989882	1497.5125 1499.4034 1514.6903
H,0,2.9888933858,-1.1091832557,1.4063739001	1522.3465 1734.0305 3040.5718
H,0,3.5641778315,-1.4780247145,-0.2102062502	3044.2947 3047.9262 3053.2964
C,0,2.9317430137,1.6810872474,-0.0591685621	3071.2646 3079.9459 3100.1243
H,0,2.3173837506,2.4766783424,-0.4565128925	3101.4332 3111.4524 3116.1149
H,0,3.8915274477,1.9671223736,0.350710662	3120.5759 3142.5766 3144.4905
O,0,-2.5852440235,-1.2138048074,-1.2056549161	3152.6453 3157.1458 3236.6001
O,0,-1.3200620709,-1.2913406615,-0.9079049675	
O,0,-2.6209600906,0.7447607776,-1.0407338306	
UM06-2X/6-311++G(2df,2p): E = -615.8380838 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1306217 Hartree	
TS-POZ2-Anti-2b 0,1	
C,0,0.7811064327,1.3958241352,-0.5173126103	- 567.7857 38.0019 80.7398
C,0,-0.6357754093,1.7336488555,-0.0265498145	116.7381 167.8105 176.5646
C,0,-1.5375391074,0.5354651987,0.0362155263	196.2412 213.4594 251.3108
C,0,-0.7911636116,-0.6524010048,1.3090424994	277.1706 294.1938 335.4351
C,0,0.7004510979,-0.3075681484,1.3567464643	355.512 359.4711 424.9923
C,0,1.2996969173,0.0372944405,-0.0133617984	447.5722 502.2287 510.0059
H,0,-0.6019849802,2.1448171185,0.9843892169	539.506 571.1547 594.9565
H,0,-1.0921365879,2.5053164831,-0.6519684464	659.4674 689.2649 727.041
H,0,0.9469530792,-0.7377315765,-0.6980663101	774.6019 805.6586 878.7474

H,0,1.4387481759,2.1990701304,-0.1912657812	917.2213 927.6643 942.0254
H,0,-1.3778978082,-0.2526324643,2.1504491497	960.3146 973.9609 1010.8542
H,0,1.2114470772,-1.1722615443,1.7822089725	1021.6601 1027.4957 1039.8331
H,0,0.8590137812,0.5269555007,2.0452662707	1071.5459 1086.592 1118.1705
H,0,0.8060508289,1.397267345,-1.6068404164	1136.0824 1175.6016 1220.9352
C,0,-2.9555150395,0.6954458673,0.5093330353	1239.2532 1257.1972 1276.1866
H,0,-3.5464693088,1.118633872,-0.3063961283	1288.9033 1304.512 1333.8832
H,0,-3.3839526394,-0.2616029584,0.7912496446	1359.6468 1371.3093 1377.4141
H,0,-2.9842777289,1.3792902022,1.3548568963	1402.2363 1415.7028 1417.864
C,0,2.8099038707,-0.08499388,0.0395946854	1424.7452 1458.5997 1471.7056
C,0,3.3225098183,-1.4719904462,-0.2292719415	1480.4689 1485.3329 1489.5403
H,0,4.3921037869,-1.5506315212,-0.0469583619	1495.6572 1500.2266 1503.2986
H,0,2.8064092845,-2.2057729475,0.3936908483	1505.0902 1736.5487 2992.524
H,0,3.1229217796,-1.7505685273,-1.2662635123	3047.0048 3053.2514 3056.3633
C,0,3.6340193074,0.9117354567,0.3403618992	3058.425 3073.8544 3081.5188
H,0,3.2930810387,1.9182410328,0.538473435	3093.9983 3103.1511 3104.8244
H,0,4.7010900151,0.7442246036,0.4046906875	3128.9064 3139.4244 3140.7794
O,0,-1.9721801178,-1.4069879151,-0.8670125842	3156.9234 3176.0136 3234.4928
O,0,-1.1497176344,-1.7930645689,0.875391868	
O,0,-1.3461666479,-0.2738939891,-1.0063345441	
UM06-2X/6-311++G(2df,2p): E = -615.8398431 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1326875 Hartree	
TS-POZ3-Syn-2a	
0,1	
C,0,0.6694642851,1.7280509416,0.1866203257	- 548.9919 26.3826 79.9783
C,0,-0.7033816092,1.9573832119,-0.4155202884	128.6192 157.4999 183.561
C,0,-1.7596732305,0.8834062433,-0.0702592865	193.8366 221.6175 248.7222
C,0,-0.9284453253,-0.6290259937,-0.7385951936	267.4262 320.3456 331.2086
C,0,0.444697467,-0.7201377475,-0.1282746612	349.0408 374.1564 435.3291
C,0,1.3279478877,0.4973755149,-0.425816817	439.745 469.9325 514.8057
H,0,-1.1273975886,2.8971878446,-0.0554887808	530.4531 573.7493 582.2177
H,0,-0.6359475806,2.0390522789,-1.5036353262	588.4035 703.1039 747.5799
H,0,1.3655764074,0.6396103007,-1.5147963651	788.7827 825.6256 879.7019
H,0,0.5636023606,1.5943057106,1.2649199486	920.5527 939.4007 954.9578
H,0,-0.9959993499,-0.5893052456,-1.8236809614	960.1821 990.7771 994.7327
H,0,0.8915421693,-1.6375498859,-0.5220200662	1020.6727 1038.3569 1050.914
H,0,0.3425140687,-0.8303238253,0.9486461336	1071.2737 1094.8723 1113.7284
H,0,1.2963412496,2.6052375428,0.0198626424	1127.1875 1148.9564 1179.9674
C,0,-3.0540085216,1.0414910256,-0.8611382945	1199.8279 1227.9699 1271.7863
H,0,-2.8830525986,1.0627141437,-1.9377715623	1280.1238 1292.731 1306.2776
H,0,-3.7367833437,0.2321920455,-0.6142456396	1343.0998 1349.8306 1365.3981
H,0,-3.5226223743,1.9836662687,-0.5728265026	1396.368 1412.2037 1419.9969
C,0,2.7468058794,0.2384734033,0.0330952498	1443.4311 1455.7487 1465.4732
C,0,3.5464842152,-0.6963252962,-0.8317200083	1477.0235 1484.4189 1489.7751
H,0,4.5428781854,-0.8541019747,-0.4246150934	1491.4337 1495.4936 1500.3421
H,0,3.0627199301,-1.6697503281,-0.9289047751	1514.7105 1735.6545 2998.8407
H,0,3.6467758616,-0.2887338497,-1.8402751892	3044.9474 3047.4656 3053.6085
C,0,3.2697276443,0.7960612659,1.1183458978	3059.7177 3061.4057 3099.5076
H,0,2.7157822616,1.4822393672,1.743121302	3100.5011 3112.3722 3118.4856
H,0,4.2861928104,0.5758684496,1.4175443507	3143.9349 3149.0822 3150.8598
O,0,-1.8698260745,-1.452239715,1.0351956932	3154.9764 3161.5233 3236.9618
O,0,-1.8648058593,-1.4567762539,-0.2655981877	
O,0,-1.8837708773,0.5576556566,1.1573661353	
UM06-2X/6-311++G(2df,2p): E = -615.8406935 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1355669 Hartree	
TS-POZ3-Syn-2b	
0,1	

C,0,0.7678756187,1.5915336612,-0.4266293784	-556.253 40.5476 94.8496
C,0,-0.6788440533,1.8608004449,-0.8285612397	136.2783 180.8846 189.2277
C,0,-1.7633717085,0.9584740586,-0.2589560214	204.2133 245.2887 265.3915
C,0,-0.8686693107,-0.582044513,0.336447096	282.8 306.1186 321.8575
C,0,0.1149986796,-0.8215610923,-0.8108496748	373.7897 385.5004 423.2434
C,0,1.2496242297,0.2052052508,-0.9031208946	448.3884 492.8266 508.3796
H,0,-0.9591151018,2.8706723166,-0.5126792318	546.2007 569.1898 599.8263
H,0,-0.7693824855,1.8227139098,-1.9169287892	677.4024 716.0573 729.4312
H,0,1.5032903539,0.2991368618,-1.9650786149	758.7203 786.5767 887.5825
H,0,0.862712822,1.6595105552,0.6536744253	892.3572 939.5116 954.7075
H,0,-1.727863296,-1.2703458746,0.3311701741	964.41 985.9437 1000.3477
H,0,-0.4495102927,-0.8343113871,-1.7455734457	1014.1862 1029.7697 1041.3385
H,0,0.5204478351,-1.8269925396,-0.6902907101	1061.3863 1081.9125 1128.8152
H,0,1.3915359606,2.3675401219,-0.8708188414	1157.9595 1184.6072 1215.5174
C,0,-2.894865124,0.5878551384,-1.1736057414	1247.6615 1257.649 1263.1732
H,0,-2.5362858901,-0.084651996,-1.9512901984	1276.4654 1321.4178 1338.2599
H,0,-3.6899420428,0.0964688612,-0.617312706	1351.296 1379.1154 1385.1124
H,0,-3.2938801716,1.4789478112,-1.6604356915	1399.0771 1409.1844 1417.7896
C,0,2.5300206416,-0.168944816,-0.1875504863	1422.2509 1455.572 1461.0288
C,0,3.7348577544,0.6283707761,-0.6059914355	1477.4745 1486.4465 1488.6513
H,0,4.6292353516,0.3003898057,-0.0806045503	1496.6888 1500.4825 1504.3973
H,0,3.9091743352,0.5343805161,-1.6805631479	1517.2985 1741.2873 2998.3701
H,0,3.591683859,1.6908792038,-0.3980297966	3014.2318 3039.0409 3048.3134
C,0,2.6041718227,-1.0918610715,0.7619950029	3052.6538 3061.8384 3093.8677
H,0,1.7394256937,-1.6432908194,1.1037137012	3097.6281 3103.4076 3107.4304
H,0,3.543831104,-1.3006644854,1.2567534703	3126.4559 3134.476 3151.2825
O,0,-1.2547804165,1.5058224541,1.782323402	3151.594 3169.3098 3234.6276
O,0,-0.4150246455,-0.2435665426,1.4778267662	
O,0,-2.2282586828,1.2720955702,0.9542931879	
UM06-2X/6-311++G(2df,2p): E = -615.8396136 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1319601 Hartree	
TS-POZ4-Anti-2b 0,1	
C,0,-0.8480758525,1.3583761661,-0.0287753855	-564.304 47.4144 70.3241
C,0,0.5172815243,1.6367505145,0.5927138668	152.0717 174.0734 180.0039
C,0,1.5450741347,0.5677601499,0.3226678744	183.7895 203.7001 252.4421
C,0,0.8342105836,-1.1252897351,0.6207477941	274.8927 323.7321 343.5632
C,0,-0.5855588103,-1.1360504796,0.0752810525	365.1901 377.9141 427.7739
C,0,-1.4485025916,0.058879116,0.5059711017	436.4247 486.0777 499.7055
H,0,0.9192283529,2.5915199205,0.2420143007	539.2812 579.6305 589.0208
H,0,0.4174371321,1.7210431144,1.6765066602	606.579 682.0449 734.2672
H,0,-1.4290697897,0.1086358158,1.6041019329	794.7397 814.6884 886.481
H,0,-0.7493118698,1.3003505495,-1.1144636178	911.1877 928.4124 946.1122
H,0,0.9285038308,-1.0198374985,1.7147376817	967.5255 986.937 1011.0509
H,0,-1.0428447943,-2.0754375511,0.3926081389	1023.6282 1043.7238 1045.1717
H,0,-0.5225660614,-1.1681809544,-1.0143890576	1070.9049 1093.2957 1103.2871
H,0,-1.5146196868,2.1929388685,0.1913844864	1133.3344 1170.8246 1212.8133
C,0,2.8098333214,0.5896595157,1.1379206379	1229.4421 1265.6935 1273.7169
H,0,2.5769842767,0.8579912283,2.1660025325	1284.4259 1297.8733 1321.4224
H,0,3.3145865231,-0.370400005,1.1060699754	1335.8848 1357.5646 1367.2676
H,0,3.4768220621,1.3463382682,0.7182986954	1408.8417 1414.1974 1417.4983
C,0,-2.8897280076,-0.1703315529,0.1045009308	1420.7157 1453.818 1471.6156
C,0,-3.655654511,-1.1239507553,0.9789653121	1473.4966 1483.185 1490.5483
H,0,-4.6539582112,-1.3072699141,0.5874332898	1497.3763 1500.0741 1502.274
H,0,-3.1435262037,-2.0829679133,1.071481073	1506.2766 1735.8812 2985.1919
H,0,-3.7502680219,-0.7165631385,1.9882290561	2986.9977 3044.3349 3048.3462
C,0,-3.4542510673,0.4153226843,-0.9447676797	3057.6041 3065.4121 3066.0366

H,0,-2.9230137507,1.1161606986,-1.5735170503	3095.8971 3097.8488 3106.2304
H,0,-4.4815724988,0.2038725603,-1.2108030322	3115.5476 3144.1631 3148.0624
O,0,2.5468585117,-0.6279457555,-1.2008545475	3150.918 3180.8732 3232.6792
O,0,1.6959522977,0.3371455809,-0.9896380286	
O,0,1.6933478378,-1.8783834682,0.0582421658	
UM06-2X/6-311++G(2df,2p): E = -615.8464515 Hartree	
RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.125689 Hartree	
TS-POZ4-Anti-2a	
0,1	
C,0,-0.802721654,1.7362846827,-0.1576914564	-553.6741 41.099 51.5473
C,0,0.5610013538,1.9602078959,0.4668006664	97.4482 160.9582 173.7134
C,0,1.6443076613,0.9343386068,0.063782896	194.6437 242.5954 261.307
C,0,0.8455119087,-0.6351930305,0.6326060426	266.8979 315.2903 347.9331
C,0,-0.5217379193,-0.7206988,0.0084023075	370.147 403.6311 407.6813
C,0,-1.4351944787,0.4553575575,0.3737647887	435.3697 481.1346 508.4803
H,0,0.9645903816,2.929948502,0.1678624814	516.5447 561.6253 590.3162
H,0,0.4857180374,1.973411795,1.557382896	618.4085 699.6201 732.4239
H,0,-1.4821206896,0.529638573,1.4691201454	772.7398 805.5626 877.9851
H,0,-0.6878415785,1.6714108111,-1.2413973942	907.6352 924.7216 955.5099
H,0,0.9061870813,-0.6605144191,1.7185295013	959.4367 992.6781 1013.9368
H,0,-0.9488632992,-1.6706944898,0.3422027911	1016.0737 1050.3124 1058.866
H,0,-0.4111009509,-0.7622345581,-1.0725116849	1069.7105 1081.158 1103.2205
H,0,-1.4511044813,2.5867431225,0.0580846741	1153.1453 1180.5531 1193.6035
C,0,2.9302018721,1.0737650917,0.8717560289	1220.1747 1246.7625 1271.0966
H,0,2.7529219209,1.0249438471,1.9464670815	1287.2143 1299.2845 1344.1096
H,0,3.6332947326,0.2972646249,0.5805349197	1344.8778 1353.5828 1369.9629
H,0,3.3779282825,2.0425134458,0.6448540476	1392.3884 1409.2877 1415.0925
C,0,-2.8449965789,0.1920735387,-0.1098964078	1429.0404 1459.6375 1469.5052
C,0,-3.6270085285,-0.8123801802,0.6905843959	1477.9309 1487.8198 1489.9339
H,0,-4.6171498034,-0.9680843047,0.2677306181	1492.4252 1498.6875 1513.932
H,0,-3.1208555616,-1.7783896119,0.7313766384	1517.3605 1740.0349 3020.2905
H,0,-3.7424273714,-0.4698436927,1.7214675125	3036.4257 3045.6355 3051.3871
C,0,-3.3750550093,0.802811292,-1.1625871615	3057.7249 3061.3317 3089.9534
H,0,-2.8341223773,1.538733265,-1.740385497	3102.703 3118.1657 3125.543
H,0,-4.3843713331,0.5777413235,-1.481695438	3126.4763 3138.7429 3143.5352
O,0,1.8157913326,-1.3259285033,-1.1816858309	3156.846 3161.7145 3244.6097
O,0,1.7827813138,0.6874538764,-1.1805847445	
O,0,1.8037857964,-1.4103297914,0.1163291124	
UM06-2X/6-311++G(2df,2p): E = -615.8340532 Hartree	
RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.125689 Hartree	
Syn-2a	
0,1	
C,0,-0.9142504049,0.8758759086,-1.2773900353	36.4282 46.0105 55.6021
C,0,0.1147217533,2.0001826258,-1.1352864517	77.4659 81.1371 122.0346
C,0,1.5669607476,1.574466574,-1.1918741218	145.2278 179.0976 193.0882
C,0,0.7199254807,0.098970331,1.2045312757	208.2571 216.1838 254.1466
C,0,-0.6520742414,-0.3815566036,0.9641236355	295.527 329.4797 339.0328
C,0,-1.5753513063,0.4690196959,0.0422800754	432.3598 451.9022 473.3408
H,0,-0.0071584076,2.7364398617,-1.9350530174	511.5957 540.4936 559.2866
H,0,-0.0284047486,2.5605209861,-0.2039866449	613.1556 707.5972 728.8716
H,0,-1.8125949055,1.3766550201,0.5993051393	756.875 804.0165 853.248
H,0,-0.4413427076,0.0134653253,-1.7528570437	882.7208 917.3393 920.9983
H,0,1.6007299001,-0.4755625271,0.940923357	947.9366 961.1572 971.0804
H,0,-1.1163514646,-0.4129211676,1.9565243221	997.7752 1012.0477 1027.2443
H,0,-0.5858583082,-1.3932073339,0.5643461076	1055.7131 1076.8041 1086.2119
H,0,-1.7060262279,1.2135968375,-1.9447514561	1102.5228 1134.1837 1197.6655
C,0,2.5752601562,2.6570810326,-0.910489243	1220.6237 1234.8991 1269.2553

H,0,2.4998698362,2.9205954359,0.1475838062	1282.0583 1312.8882 1345.1004
H,0,3.5784870126,2.3038671174,-1.129624893	1364.2075 1388.8934 1406.2582
H,0,2.352024106,3.5575920135,-1.4821144879	1409.1266 1420.2707 1422.5003
C,0,-2.8599830697,-0.3180916996,-0.1322710811	1450.3112 1454.5488 1461.1947
C,0,-3.7288808205,-0.4208539319,1.0915549318	1471.8902 1485.0184 1491.0795
H,0,-4.6769478862,-0.9011179721,0.8591093579	1499.5546 1507.3785 1650.9397
H,0,-3.2448768168,-1.0030796452,1.8783841658	1733.0707 1826.4168 3026.3366
H,0,-3.9294335094,0.5682840436,1.5073519375	3031.5573 3050.6217 3052.5354
C,0,-3.2076094219,-0.8984732281,-1.275110149	3059.0233 3070.2846 3082.4736
H,0,-2.5960249446,-0.8446013849,-2.1646895879	3107.8097 3113.2716 3116.1897
H,0,-4.1326279984,-1.4547368852,-1.3528738133	3120.2449 3142.3989 3154.8132
O,0,-0.0422751777,1.9840632415,2.1419277856	3179.2977 3221.0773 3237.0632
O,0,1.9032839933,0.4352249141,-1.4143509273	
O,0,0.9917753817,1.1725414147,1.776422506	
UM06-2X/6-311++G(2df,2p): E = -615.8999996 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.179262 Hartree	
Anti-2a 0,1	
C,0,-0.876195693,0.953986456,-1.4426487224	33.8777 62.6457 66.2765
C,0,0.4389374612,1.7290769687,-1.4654932415	116.2399 127.7486 138.5119
C,0,1.6923957565,0.8754503215,-1.51673301	147.8455 151.4345 175.384
C,0,0.8922480883,-0.2402331213,1.0292071934	203.0016 236.5728 244.4141
C,0,-0.4031767218,-0.6849557785,0.4644060128	275.1591 305.8931 346.7706
C,0,-1.3195697677,0.4354374591,-0.0681039556	381.482 440.3326 461.9234
H,0,0.479856851,2.3607420912,-2.3588031033	488.6697 525.1325 548.5541
H,0,0.5273580756,2.4171195204,-0.6197319768	615.631 655.8004 731.1152
H,0,-1.277920162,1.2676207529,0.6418653251	760.9571 777.2434 828.1393
H,0,-0.7935143784,0.1182952873,-2.1399571838	873.5917 911.7294 941.7031
H,0,1.7519533682,-0.8984692354,1.1407725863	958.8628 967.2251 988.5084
H,0,-0.9032173575,-1.2515505391,1.2588213146	999.0042 1012.4472 1024.5307
H,0,-0.1845550367,-1.4008998867,-0.3300097547	1056.7698 1072.7323 1076.2982
H,0,-1.6687821577,1.6042848573,-1.8137783058	1110.6755 1132.2696 1187.5108
C,0,2.9910252631,1.5876615288,-1.2734396588	1214.2829 1240.3196 1268.3622
H,0,3.0787934142,1.7335155231,-0.1900995076	1298.3127 1323.6341 1350.796
H,0,3.8227549413,0.9849283159,-1.6265582867	1369.0361 1387.5287 1405.144
H,0,2.9968645557,2.5710618313,-1.742416866	1412.9567 1417.1412 1417.5704
C,0,-2.7456991274,-0.0841254293,-0.0560769733	1436.715 1450.4342 1461.2385
C,0,-3.4291233404,-0.0256588014,1.2815863893	1474.6375 1484.467 1486.774
H,0,-4.4057898193,-0.5036036558,1.2524236764	1490.5554 1499.2065 1667.0549
H,0,-2.8348297895,-0.5088529247,2.0604974943	1742.2368 1815.8298 3023.3311
H,0,-3.5605845877,1.0136387965,1.5903993308	3035.6701 3039.9176 3040.4493
C,0,-3.3550699117,-0.5662044763,-1.1318591741	3044.412 3068.2627 3080.4767
H,0,-2.8820107179,-0.5948969155,-2.103387509	3089.7333 3102.2756 3110.2516
H,0,-4.3652475101,-0.9491060017,-1.0698220135	3115.5258 3136.982 3160.4514
O,0,2.2611010344,1.2945393831,1.9252026467	3163.4182 3178.459 3242.0449
O,0,1.6386157788,-0.3173833457,-1.7149431837	
O,0,1.0361064503,0.9273964884,1.4166828671	
UM06-2X/6-311++G(2df,2p): E = -615.8998347 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1781127 Hartree	
Syn-2b 0,1	
C,0,-0.7046638752,-1.5139144069,-0.0938654859	37.7243 54.4064 69.3563
C,0,0.6559516682,-1.69723173,-0.7676793813	98.9522 133.3527 147.6635
C,0,1.8122206946,-1.0767867533,-0.0613630729	152.5073 160.1846 179.6229
C,0,0.5437483268,1.624897128,0.0736158457	181.8542 259.3039 298.8685
C,0,-0.6852128797,0.9705416574,0.6396873156	321.7543 325.8695 345.0936
C,0,-1.3332504262,-0.1173232949,-0.2378944462	355.8975 381.9334 473.6247

H,0,0.8820578448,-2.7627133892,-0.8854998678	505.6805 562.0977 579.018
H,0,0.6482452221,-1.2774875582,-1.7768946494	635.6001 684.1201 727.0459
H,0,-1.2070885278,0.1968658404,-1.2796416322	743.157 805.3625 828.2671
H,0,-0.6286020485,-1.7854639995,0.9601843676	898.485 910.8181 953.4777
H,0,1.0189847419,2.3792126141,0.7222856014	957.2076 980.3736 986.8258
H,0,-1.390548068,1.7895640025,0.8191196313	996.9556 1027.8665 1040.0782
H,0,-0.4358807116,0.5876892894,1.6328325599	1053.8346 1062.7364 1080.8698
H,0,-1.3893875639,-2.2278172824,-0.5521494662	1108.951 1142.0889 1212.99
C,0,3.1279000061,-0.8513835289,-0.6806367828	1238.4805 1258.7283 1269.4533
H,0,3.1892013754,-1.3232704451,-1.6566626331	1288.2354 1323.3562 1351.606
H,0,3.2694928838,0.2290535076,-0.7653417155	1384.7024 1392.5319 1414.1391
H,0,3.9034126542,-1.2042510538,0.0002895672	1416.3805 1423.9174 1426.9783
C,0,-2.8234650681,-0.1264569981,0.053195028	1454.8367 1460.0419 1465.9056
C,0,-3.6116284696,0.9431321657,-0.6498202301	1469.9551 1479.2603 1489.3816
H,0,-4.6441815722,0.9690485949,-0.308352784	1493.0751 1507.6576 1650.5676
H,0,-3.1732917705,1.9312709433,-0.4945895987	1738.5883 1838.7517 2981.1803
H,0,-3.6062939778,0.7655196611,-1.7275006611	3016.9882 3034.6871 3042.4156
C,0,-3.4026144905,-0.9908926998,0.877412157	3048.433 3057.0931 3059.8186
H,0,-2.8504970327,-1.7749595384,1.3771563201	3078.3636 3087.4079 3114.5621
H,0,-4.4643073373,-0.9385101378,1.0795174206	3116.2814 3138.5269 3144.0411
O,0,2.5941782557,0.0020826544,1.7523589657	3154.5617 3167.0372 3235.4862
O,0,1.6055552322,-0.7105353214,1.1145035851	
O,0,1.0002465038,1.379681109,-1.0138149681	
UM06-2X/6-311++G(2df,2p): E = -615.9016464 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1801911 Hartree	
Anti-2b 0,1	
C,0,3.0586454817,-4.1410562224,-1.260335828	57.1323 64.5969 96.3442
C,0,2.3328786564,-3.3559140969,-0.1449142268	105.3741 145.9392 165.969
C,0,2.5708077306,-1.8919498075,-0.0698021119	181.7531 196.5801 207.518
C,0,5.3762192594,-1.3086888027,-1.7341186714	216.4804 252.7108 272.4352
C,0,4.6274385006,-2.4588392711,-2.3348752214	297.9348 323.2434 336.183
C,0,4.5195489568,-3.7246802166,-1.4543184072	362.8453 436.1017 489.9251
H,0,1.2551532193,-3.4713963322,-0.296890767	496.6775 548.7836 553.5008
H,0,2.6061915228,-3.7728825123,0.8244629143	619.5015 674.0631 711.5423
H,0,4.9388872517,-3.4702325499,-0.4737990088	733.0906 796.8376 826.6514
H,0,2.5062678831,-4.0324622399,-2.1911398194	872.8658 918.011 943.398
H,0,5.5113391842,-0.440685289,-2.4054621716	953.5795 957.0849 988.4064
H,0,5.0982014176,-2.6830917338,-3.2971091906	995.7697 1023.3535 1037.3756
H,0,3.6310184579,-2.0792788706,-2.6045582938	1060.2849 1066.1678 1074.8264
H,0,3.0153061945,-5.1880501159,-0.9615646254	1117.5341 1132.8997 1202.1038
C,0,3.213715849,-1.2493436982,1.1032807807	1229.4627 1244.7525 1273.984
H,0,4.2186055256,-1.6563368131,1.2254161758	1295.9297 1318.3203 1348.811
H,0,3.2731899793,-0.1729052479,0.9730121984	1384.6521 1389.7953 1410.8059
H,0,2.6401580237,-1.4898596229,2.0006673397	1415.5827 1417.3486 1429.1473
C,0,5.4099595587,-4.8043609649,-2.03202103	1446.7437 1452.632 1456.4379
C,0,6.8811099389,-4.5281308283,-1.895864114	1458.8829 1487.7233 1490.4289
H,0,7.4793163585,-5.3133783108,-2.3528798456	1494.7425 1502.935 1654.4858
H,0,7.1480791668,-3.5774058012,-2.3640241452	1735.8052 1838.4874 3021.0165
H,0,7.1569192938,-4.4413609062,-0.8429433255	3035.1262 3036.9084 3041.2784
C,0,4.9531951691,-5.8895765309,-2.6449735063	3045.4368 3053.3685 3062.3551
H,0,3.8971066125,-6.092634532,-2.7567734921	3088.7803 3091.8792 3096.0725
H,0,5.6364368883,-6.6149625389,-3.066803076	3108.8365 3113.9356 3140.1713
O,0,1.5667547186,-1.6794479909,-2.0667232634	3154.1251 3174.2465 3233.7086
O,0,2.1691638821,-1.1210300001,-0.9695998867	
O,0,5.8037214487,-1.268715573,-0.6090625709	
UM06-2X/6-311++G(2df,2p): E = -615.9044705 Hartree	

RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.182069 Hartree	
TS-2POZ-1POZ	
0,1	
C,0,0.5923478568,1.270722079,-0.7146985843	-89.2648 49.4892 76.1294
C,0,-0.8916352447,1.0724293344,-1.0141403099	152.6727 174.7571 191.0722
C,0,-1.6636578602,0.5164509222,0.1841762367	210.5906 233.1837 252.3958
C,0,-0.9696943767,-0.7144672297,0.7639540641	274.108 343.9546 375.6502
C,0,0.5327179865,-0.6118941115,0.9297392345	392.9027 415.8879 451.0965
C,0,1.2461182327,-0.0476892885,-0.3094020916	487.7478 534.2571 552.0506
H,0,-1.3574607342,2.0082453457,-1.3265233132	616.9331 674.3913 723.8579
H,0,-1.0043496472,0.36526333,-1.8374216728	741.7822 762.644 809.8251
H,0,1.0915591658,-0.7635909781,-1.1254101341	875.0799 904.1775 910.102
H,0,0.7238550157,2.0039001533,0.0871781466	933.0219 949.1597 959.702
H,0,-1.4553609016,-1.0014349199,1.7027629444	975.195 999.8064 1011.6689
H,0,0.9150959252,-1.5980113406,1.1926848505	1022.4597 1036.6573 1042.7189
H,0,0.7293997354,0.0445988637,1.782913226	1064.9007 1079.0886 1108.6503
H,0,1.0908862271,1.6776667697,-1.595149199	1150.1276 1175.4697 1186.7739
C,0,-2.0044190192,1.564763914,1.224248089	1216.2262 1256.8154 1269.5664
H,0,-2.6362261886,2.3352554593,0.7847352341	1293.1918 1311.4986 1320.6711
H,0,-2.5338525856,1.1151791149,2.0624496539	1342.1113 1366.8009 1373.4394
H,0,-1.0942920703,2.0387302132,1.5915753292	1384.9714 1408.5177 1412.6464
C,0,2.7375572921,0.0318499137,-0.0686530469	1418.6707 1423.0449 1459.4788
C,0,3.4258483946,-1.2827300206,0.1856700888	1477.8993 1488.2053 1489.6492
H,0,4.5074681919,-1.1694089288,0.1601635217	1495.6373 1499.5882 1508.6002
H,0,3.1550259854,-1.6904134854,1.1611872369	1511.2918 1736.4734 3020.7592
H,0,3.1349849792,-2.0237085007,-0.5618543934	3038.358 3040.0007 3047.2274
C,0,3.418804881,1.171905168,-0.0792620972	3057.3028 3058.2418 3061.8632
H,0,2.9491491735,2.1288784859,-0.2573010822	3090.2804 3093.6915 3107.0348
H,0,4.4875962012,1.1787237754,0.0903765281	3108.6775 3135.4698 3139.2148
O,0,-2.6290869684,-1.4456608109,-0.5369716182	3146.1682 3161.9956 3245.4888
O,0,-1.2657099583,-1.6693071243,-0.2345339007	
O,0,-2.8932742892,-0.0556125634,-0.250895621	
UM06-2X/6-311++G(2df,2p): E = -615.87979824 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1593155 Hartree	
TS-Syn-2a-H-Shift	
0,1	
C,0,0.3135829299,-1.5098544974,0.5678873447	-1563.5397 43.6585 48.8944
C,0,-1.1415698961,-1.2755445288,0.9607629137	52.9589 63.9569 89.2945
C,0,-2.0906974588,-1.0810935792,-0.211739418	112.9413 154.0028 156.9993
C,0,-0.2776923578,1.801785714,-0.2575117415	174.6527 188.6662 278.1802
C,0,0.4906697083,0.6977742785,-0.6565941129	303.112 337.3952 349.795
C,0,1.0991947127,-0.2065439533,0.406742165	421.9444 462.1767 475.085
H,0,-1.5360416928,-2.1451190803,1.4971045412	498.9554 531.3688 542.8594
H,0,-1.2474250705,-0.4366676918,1.655536527	585.6794 620.3649 732.7798
H,0,1.050963142,0.3291600012,1.3648389751	746.7659 774.4304 826.3662
H,0,0.3249450069,-2.0697690619,-0.3684745085	848.408 908.9727 928.3811
H,0,-0.62348967,2.0452160478,0.7435711342	950.7151 960.9092 966.7501
H,0,1.0311651587,1.5007445055,-1.531268714	985.3643 995.0313 1017.9613
H,0,0.1053047503,0.1699626205,-1.5335875967	1038.7741 1070.3168 1079.6942
H,0,0.808356523,-2.1229001082,1.3213513203	1109.1013 1143.7277 1182.0181
C,0,-3.3936173727,-0.3866596298,0.0960521238	1190.7854 1219.8106 1236.0548
H,0,-3.1930416179,0.6710849587,0.2834760406	1260.7537 1289.5262 1334.5316
H,0,-4.0761716134,-0.4782801403,-0.7432955384	1342.8381 1375.6515 1379.5052
H,0,-3.8426471307,-0.7936200222,1.0026794912	1395.236 1404.3592 1416.4775
C,0,2.5759947078,-0.4056952763,0.1134681955	1431.8737 1459.3345 1465.3271
C,0,3.4337717472,0.8079659298,0.3350861002	1468.6942 1481.9739 1484.9693
H,0,4.4695465544,0.6161761255,0.0638563961	1495.7064 1504.2562 1602.6466

H,0,3.0764929679,1.6565577255,-0.2511316337	1735.572 1851.4284 1869.0101
H,0,3.4025488133,1.108429933,1.3852809535	2997.8714 3035.044 3044.9241
C,0,3.0853981427,-1.5567840592,-0.3066418705	3046.2938 3064.0066 3074.6344
H,0,2.4813139808,-2.4395902867,-0.4595994555	3087.7993 3103.7146 3113.2091
H,0,4.1430411329,-1.6473831158,-0.5162142387	3116.7321 3139.8502 3158.2824
O,0,0.2710820763,2.4694455868,-2.2543196761	3164.5445 3170.5655 3248.5026
O,0,-1.8298084383,-1.4830485972,-1.3158463584	
O,0,-0.4014359462,2.7716283817,-1.0877222089	
UM06-2X/6-311++G(2df,2p): E = -615.8723957 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1534784 Hartree	
TS-Syn-2a-H-Shift-02	
0,1	
C,0,0.3037639076,-1.4882125602,0.7480566402	-1566.8949 45.3998 60.2303
C,0,-1.1789322196,-1.2309249126,0.9959350676	66.7825 82.5563 82.951
C,0,-2.0463239247,-1.3714304238,-0.24750525	97.3142 120.5912 175.6108
C,0,0.4319457903,1.9137467811,-0.7912897489	190.1262 224.5327 286.2038
C,0,0.4403615131,0.5097530998,-0.7700572309	307.0279 327.1933 346.5036
C,0,1.0845445971,-0.2150512687,0.402743394	432.5072 451.6206 477.3722
H,0,-1.5814245091,-1.9592473935,1.7074944234	496.2302 519.3814 539.4542
H,0,-1.3564967554,-0.2497321076,1.445268071	596.73 623.9952 726.8468
H,0,1.0142290355,0.4500973477,1.2739152649	752.52 772.5536 824.5888
H,0,0.3868496366,-2.2055403535,-0.0696731699	840.1773 906.9651 925.4851
H,0,0.9763430045,2.5947154354,-0.1432759823	961.5698 966.5757 970.8447
H,0,0.5978388309,0.0377926924,-1.7445086041	979.4006 1003.1879 1014.3233
H,0,-0.8028680562,0.5916673549,-1.1613999056	1040.4434 1069.9097 1083.8737
H,0,0.7614476096,-1.9401909055,1.6281270473	1104.3764 1148.7412 1178.5216
C,0,-3.382450847,-0.6767423803,-0.21381694	1185.8216 1224.8872 1235.186
H,0,-3.2123081371,0.3842423322,-0.4166376319	1262.3438 1293.0974 1335.8764
H,0,-4.033422683,-1.0801528618,-0.9838191333	1347.6027 1366.2728 1378.4939
H,0,-3.8466372038,-0.7589667918,0.7689435462	1394.5097 1403.1228 1413.9541
C,0,2.5641724802,-0.4510508918,0.1593211562	1424.5912 1456.2726 1462.3073
C,0,3.3984864301,0.7920018012,0.0096457634	1469.5062 1481.6561 1489.2092
H,0,4.4581039726,0.5507326076,-0.0363917431	1496.8448 1505.4441 1605.9163
H,0,3.1390178771,1.3350573617,-0.9016723557	1734.6719 1845.6134 1916.9115
H,0,3.2385136452,1.4721429108,0.8505361375	2998.9745 3042.9973 3044.5553
C,0,3.1105465429,-1.6581949315,0.0779904771	3050.2927 3064.9556 3072.5055
H,0,2.5336311652,-2.5663575301,0.1739979385	3085.531 3100.1259 3121.3244
H,0,4.1725323088,-1.7718080052,-0.0964863138	3124.0258 3142.2697 3157.91
O,0,-1.2769446978,1.5385394665,-2.0918465616	3158.5126 3181.6068 3241.1537
O,0,-1.6832565389,-2.0092466431,-1.2026981106	
O,0,-0.4817674647,2.4915125499,-1.4815171356	
UM06-2X/6-311++G(2df,2p): E = -615.8736858 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.154405 Hartree	
TS-Syn-2a_Dioxirane1	
0,1	
C,0,0.3281342535,-1.2354161642,0.8981302721	-699.6077 25.6489 69.7056
C,0,-1.1412491794,-0.8675103903,1.097928275	78.5464 82.8689 129.3957
C,0,-2.0583911405,-1.274235545,-0.0527033091	136.1141 140.9103 155.4855
C,0,-0.1518840648,1.6369195587,-0.8188751595	158.0544 208.4243 237.7377
C,0,0.5505340351,0.3596684555,-1.0730545774	261.879 300.871 322.5746
C,0,1.1733694093,-0.1159938731,0.2844598024	382.3002 422.4296 450.1669
H,0,-1.544442805,-1.3999903432,1.9656371154	485.2764 521.5665 554.6933
H,0,-1.2873435076,0.1918955195,1.3221953585	612.5091 644.9306 716.0574
H,0,1.1500619513,0.7290480692,0.9882019126	740.0621 769.6204 809.2414
H,0,0.3612222163,-2.1148447369,0.2541107896	836.7478 881.8736 915.9028
H,0,0.4761285691,2.4747570953,-0.4853983238	952.571 953.0786 965.1524
H,0,1.3409211805,0.5589033557,-1.7983196692	991.1336 1006.8404 1027.5105

H,0,-0.1135732532,-0.386253968,-1.4940883634	1051.1096 1072.7615 1073.8504
H,0,0.7801749529,-1.5103427103,1.8514479021	1107.9022 1135.5087 1186.8414
C,0,-3.4081388318,-0.6156479928,-0.1070746919	1214.4693 1236.4441 1274.1905
H,0,-4.1137628736,-1.2626981751,-0.6207921855	1281.7282 1313.4437 1352.1288
H,0,-3.7721749721,-0.3518384768,0.8850750385	1383.4026 1388.2728 1395.7256
H,0,-3.2884064296,0.3003837494,-0.6922315863	1409.9903 1419.1516 1419.7349
C,0,2.6358221072,-0.4593635698,0.0978868837	1442.2805 1444.3894 1455.5374
C,0,3.541438255,0.7268479201,-0.0827722799	1473.3442 1483.7444 1485.0668
H,0,4.5619890076,0.4207340094,-0.3014537584	1489.699 1496.6408 1603.4583
H,0,3.2013131497,1.3728435054,-0.8959229355	1745.7275 1819.1324 3032.1048
H,0,3.5513584976,1.3375173848,0.8232827751	3043.0408 3046.8986 3054.0138
C,0,3.1014939581,-1.7016433541,0.0964996578	3058.1858 3070.0558 3079.497
H,0,2.4645308498,-2.5619183943,0.2422880103	3089.3764 3096.9531 3105.0419
H,0,4.1555868782,-1.8938397174,-0.0552250847	3116.0256 3126.9198 3138.9824
O,0,-1.6245363893,1.3342165612,-2.0950390284	3151.1171 3168.5399 3233.1483
O,0,-1.7162659399,-2.0997633671,-0.8611446192	
O,0,-1.3963120447,1.837190924,-0.7259337908	
UM06-2X/6-311++G(2df,2p): E = -615.8556258 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1395845 Hartree	
TS-Syn-2a_SOZ1	
0,1	
C,0,0.2642507105,-1.3435615778,0.4850114955	-334.5995 65.4252 90.2179
C,0,-1.0883659538,-1.0669723278,1.1251410307	132.6118 158.1045 172.4828
C,0,-2.0294160209,-0.2836694776,0.240791967	191.1736 197.4827 210.4569
C,0,-0.5015796595,1.4217095761,-1.2803482674	233.3935 260.9468 267.0224
C,0,0.7381054097,0.6257922979,-1.0909508979	327.2125 355.936 385.39
C,0,1.1176136527,-0.0962865229,0.2167970883	442.8407 458.6994 478.8277
H,0,-1.5871402751,-2.0175938203,1.3459551261	523.5743 532.7656 554.2497
H,0,-0.9764793521,-0.5450907635,2.0759904341	611.3996 725.5577 756.6027
H,0,0.9887334067,0.602672913,1.042329891	778.7729 785.556 848.6115
H,0,0.1118114031,-1.8918672782,-0.44722682	887.5479 917.6133 944.1835
H,0,-0.7269607531,1.7309638806,-2.2981133636	954.7595 968.1632 984.2268
H,0,1.5203321754,1.3612367977,-1.3341182854	996.5271 1004.6128 1028.2885
H,0,0.7598360028,-0.0931903362,-1.9127430391	1051.7518 1070.1594 1075.1004
H,0,0.8276828599,-1.9979397334,1.1508154152	1098.2098 1143.6226 1189.0423
C,0,-3.386164952,0.0546054731,0.7992761861	1212.6012 1233.0698 1271.615
H,0,-3.3367867562,0.2865603643,1.859905781	1305.9411 1319.3136 1347.8979
H,0,-3.7987953791,0.9003235763,0.2555337828	1396.6484 1404.6315 1408.3089
H,0,-4.0408284592,-0.8080991854,0.652958328	1413.761 1418.0739 1418.3314
C,0,2.6019074611,-0.4108803551,0.1009771232	1436.4183 1455.0667 1465.1768
C,0,3.5226546145,0.6972655054,0.5279843889	1475.5874 1482.5183 1485.1291
H,0,4.5639411792,0.4559805323,0.3249488606	1492.008 1498.1996 1617.342
H,0,3.2814204584,1.6351346629,0.022164936	1669.0979 1737.0292 2995.2557
H,0,3.4103061543,0.8855202302,1.5978290192	3032.1868 3041.2531 3053.8694
C,0,3.0631998033,-1.5664845214,-0.3609009129	3062.2221 3082.2675 3093.0454
H,0,2.4041462857,-2.37376152,-0.6512684756	3095.4384 3100.4872 3108.2927
H,0,4.1263406391,-1.7448909834,-0.4559934405	3136.4771 3138.3547 3150.2269
O,0,-1.1385893192,1.5873898617,0.8294152847	3168.0667 3194.9864 3231.2371
O,0,-1.8414151689,-0.2412676267,-0.9838387782	
O,0,-1.1588645173,2.0924301785,-0.4446083276	
UM06-2X/6-311++G(2df,2p): E = -615.893836 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1753692 Hartree	
TS-Syn-2a_SOZ2	
0,1	
C,0,-0.4463960408,1.3447157643,-0.2643362028	-334.4756 61.1574 83.8651
C,0,0.8647125126,1.6925956764,0.4415428261	138.6564 155.5222 163.7641
C,0,1.7703798702,0.5342065509,0.797677349	172.6249 186.9376 195.3848

C,0,0.6176013677,-1.8137531848,-0.0163002964	226.4205 260.7097 294.3083
C,0,-0.6999725628,-1.2070806566,-0.361492057	332.2969 348.9704 387.2342
C,0,-1.1950126955,0.1185814884,0.27392926	440.0089 471.4065 507.7013
H,0,1.4146972166,2.4166227681,-0.1586436295	518.2571 526.3688 558.9524
H,0,0.6446461494,2.1768894079,1.3997346244	612.2415 684.1275 731.2223
H,0,-1.0465554943,0.0452282913,1.3520978458	779.0971 827.8627 857.043
H,0,-0.2475863939,1.2020166425,-1.3263913367	899.3207 929.4534 943.7424
H,0,0.6760450474,-2.7226416548,0.5738685429	956.7217 984.881 987.6964
H,0,-1.4350380543,-1.9844880324,-0.1459645647	1003.2834 1025.5973 1028.7038
H,0,-0.665794884,-1.0543652441,-1.4443440569	1041.0726 1071.2275 1078.4915
H,0,-1.1050543896,2.2090577163,-0.173569395	1097.8697 1128.4054 1197.8519
C,0,3.257326103,0.7698856537,0.7638616142	1209.5864 1232.7905 1282.5435
H,0,3.557106756,1.3127624679,-0.1277251467	1297.0672 1327.4784 1345.4192
H,0,3.5286626428,1.3588976373,1.6444802444	1354.8789 1387.2121 1392.894
H,0,3.7733371208,-0.1854353039,0.8116172949	1403.9746 1413.0598 1426.611
C,0,-2.6914634614,0.1735849023,0.0098195118	1454.4973 1462.8681 1466.9513
C,0,-3.5441768583,-0.5466069075,1.0155362942	1471.5825 1483.7527 1484.4798
H,0,-4.5905113834,-0.5617112791,0.7175965582	1493.2153 1502.4829 1602.0611
H,0,-3.2119344978,-1.5780201739,1.1548424448	1663.7506 1738.0162 3025.6052
H,0,-3.4669956974,-0.0606171634,1.9905915048	3033.6684 3043.4508 3045.8478
C,0,-3.2159421181,0.7852593715,-1.0446502111	3064.1492 3082.3126 3086.1547
H,0,-2.6057209568,1.3155076318,-1.7637352978	3101.7217 3110.1599 3114.784
H,0,-4.2836935362,0.7775448819,-1.2203442708	3129.6654 3135.7109 3149.2881
O,0,1.6699435139,-1.6098868896,-0.6794706384	3169.8372 3200.1951 3229.66
O,0,1.7215543839,-0.3472206624,-1.2047674543	
O,0,1.3203385204,-0.4211718199,1.4468431927	
UM06-2X/6-311++G(2df,2p): E = -615.889581 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1721408 Hartree	
TS-Syn-2b_SOZ1	
0,1	
C,0,-0.4057430945,1.3402904184,-0.1006427024	-260.2951 49.9359 72.7073
C,0,0.9311443497,1.4847361609,0.6476335323	136.1448 153.8574 160.3405
C,0,2.167912914,0.7474926961,0.2418006355	192.3947 209.7002 225.3388
C,0,0.7015445602,-1.2860707533,-0.9356919307	230.2014 301.9218 308.4802
C,0,-0.7719170635,-1.1604360316,-0.6341107476	337.9391 361.8197 398.0817
C,0,-1.1927149371,0.0615592084,0.2070900603	429.604 440.4116 466.5828
H,0,1.2073404648,2.54040628,0.6186126705	498.1112 561.0122 586.5318
H,0,0.7715886175,1.1995281734,1.6923826251	625.9747 667.7141 725.6497
H,0,-0.9935456264,-0.1940220465,1.2513365537	766.6917 817.4738 869.8628
H,0,-0.244625337,1.464024563,-1.1703327264	902.5326 912.1686 949.5337
H,0,1.0993422274,-2.3083037097,-0.9525696379	965.6559 984.7867 995.3338
H,0,-1.1062988522,-2.0759506803,-0.1473753669	1015.5154 1032.6308 1054.9184
H,0,-1.2692027747,-1.1086556932,-1.6089274765	1066.5807 1071.4098 1078.0894
H,0,-1.006671832,2.1840227941,0.24081469	1095.2743 1150.3186 1192.5135
C,0,3.3028679257,1.451209842,-0.404456739	1229.5722 1279.3832 1290.2204
H,0,3.6256718915,2.2877731143,0.2167941376	1320.8382 1334.6957 1350.4864
H,0,4.1279069721,0.7686613931,-0.5820383704	1371.391 1386.2891 1407.0329
H,0,2.9451814073,1.850331467,-1.3537356119	1413.6433 1416.0126 1432.2302
C,0,-2.6940007013,0.2333988144,0.0675197041	1455.4876 1458.2974 1475.7744
C,0,-3.5221493891,-0.8222980846,0.7477429437	1476.5564 1480.3691 1488.3491
H,0,-4.5852415562,-0.6095471567,0.6567318438	1489.0681 1502.5144 1605.7872
H,0,-3.3359226232,-1.8078847143,0.3169839913	1666.1921 1732.1519 3043.082
H,0,-3.2681729902,-0.8863382432,1.8078301419	3043.8779 3046.479 3053.3351
C,0,-3.2642525105,1.2094642894,-0.6298974592	3059.7209 3066.9439 3070.0479
H,0,-2.6917980698,1.9709495302,-1.1413117759	3099.9969 3105.1272 3115.3316
H,0,-4.3410756401,1.2700829981,-0.7194971191	3127.307 3129.1147 3134.4329
O,0,2.4415316301,-0.3933803209,0.7143317613	3150.0319 3183.053 3229.1594

O,0,1.3314705235,-0.3844676047,-1.4965426672 O,0,1.3310399238,-1.1266305439,1.0379307002	
UM06-2X/6-311++G(2df,2p): E = -615.8949978 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1762558 Hartree	
TS-Syn-2b_SOZ2 0,1 C,0,-0.161405534,-1.437679361,0.0575879062 C,0,1.3156742075,-1.3002173082,-0.3202801074 C,0,2.3786244046,-0.7095968442,0.5464006672 C,0,0.5599352602,1.173050232,1.5239444251 C,0,-0.8469119314,0.69196168,1.2886430146 C,0,-0.9880761154,-0.145294498,0.0125121363 H,0,1.7113622433,-2.3110227481,-0.5008719399 H,0,1.4052098921,-0.7851070954,-1.2795745503 H,0,-0.6126516349,0.4650045075,-0.8159162239 H,0,-0.2593025017,-1.923878948,1.0249674437 H,0,0.7313822892,1.6958927089,2.4731983475 H,0,-1.4786403694,1.5838266475,1.2243210871 H,0,-1.1876768591,0.12415388,2.1556665607 H,0,-0.5777402367,-2.1141632995,-0.691837504 C,0,3.7016106496,-0.4322286789,-0.0763056813 H,0,4.4653422074,-0.310776914,0.6859452594 H,0,3.9766537328,-1.2218337375,-0.7739297487 H,0,3.6001537257,0.500977782,-0.632132416 C,0,-2.4624024258,-0.3979821316,-0.2372398883 C,0,-3.205237078,0.7331055546,-0.8916804063 H,0,-4.2702897195,0.5223129503,-0.9631692889 H,0,-3.0760988312,1.666446076,-0.3406576142 H,0,-2.8179112585,0.9062044806,-1.8982952378 C,0,-3.0762765596,-1.5226059005,0.1118848123 H,0,-2.5505968645,-2.3465700988,0.5756009089 H,0,-4.1377694353,-1.6528010298,-0.0539506696 O,0,1.1532345535,-0.5879405048,2.4044345376 O,0,2.3839685966,-0.6422679152,1.8057978319 O,0,1.3625790924,1.3122187141,0.5952836581	-232.0614 60.8604 70.1968 144.5444 156.7553 159.228 182.0148 210.4585 221.4348 240.4731 285.7637 299.956 343.7449 376.2196 388.3237 429.0573 441.2107 465.6779 503.6793 534.599 558.1743 650.8605 690.2353 729.1375 761.3737 793.0579 847.0335 900.2274 925.1881 948.0579 962.2961 977.1055 987.9375 1009.2079 1025.7012 1048.6556 1069.037 1073.2056 1084.6013 1109.5459 1140.1345 1195.1613 1231.92 1245.74881287.9867 1308.9993 1323.2537 1357.198 1383.404 1391.7823 1402.8827 1415.8035 1419.6051 1439.0586 1449.2994 1454.3451 1463.1534 1469.135 1484.4112 1488.0007 1492.7046 1499.3885 1616.9128 1664.5667 1734.0585 3005.3359 3034.4327 3039.041 3045.3756 3058.6361 3064.3389 3070.4976 3087.2246 3098.1442 3101.5576 3134.5642 3136.0507 3140.3661 3147.216 3173.4683 3226.9664
UM06-2X/6-311++G(2df,2p): E = -615.8983847 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1786413 Hartree	
TS-Anti-2b_SOZ1 0,1 C,0,0.3684192772,-1.3335579862,0.2310305101 C,0,0.0337440076,-2.012663609,1.5799296599 C,0,-0.4016021883,-1.0279099204,2.6149992389 C,0,-0.5521770158,1.3603943689,1.4683049707 C,0,0.7392687086,1.2556022548,0.6875649168 C,0,1.3393050766,-0.136886217,0.3104740416 H,0,-0.7354930146,-2.7696624548,1.4389627298 H,0,0.930184679,-2.5104736201,1.9593102937 H,0,2.0785294658,-0.3745025191,1.079216794 H,0,-0.5575665204,-1.0483578119,-0.2623943794 H,0,-0.8151867616,2.3724622994,1.7987200936 H,0,1.4918467232,1.8585846689,1.1930679041 H,0,0.4954737427,1.7811356354,-0.2451376489 H,0,0.8439445891,-2.1019044936,-0.3786307906 C,0,-1.6528213013,-1.1333268151,3.40062848 H,0,-2.4903049643,-1.3518292831,2.7453852008 H,0,-1.5165126561,-1.9754661357,4.0880491402 H,0,-1.8293715005,-0.2212639886,3.9582468947	-351.5682 52.1689 67.6838 151.2935 171.0367 178.4161 188.7662 208.7463 235.0911 260.5097 297.745 304.6087 325.8648 340.0731 378.7221 428.6468 443.9625 471.8304 507.002 555.7417 560.1892 615.1959 707.3942 729.3412 780.7394 812.3474 842.2876 877.0235 912.6228 938.6795 950.3266 956.6722 979.4295 1011.2599 1015.298 1028.3604 1045.0096 1053.3036 1072.6507 1091.3706 1140.8258 1185.9712 1229.4951 1265.3022 1274.9941 1306.171 1328.1262 1334.6941 1359.121 1372.9664 1388.8608 1409.1517 1413.8047 1423.8361

C,0,2.1181636852,0.0607983359,-0.9805108873	1449.1538 1452.0589 1456.7633
C,0,3.3670491292,0.8883988274,-0.8466556422	1479.3235 1486.8148 1488.4086
H,0,3.8897244411,0.9718680755,-1.7972164461	1494.2368 1502.1756 1574.3098
H,0,3.1375148351,1.8958169943,-0.4947097523	1682.4356 1730.635 3010.6445
H,0,4.0440461128,0.4437866799,-0.1140552563	3040.7427 3042.4182 3060.6078
C,0,1.7291752316,-0.4118451973,-2.1589636218	3061.8113 3073.5988 3075.0458
H,0,0.8301378625,-0.9994182148,-2.2830880369	3098.8095 3111.2558 3125.2297
H,0,2.3064032525,-0.2123335403,-3.0523279324	3135.9868 3139.7369 3152.6757
O,0,0.1818333053,0.9959974999,3.4164075532	3156.5402 3217.1098 3236.9869
O,0,0.5530588987,-0.2554308134,2.9463460715	
O,0,-1.4121621909,0.48415795,1.4048841104	
UM06-2X/6-311++G(2df,2p): E = -615.8816608 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1626 Hartree	
TS-Anti-2b_SOZ2 0,1	
C,0,0.433023548,-1.2845775118,0.1298972264	-379.2203 57.2001 79.9304
C,0,-0.7655466578,-1.3479177944,1.0842495155	166.5535 186.629 202.7316
C,0,-1.7975221212,-0.3155449533,0.7654414517	210.3923 219.8714 240.5141
C,0,-0.5289061178,1.9252194514,0.2631742695	261.3221 288.526 305.7779
C,0,0.5445473381,1.2454844366,-0.5669000226	339.719 352.4983 375.8343
C,0,1.2245093481,0.0394783608,0.1304677349	423.1984 475.0605 487.6533
H,0,-1.2286365749,-2.339175213,1.050398703	520.4758 548.6319 555.4509
H,0,-0.4588071636,-1.1783898043,2.1171897295	617.1604 675.8662 735.0461
H,0,1.379570208,0.3267334775,1.1751519153	776.7021 811.1171 840.8433
H,0,0.0950915682,-1.5130996336,-0.8811338405	873.8176 919.6853 934.2401
H,0,-0.8034867502,2.9500240864,-0.0046071113	951.9703 958.2488 985.2242
H,0,1.3003724516,2.0136216252,-0.7566379867	1002.9794 1021.3659 1031.2555
H,0,0.150040859,0.9642687812,-1.5427498936	1038.9937 1058.4465 1072.5326
H,0,1.1215197729,-2.0800504179,0.4170168233	1103.3145 1124.0828 1189.0651
C,0,-2.9158882398,0.0368868325,1.6729345632	1214.1771 1248.7184 1269.6669
H,0,-3.6216955112,-0.7996254455,1.6465117775	1296.0617 1321.31 1345.3053
H,0,-2.5523818227,0.1587466177,2.6883060935	1364.5792 1374.4417 1393.9217
H,0,-3.4038918853,0.942308237,1.3317073182	1410.8404 1415.5815 1420.4438
C,0,2.5978181878,-0.1300355565,-0.4970813342	1445.4012 1454.9598 1459.5653
C,0,3.6685741861,0.7605290992,0.068156668	1462.7919 1487.1501 1488.5566
H,0,4.597484017,0.6770868284,-0.4923447928	1492.5778 1498.6412 1566.2492
H,0,3.3575695478,1.8072174737,0.0661045115	1660.2839 1736.6196 3040.997
H,0,3.8656377354,0.4953949416,1.1093057697	3045.6395 3049.9403 3051.1804
C,0,2.8489563729,-0.9789969368,-1.4863969899	3057.7685 3068.8821 3095.1161
H,0,2.0893863098,-1.6331680858,-1.8925090093	3101.9468 3113.7207 3116.607
H,0,3.8351653281,-1.0442965034,-1.9267719178	3121.4961 3140.3552 3153.0739
O,0,-2.2360010886,1.274713387,-0.7636801792	3158.7571 3206.1894 3240.9166
O,0,-1.7996394389,-0.0078272368,-0.4703091663	
O,0,-0.7947738969,1.4783450169,1.3825934134	
UM06-2X/6-311++G(2df,2p): E = -615.8871396 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1681034 Hartree	
SOZ1 0,1	
C,0,0.256049809,-1.3030735366,0.4951537133	57.2876 94.3891 144.9905
C,0,-1.0957990113,-0.9960515476,1.1455330063	170.709 180.2523 215.0518
C,0,-1.852125642,0.1452911082,0.4802731165	236.3157 252.9499 275.864
C,0,-0.6884326854,1.1622189705,-1.1557298497	303.5431 368.0676 383.2465
C,0,0.7390683871,0.6505415014,-1.0733449361	408.3501 429.8372 450.5775
C,0,1.1513058595,-0.0836036309,0.2206167076	513.1753 548.264 610.6092
H,0,-1.7191439544,-1.8915500738,1.1242882505	639.89 646.797 726.7471
H,0,-0.9639949052,-0.7238136727,2.1953402675	800.5202 817.4591 848.2661
H,0,1.0577943056,0.6166887333,1.053857314	874.1462 890.2116 910.0549

H,0,0.0837323278,-1.8354861745,-0.4427221444 H,0,-0.8877265077,1.6111265028,-2.1293172545 H,0,1.3975611475,1.5025125224,-1.2523070749 H,0,0.8762989395,-0.0410543759,-1.9091634452 H,0,0.7921974946,-1.9899343686,1.1507047792 C,0,-3.3352587338,0.1710231049,0.7619331039 H,0,-3.5116718195,0.1250092231,1.8357125687 H,0,-3.7563057776,1.0926784849,0.3653065742 H,0,-3.8171534274,-0.6805421569,0.284044771 C,0,2.6218531277,-0.4376652385,0.0909136953 C,0,3.578345402,0.6687435916,0.4369859937 H,0,4.6093794784,0.3824062461,0.2400194375 H,0,3.3586788516,1.5760098532,-0.1292295053 H,0,3.4855449779,0.9289883026,1.4935923884 C,0,3.0490605531,-1.6252736182,-0.3212194828 H,0,2.3683956017,-2.431311359,-0.5603754735 H,0,4.1058795515,-1.8298860049,-0.431871086 O,0,-1.2267518525,1.3569383485,0.9587613457 O,0,-1.6459963595,0.1629714172,-0.9170415376 O,0,-1.0060767082,2.1481818371,-0.2007048232	926.7692 947.2923 949.0292 969.4967 996.7461 1006.0603 1029.3192 1046.7932 1058.5601 1072.0719 1086.9032 1118.7489 1145.8774 1183.175 1204.5451 1215.164 1251.1459 1265.2788 1291.6761 1308.1353 1316.7399 1351.477 1372.9609 1376.0605 1394.6212 1403.2765 1414.8303 1416.5413 1420.0959 1456.3268 1472.4786 1482.731 1486.9249 1490.3277 1492.9088 1497.3595 1509.6712 1733.5108 3043.3461 3048.742 3052.6086 3057.6491 3061.0666 3074.6223 3094.568 3098.1466 3102.268 3107.5346 3134.1482 3135.7806 3140.9312 3151.0465 3151.4902 3231.8526
UM06-2X/6-311++G(2df,2p): E = -615.9650853 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.2395947 Hartree	
SOZ2 0,1 C,0,-0.1495358248,-1.4427778404,-0.0763848487 C,0,1.3201005891,-1.2445155992,-0.4642259672 C,0,2.1744901061,-0.3351564954,0.4136768518 C,0,0.6785665556,0.8004316972,1.656930995 C,0,-0.770715933,0.6940449082,1.2296462738 C,0,-0.9778848566,-0.1497291874,-0.0464704845 H,0,1.8166268879,-2.2159828978,-0.5057502917 H,0,1.3593375194,-0.8237088765,-1.4727638169 H,0,-0.6442960978,0.4665571613,-0.8891093262 H,0,-0.2238874103,-1.9695085749,0.8749207825 H,0,0.8544470621,1.6310587534,2.3441680685 H,0,-1.1588832099,1.7013706339,1.0759548869 H,0,-1.3276933399,0.253552785,2.0606622086 H,0,-0.581342319,-2.0957585734,-0.8362779078 C,0,3.5785061065,-0.1586665331,-0.1122287291 H,0,3.5397368775,0.2877875963,-1.1036118787 H,0,4.1343786719,0.4941913989,0.5559014429 H,0,4.0771731737,-1.1238387847,-0.1780918307 C,0,-2.4674811512,-0.3751134307,-0.2242495534 C,0,-3.2679097163,0.8442730825,-0.5932185963 H,0,-4.3092975411,0.5896408561,-0.778494564 H,0,-3.2413746459,1.5920233006,0.2015879206 H,0,-2.8604996012,1.3170903143,-1.489461559 C,0,-3.054511243,-1.5516176125,-0.0381263179 H,0,-2.5009148285,-2.4382131937,0.2375446514 H,0,-4.1252350974,-1.6605634992,-0.1515765242 O,0,1.0229301412,-0.4367468598,2.2955396164 O,0,2.2786728491,-0.8016631322,1.7458345612 O,0,1.568640936,0.933388073,0.5809946468	35.8261 72.1276 174.1254 180.4756 193.265 213.7538 229.378 243.0664 263.4604 294.0322 348.4414 386.913 412.0959 430.7639 440.6754 506.6972 555.0811 604.6004 629.6099 679.6419 717.7653 758.343 819.0817 838.2508 878.2095 896.5782 903.9793 921.8896 949.4392 954.7557 974.9288 992.6836 1010.0061 1024.4781 1053.2613 1061.5092 1071.8439 1094.6841 1137.9793 1147.6092 1194.2949 1197.1594 1238.086 1242.517 1264.4597 1290.5724 1306.1183 1330.7572 1354.9115 1369.2609 1373.8647 1405.8627 1413.9501 1419.5555 1421.1331 1428.6288 1457.88 1473.4868 1480.5978 1492.3452 1492.8806 1498.1999 1499.8795 1505.6532 1733.4019 3026.9757 3045.5173 3047.9501 3058.5552 3063.6692 3081.2222 3102.6606 3103.8344 3105.9888 3115.187 3126.7069 3142.7775 3155.6617 3162.2646 3172.3877 3236.9777
UM06-2X/6-311++G(2df,2p): E = -615.9644064 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.2389387 Hartree	
TS-Syn-2b_Dioxirane2 0,1	

C,0,-0.0233523426,-0.6199250717,0.0611007573	-482.7934 37.2107 63.4115
C,0,-1.0600920732,0.4756727275,0.2804322124	67.3727 107.9382 118.7843
C,0,-2.4705634667,0.0054385767,0.1942353034	128.8659 161.7124 180.1153
C,0,1.4333435697,2.3649296109,-0.1895564391	200.2547 213.8545 251.1733
C,0,1.7418846204,1.009020292,-0.7617992786	266.4622 309.6527 333.5183
C,0,1.4140795746,-0.1309497295,0.2373591539	353.2976 403.7014 431.7136
H,0,-0.9189065049,1.0099244551,1.2242006308	460.3311 511.9687 553.4953
H,0,-0.9902507726,1.2504447674,-0.4965390775	593.7133 663.3719 722.8343
H,0,1.5116348833,0.2798277979,1.2518091229	736.9365 763.2233 794.261
H,0,-0.1569295011,-1.0243035683,-0.9425212241	850.5705 879.1255 917.2802
H,0,2.0096419919,2.6214390385,0.7231852732	952.3864 964.0982 975.6298
H,0,2.8115400849,1.003955945,-0.9853126501	995.5517 1016.5603 1026.9376
H,0,1.201231102,0.8690799812,-1.6983448926	1044.0804 1068.4095 1073.9661
H,0,-0.2065212376,-1.4426040435,0.7539440008	1112.9661 1137.2038 1193.7256
C,0,-3.5525704551,0.8750957376,0.7311765545	1211.0676 1237.3813 1274.4187
H,0,-3.2798672227,1.1761587253,1.746076584	1292.2082 1322.4088 1347.0021
H,0,-3.6297988119,1.7825562311,0.1315906751	1375.883 1391.6778 1409.2071
H,0,-4.5018172058,0.353628651,0.7031395534	1415.0223 1425.5155 1432.1803
C,0,2.4440514014,-1.238465905,0.128119424	1443.581 1451.2145 1456.4295
C,0,3.7737010055,-0.9298226081,0.7577608423	1459.4504 1480.759 1489.0951
H,0,4.4909671992,-1.7288904874,0.5844982782	1494.611 1501.1383 1580.2487
H,0,4.2004212645,-0.0009733496,0.372978937	1738.8173 1838.6917 2977.1474
H,0,3.6580371362,-0.7990442196,1.8363369879	3032.9162 3040.5899 3044.4364
C,0,2.2070528586,-2.4022053326,-0.4638475441	3045.4945 3052.6012 3067.947
H,0,1.249156843,-2.6544017794,-0.8959654155	3078.4929 3083.7283 3098.4755
H,0,2.981551655,-3.1550215544,-0.5278234711	3122.9464 3127.4537 3143.0367
O,0,-3.6385014552,-0.6867823485,-1.261656635	3155.5135 3180.5187 3237.8836
O,0,-2.6711710132,-1.1645158799,-0.2545062232	
O,0,0.6330186824,3.1399101004,-0.6332504399	
UM06-2X/6-311++G(2df,2p): E = -615.8633022 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1454411 Hartree	
TS-Anti-2b_Dioxirane2 0,1	
C,0,0.008547468,-0.6205350276,-0.007570002	-520.1978 62.5134 64.911
C,0,-1.0375203701,0.4679981773,0.2024516705	88.7499 116.9164 133.4563
C,0,-2.4432996245,-0.0030011913,0.0613031387	157.5719 175.214 214.0447
C,0,1.4645653431,2.3719154966,-0.1469605714	226.0644 242.186 247.4842
C,0,1.7946735974,1.0294006087,-0.7384264097	268.4491 311.8212 347.0751
C,0,1.4383680072,-0.1327052619,0.2248295729	379.3514 393.2729 435.9187
H,0,-0.9277499611,0.9818422421,1.1616028612	464.3204 513.6075 552.2448
H,0,-0.9451205732,1.2596426915,-0.5549094662	592.3595 669.4976 724.2331
H,0,1.5026170773,0.2560646402,1.2505458496	733.9343 771.3727 804.5951
H,0,-0.0920643931,-1.0032181265,-1.0234698923	872.8848 879.5108 915.2765
H,0,2.0109565945,2.6096004624,0.7889756628	948.5761 955.7609 974.6547
H,0,2.8708869713,1.0312935753,-0.9279198718	989.6211 996.9741 1023.0024
H,0,1.2843548208,0.9088444247,-1.694485073	1043.051 1068.5297 1074.0388
H,0,-0.1943247849,-1.4584656836,0.6610842682	1114.6528 1136.0336 1195.0229
C,0,-3.5440856792,0.8526122142,0.5824019969	1211.0158 1226.8999 1266.0366
H,0,-3.3044982482,1.1319807695,1.61176066	1290.1983 1313.9722 1346.8549
H,0,-3.6046615976,1.7727927119,0.0005509229	1379.2474 1393.3546 1413.6876
H,0,-4.490583511,0.3300285642,0.5128933804	1418.1034 1423.8968 1426.1035
C,0,2.4742134836,-1.2355618574,0.1243374987	1428.4267 1449.8162 1450.8594
C,0,3.7824063835,-0.9381073937,0.8024445816	1456.4165 1471.809 1487.873
H,0,4.5069186626,-1.7318064331,0.6347425479	1495.7992 1502.515 1591.1096
H,0,4.2186534768,-0.0002632438,0.4516667436	1735.2179 1825.6252 3019.7527
H,0,3.6322525647,-0.8310824042,1.8793879634	3030.5021 3036.174 3044.4448
C,0,2.2591872302,-2.3865904072,-0.4999858223	3049.1467 3053.4282 3069.6907

H,0,1.3161467924,-2.6311868004,-0.9676833556 H,0,3.0373153012,-3.1363173989,-0.5556608984 O,0,-3.5626523559,-0.6655713058,-1.445654642 O,0,-2.6264796794,-1.163274797,-0.4189223373 O,0,0.6766656638,3.1548167436,-0.5989104775	3090.3061 3101.6348 3104.7511 3117.1026 3119.4384 3137.1844 3155.5971 3184.3169 3236.8492
UM06-2X/6-311++G(2df,2p): E = -615.8721786 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E =-615.152717 Hartree	
Dioxirane2 0,1 Redundant internal coordinates found in file. C,0,-0.059539249,-0.6717121698,-0.2802045567 C,0,1.0686797055,0.3471976337,-0.4432557262 C,0,1.1831008077,1.0406161936,-1.7763762613 C,0,-1.3234093426,2.3799195527,-0.1595494552 C,0,-1.6782512058,1.1014821617,0.5512671782 C,0,-1.4946998775,-0.1396141412,-0.3583357495 H,0,1.0170458019,1.1231877321,0.3228696268 H,0,2.0204498957,-0.1661978372,-0.2839496825 H,0,-1.6903522402,0.1735569219,-1.3864814115 H,0,0.0854523211,-1.1212824996,0.7040205791 H,0,-1.9615151693,2.6152305138,-1.0328670129 H,0,-2.7283062207,1.1915612536,0.840459923 H,0,-1.0855473475,1.0069411654,1.4620026275 H,0,0.0566808671,-1.4710208359,-1.0128547144 C,0,2.3343848145,1.9861880258,-1.9401544 H,0,2.2294057386,2.7997926295,-1.222135118 H,0,3.277315209,1.4743220918,-1.7512075458 H,0,2.3299954115,2.3887721885,-2.9494408385 C,0,-2.5437473428,-1.1856878821,-0.0301403233 C,0,-3.9114364646,-0.8867612555,-0.5800658404 H,0,-4.6478761586,-1.610507622,-0.2379254922 H,0,-4.2529207697,0.1101645084,-0.2935800879 H,0,-3.8865591869,-0.9071050055,-1.6718475898 C,0,-2.3103058406,-2.292515519,0.6649607712 H,0,-1.3332895976,-2.5539494699,1.0440224481 H,0,-3.1109253605,-2.991189717,0.8698672102 O,0,0.8152433537,0.305234206,-2.8977292057 O,0,0.0112337499,1.429681853,-2.4159786105 O,0,-0.4284221225,3.1182904429,0.1524139182	34.6953 43.0259 69.7986 77.5102 89.1594 96.5467 152.1349 168.3309 189.9229 199.7848 224.806 264.4504 316.3118 335.9493 396.3843 413.189 430.593 457.3388 494.9425 523.1591 570.5972 581.1984 727.7044 758.8391 794.0902 795.8987 874.6976 884.4058 941.8401 950.5031 964.8171 981.6071 992.9134 1021.0408 1022.6981 1057.6743 1063.1855 1076.9643 1102.9891 1125.5627 1151.7635 1206.1248 1221.5098 1243.2061 1277.3292 1290.7636 1315.5873 1341.4956 1361.2106 1398.8214 1415.8512 1418.3245 1426.982 1429.2583 1456.2036 1458.4508 1461.1795 1480.4719 1489.8114 1493.2378 1498.0966 1505.9672 1513.815 1738.6469 1863.462 2950.7031 3006.4914 3039.8949 3040.0841 3047.9249 3067.1079 3070.7501 3090.8717 3095.2796 3114.7334 3121.3132 3133.6612 3136.7495 3158.7058 3172.883 3243.1019
UM06-2X/6-311++G(2df,2p): E = -615.9350402 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.2108321 Hartree	
Dioxirane1 0,1 C,0,-0.4006174253,-1.4967620855,-0.3561215971 C,0,1.0307108331,-1.4265007599,-0.8774062844 C,0,2.0892964492,-1.0518792572,0.1380223496 C,0,0.4227314216,1.6559697602,0.8123586684 C,0,-0.6426151003,0.6326349812,1.0630379074 C,0,-1.109197514,-0.1446959778,-0.1878038501 H,0,1.3306978969,-2.4082420917,-1.2606672673 H,0,1.1132938302,-0.7426243007,-1.7254428364 H,0,-0.8789091169,0.4709937511,-1.0639628738 H,0,-0.4053228864,-2.0392873325,0.5917223071 H,0,0.8978102049,2.0855315643,1.691705742 H,0,-1.4755697743,1.1837813261,1.5082180692 H,0,-0.284039377,-0.0611220794,1.8223470969 H,0,-0.9821420735,-2.0876820926,-1.0645904493	61.467 66.9253 83.5674 99.8445 114.1166 138.9135 148.2939 164.5376 169.6154 212.2156 246.318 264.0132 312.9834 333.0067 404.9572 428.8109 466.0436 492.1781 520.4812 555.4605 613.7529 628.9381 728.5501 766.1336 811.8903 852.8558 854.2158 905.5178 927.1725 945.5537 950.6037 972.4187 991.715 1004.1016 1024.2722 1048.0559 1073.6899 1076.5986 1101.6684 1128.8557 1173.4833 1197.7201

C,0,3.453368328,-0.7292162622,-0.416619217	1223.169 1254.7626 1275.1536
H,0,4.1858919025,-0.7005203838,0.3846927364	1301.0386 1322.8516 1342.8227
H,0,3.7465721923,-1.4534097608,-1.176854704	1349.7816 1386.6877 1400.587
H,0,3.4025537024,0.2494946029,-0.8974250748	1410.6502 1416.5708 1417.3835
C,0,-2.6197152855,-0.2716994815,-0.1279538214	1453.6688 1455.5523 1472.3178
C,0,-3.3646192637,0.9661222064,-0.5413292921	1473.3396 1485.6322 1487.4074
H,0,-4.4326233382,0.8753511338,-0.3546541618	1490.4608 1492.8057 1501.4769
H,0,-2.9915220371,1.8477879599,-0.0154616685	1742.6627 1833.1682 3037.8874
H,0,-3.2111650631,1.1554505883,-1.6061235576	3041.0478 3042.1994 3055.4012
C,0,-3.2494502569,-1.3690418739,0.2734818467	3057.9586 3058.9769 3092.4888
H,0,-2.720263998,-2.268741818,0.5561279331	3096.0357 3105.789 3122.8875
H,0,-4.329821118,-1.4000192743,0.3293658064	3125.168 3143.3425 3151.3029
O,0,1.2676485168,1.5266998292,-0.2766922807	3155.5451 3177.9362 3233.2494
O,0,1.8637258905,-1.0200613456,1.3237476442	
O,0,0.2276166901,2.5522023639,-0.228219211	
UM06-2X/6-311++G(2df,2p): E = -615.9389641 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.213447 Hartree	
TS-Syn-2b-H-Shift 0,1	
C,0,-0.1923015381,-1.3224072452,-0.4321233483	-1552.5099 25.2869 56.4886
C,0,1.1595804551,-0.9196874441,-0.9890555316	59.9468 83.3078 90.3711
C,0,2.3282685193,-0.9938307992,-0.1930703251	116.1825 140.9182 176.0696
C,0,0.6119831171,1.4450484401,0.7758431485	192.0571 234.8262 249.949
C,0,-0.7088502607,0.7435733409,0.9461819742	289.0512 326.6055 341.8285
C,0,-1.1379362595,-0.1248243845,-0.2537894762	344.1761 413.3744 484.6982
H,0,1.3519934644,-1.2559413634,-2.0101503556	493.8566 508.1231 553.144
H,0,1.6246897038,0.2250667625,-1.4353947971	572.8103 608.5818 707.198
H,0,-1.067232216,0.4924759143,-1.1571813163	726.5186 775.0624 806.6832
H,0,-0.083761833,-1.8326749692,0.5289456366	850.5458 896.2662 916.2591
H,0,0.7078477994,2.0884027983,-0.1193539475	951.2041 962.3985 982.3529
H,0,-1.4506841983,1.5339170224,1.0990613833	993.7942 1023.7055 1033.74
H,0,-0.6740474618,0.1391754717,1.8541615326	1061.2397 1065.1819 1076.5818
H,0,-0.6658626834,-2.0365336963,-1.1053241871	1104.1741 1127.7313 1142.5732
C,0,2.5164373646,-1.6301672693,1.1335208398	1198.9434 1243.509 1272.0519
H,0,2.1938703276,-2.6695700165,1.1149632694	1291.1061 1301.9823 1329.7334
H,0,3.5587139889,-1.5590392291,1.4330737664	1357.544 1387.797 1399.8824
H,0,1.9130890517,-1.0859950235,1.8637558436	1410.8823 1418.4523 1423.1744
C,0,-2.5937617255,-0.508250833,-0.0799171656	1451.4034 1458.4631 1468.176
C,0,-3.5879472444,0.5523605832,-0.4612161064	1473.6636 1491.4646 1497.4143
H,0,-4.6063842668,0.2429975327,-0.236411252	1500.262 1507.4595 1573.9854
H,0,-3.3937992988,1.4914289382,0.0606448667	1737.2698 1846.661 1895.6148
H,0,-3.5191230247,0.7660336085,-1.5301846722	2987.1883 3019.6784 3045.0421
C,0,-2.9785463326,-1.6905301843,0.3854835308	3046.9416 3051.827 3055.026
H,0,-2.2732027807,-2.4676581348,0.6459347495	3087.2254 3100.9519 3102.9721
H,0,-4.0273469612,-1.9200918927,0.5201314615	3118.0967 3124.9985 3146.8155
O,0,2.9549371661,0.4806981809,-1.7058492225	3155.3593 3161.8043 3235.5741
O,0,3.3057797911,-0.2533818732,-0.5821573169	
O,0,1.5185424465,1.3595131546,1.5604491275	
UM06-2X/6-311++G(2df,2p): E = -615.8757229 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1552784 Hartree	
TS-Anti-2b-H-Shift 0,1	
C,0,0.4916984537,-1.3606712048,0.2765415789	-1598.5987 52.3349 60.9086
C,0,-0.8519944559,-1.363005117,1.011849181	78.4369 94.9594 120.0889
C,0,-2.0185875501,-0.7898998838,0.2843734005	152.2857 159.0138 182.6135
C,0,-0.4648861715,1.8219118476,-0.0523662809	200.1336 238.5915 262.9214
C,0,0.683936664,1.0435063937,-0.6301211625	283.2872 316.5416 356.3151

C,0,1.2738681874,-0.0385146885,0.2891465495 H,0,-1.1255469456,-2.3895308654,1.2721998848 H,0,-0.7874692983,-0.8191842986,1.9574555228 H,0,1.2430589392,0.3572302135,1.3099273271 H,0,0.3434261748,-1.6976838368,-0.7510296578 H,0,-0.9459464863,2.5370281566,-0.742232728 H,0,1.4426524968,1.7921690426,-0.8848263728 H,0,0.3650850481,0.6199442334,-1.5857960756 H,0,1.1185234833,-2.1102874546,0.7602433457 C,0,-3.2423636292,-0.351887633,0.8144756824 H,0,-3.2916816477,-0.251071109,1.8887031634 H,0,-3.259924476,0.5275035101,-0.1792442623 H,0,-4.1302797474,-0.7783898705,0.3516094622 C,0,2.7348455447,-0.2268162899,-0.0777424008 C,0,3.6675714783,0.803050059,0.4960173553 H,0,4.6768226786,0.6909874756,0.1056478528 H,0,3.3261502963,1.8173899587,0.2791761542 H,0,3.7033718541,0.7119569877,1.5838345647 C,0,3.1747560806,-1.2071089985,-0.8573172866 H,0,2.5186933442,-1.9641251968,-1.2641785919 H,0,4.2228180927,-1.2818399352,-1.1157402073 O,0,-2.8618138371,0.2747806673,-1.4565444189 O,0,-1.8153304008,-0.5009584574,-0.9589366572 O,0,-0.8510219311,1.7173565641,1.0819915673	435.2776 482.7509 522.4058 539.9124 552.385 566.6658 647.6965 682.88 708.2546 730.8614 741.9831 810.9879 849.4835 899.9892 921.0416 932.3154 949.7539 958.7958 988.3958 1003.4193 1020.2293 1033.3018 1057.4633 1069.7466 1074.2139 1114.5243 1136.3623 1200.6662 1230.6354 1274.3664 1283.1206 1308.0592 1325.1585 1348.2385 1354.625 1387.9296 1412.258 1416.5077 1421.8632 1426.0783 1448.0219 1454.8175 1461.3227 1488.2652 1491.9434 1497.9867 1520.1184 1566.7342 1737.5215 1847.7747 1884.6162 3012.8275 3034.5295 3036.6008 3044.7025 3053.3354 3061.6283 3092.7614 3093.6997 3096.9224 3107.0039 3112.4598 3142.9359 3154.3206 3228.4244 3235.2529
UM06-2X/6-311++G(2df,2p): E = -615.877845 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1556657 Hartree	
VHP3 0,1 C,0,0.029741528,-1.8831787058,-0.1319273463 C,0,1.4389417719,-1.6995994879,-0.6866946179 C,0,2.3465290243,-0.771805236,0.1011823008 C,0,0.331425569,1.4543906664,-0.5728649571 C,0,-0.3234584708,0.5421085311,0.1254688905 C,0,-0.8989077735,-0.7067465276,-0.4824181187 H,0,1.9643897851,-2.6607541486,-0.7105678777 H,0,1.4110414874,-1.3530542449,-1.7238483452 H,0,-0.8964682956,-0.5902966031,-1.5741193513 H,0,0.0896495092,-1.9917478338,0.9526456741 H,0,0.3704399367,1.4764886058,-1.6566477781 H,0,1.7490603868,1.6052687233,1.4717362694 H,0,-0.3190251164,0.5873936119,1.2064332903 H,0,-0.3966476571,-2.8041982888,-0.5317581276 C,0,3.4679173712,-0.1317376106,-0.6747292488 H,0,3.039771768,0.6519584962,-1.3050973854 H,0,4.1931625509,0.311096798,0.0019130811 H,0,3.9496822002,-0.8539710661,-1.3341874191 C,0,-2.3411420958,-0.9021907891,-0.0587579054 C,0,-3.2838515703,0.1598361032,-0.549775962 H,0,-4.3049609751,-0.0380563602,-0.2312438745 H,0,-2.9845241897,1.1414964095,-0.1787341783 H,0,-3.264345731,0.2149037299,-1.6408650021 C,0,-2.7560235404,-1.9119512186,0.6965234181 H,0,-2.089402409,-2.6797851612,1.0621446306 H,0,-3.797276581,-1.9963212747,0.979254326 O,0,1.212514238,2.4031440739,1.3201029311 O,0,2.1954365163,-0.5561006955,1.280806949 O,0,1.1184427029,2.4580075232,-0.0864776653	36.4282 46.0105 55.6021 77.4659 81.1371 122.0346 145.2278 179.0976 193.0882 208.2571 216.1838 254.1466 295.527 329.4797 339.0328 432.3598 451.9022 473.3408 511.5957 540.4936 559.2866 613.1556 707.5972 728.8716 756.875 804.0165 853.248 882.7208 917.3393 920.9983 947.9366 961.1572 971.0804 997.7752 1012.0477 1027.2443 1055.7131 1076.8041 1086.2119 1102.5228 1134.1837 1197.6655 1220.6237 1234.8991 1269.2553 1282.0583 1312.8882 1345.1004 1364.2075 1388.8934 1406.2582 1409.1266 1420.2707 1422.5003 1450.3112 1454.5488 1461.1947 1471.8902 1485.0184 1491.0795 1499.5546 1507.3785 1650.9397 1733.0707 1826.4168 3026.3366 3031.5573 3050.6217 3052.5354 3059.0233 3070.2846 3082.4736 3107.8097 3113.2716 3116.1897 3120.2449 3142.3989 3154.8132 3179.2977 3221.0773 3237.0632

UM06-2X/6-311++G(2df,2p): E = -615.9398142 Hartree
RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.2137096 Hartree

VHP2
0,1

C,0,0.4983487953,-1.3232011786,0.2132408271	25.1422	43.3685	67.9963
C,0,-0.8938790857,-1.0112066621,0.675257925	87.4017	118.6166	121.1379
C,0,-1.927314929,-0.787995259,-0.1310614408	145.3685	153.4467	180.133
C,0,-0.3149675657,1.7497129641,0.0069097216	189.7588	223.0075	257.6658
C,0,0.9001510078,1.0505007595,-0.5478269279	270.6928	311.3962	335.7838
C,0,1.4206623245,-0.0993522424,0.3316166378	363.6112	386.8393	464.3319
H,0,-1.0480954314,-0.8975398146,1.7393995976	475.4139	496.1205	519.3145
H,0,-3.2327376369,0.8622878653,1.6518248337	535.8178	579.6648	637.0746
H,0,1.3836224876,0.246446801,1.3731778626	718.5641	754.9213	828.0834
H,0,0.497597144,-1.6642589058,-0.8216600368	868.7242	912.8024	914.1108
H,0,-0.3274852306,1.8538482919,1.1110545015	956.6116	960.5095	978.3361
H,0,1.6643911459,1.8304047857,-0.6299470471	996.0649	1023.0001	1058.4684
H,0,0.6869355663,0.7069061387,-1.5618160823	1065.3921	1070.8076	1077.2216
H,0,0.9181158711,-2.1336459483,0.8122851136	1084.6389	1123.2439	1142.4621
C,0,-1.9751643385,-0.8393772184,-1.6223660603	1187.6968	1228.2398	1259.564
H,0,-1.1476470955,-1.409144407,-2.0321615772	1282.8596	1291.8164	1315.8323
H,0,-2.9106825756,-1.2941105871,-1.9457722797	1359.4517	1371.6037	1401.7613
H,0,-1.9412198396,0.1808826984,-2.0128191056	1417.3054	1424.3296	1431.4118
C,0,2.8745228942,-0.3865666417,0.0167451778	1435.1106	1449.8033	1454.1347
C,0,3.8619922555,0.5900300688,0.5934910784	1480.7012	1482.999	1491.0362
H,0,4.8779267511,0.3612251923,0.2785480964	1496.2321	1505.2474	1735.6404
H,0,3.6369139253,1.6160048011,0.2959508012	1764.5103	1847.2746	2952.5072
H,0,3.8247303889,0.5629485839,1.6848794178	3012.4545	3043.3391	3049.1634
C,0,3.2719594045,-1.4237161996,-0.7106661938	3054.8229	3065.2598	3096.5026
H,0,2.5809680688,-2.151048343,-1.1124215212	3110.6594	3112.9976	3117.649
H,0,4.3211221736,-1.580396608,-0.9245907403	3145.4545	3161.1019	3171.9994
O,0,-3.2055093159,-0.1029140396,1.6703567204	3210.5241	3242.528	3818.1094
O,0,-3.1732986104,-0.3951687423,0.2914000727			
O,0,-1.1920026096,2.2319140465,-0.6577147924			

UM06-2X/6-311++G(2df,2p): E = -615.9328296 Hartree
RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.2074544 Hartree

VHP1
0,1

C,0,-0.5491046231,-1.5129538941,-0.3561144602	47.4467	52.1099	66.5651
C,0,0.8639387392,-1.5328303844,-0.9618151603	93.364	123.4858	148.108
C,0,1.9602273584,-1.010188581,-0.0754915534	170.1079	174.0784	198.297
C,0,0.5001196195,1.734078888,-0.4301615615	200.2835	206.233	245.1502
C,0,-0.434370016,0.9047845107,0.413530651	294.3165	338.3188	344.5981
C,0,-1.2358398276,-0.1478786412,-0.3721709651	379.5069	435.0563	470.9289
H,0,1.1146171982,-2.5688703222,-1.202433311	505.335	552.0504	557.5558
H,0,0.8908337928,-0.9668728125,-1.8933068151	639.7374	666.4037	719.4825
H,0,-1.2642795624,0.1992933177,-1.4104006809	748.4224	767.6057	825.775
H,0,-0.5023314097,-1.8956926992,0.6642662077	863.9151	887.0831	903.6752
H,0,1.2224984681,2.3473780445,0.1394572604	916.8712	952.9496	959.3415
H,0,-1.095895493,1.628192687,0.902945406	981.6417	993.9136	1010.2944
H,0,0.1377839063,0.4467613491,1.2253321094	1033.7915	1066.6715	1068.873
H,0,-1.1680380779,-2.2093061702,-0.9235389466	1078.4738	1107.7094	1136.5865
C,0,2.8992021502,-0.1383870087,-0.416919405	1193.8852	1240.4438	1273.0116
H,0,2.8699190575,0.2876932572,-1.4073078562	1281.2902	1300.9075	1314.0874
H,0,3.5457398345,-1.8235207084,1.9347514054	1355.9655	1370.6126	1386.9408
H,0,3.6715291309,0.1742265821,0.266047529	1412.4762	1417.3192	1419.6675
C,0,-2.6690347519,-0.1851826026,0.1166591686	1431.8337	1445.7685	1458.41
C,0,-3.5134861886,0.971733442,-0.3416913866	1463.919	1487.9848	1490.2661

H,0,-4.4988635544,0.9579297132,0.1192279246	1494.3322 1501.6509 1738.7932
H,0,-3.0399210468,1.9290216889,-0.1139367815	1739.6676 1848.7688 2987.8871
H,0,-3.635624465,0.9375180645,-1.4264253601	3036.3923 3042.8624 3045.3956
C,0,-3.1691454908,-1.1490021141,0.880933469	3058.1742 3065.3439 3081.46
H,0,-2.5861738888,-2.0009932637,1.2007424926	3090.2803 3104.1761 3118.0992
H,0,-4.1987933007,-1.1121658213,1.2122348978	3135.2975 3159.7714 3194.9596
O,0,2.8457540618,-1.1683360816,2.0509777697	3245.9001 3290.875 3810.5038
O,0,1.8625140509,-1.621232474,1.1509810897	
O,0,0.4700445684,1.7895877643,-1.6295435372	
UM06-2X/6-311++G(2df,2p): E = -615.9291012 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.2030062 Hartree	
TS-SOZ1-decomposition 0,1	
C,0,-0.4464747395,1.4393469446,-0.1006997551	-1420.1345 63.284 88.7017
C,0,0.9501637798,1.6068455969,0.515101521	134.9857 157.3285 163.25
C,0,1.8607838181,0.3795744617,0.4943998222	196.5372 234.9438 249.7319
C,0,0.7676098564,-1.2036112125,-0.8205473274	270.1541 292.7103 301.9732
C,0,-0.7279528568,-0.9902930459,-0.8463363527	347.9417 399.5217 421.4094
C,0,-1.1603796681,0.1024017897,0.1672193507	426.3664 458.4251 484.4244
H,0,1.459135189,2.4285033629,0.0102448584	513.3377 547.8493 601.4067
H,0,0.8605311298,1.882895869,1.5678514939	628.2681 682.6278 734.1178
H,0,-0.8939134495,-0.2504728326,1.1652486978	771.8176 804.5658 847.6974
H,0,-0.3734556573,1.5891858217,-1.1794049859	886.6233 924.3581 934.2553
H,0,1.0857612023,-2.3243157585,-1.2396561115	943.6399 955.7555 961.9905
H,0,-1.2303421169,-1.9332820544,-0.6359497279	992.5451 1005.7234 1020.8233
H,0,-1.0095276359,-0.6596959742,-1.847183998	1036.0327 1048.2588 1072.6859
H,0,-1.0725591366,2.2444016712,0.2846162836	1092.1819 1114.5632 1171.3807
C,0,3.3426586162,0.6314499868,0.3832882294	1209.937 1235.8323 1272.1611
H,0,3.6697458865,1.1654558259,1.2771359177	1283.3048 1297.9583 1341.7553
H,0,3.8610179092,-0.3231058428,0.3344264949	1351.9735 1363.778 1374.9951
H,0,3.578185159,1.2277546673,-0.4952178239	1392.048 1415.5326 1417.9954
C,0,-2.6727109471,0.196501579,0.0916559808	1423.9345 1455.2284 1470.0015
C,0,-3.4173812908,-0.8194426183,0.911141657	1475.3602 1482.9263 1485.0827
H,0,-4.4912175803,-0.7545618228,0.7486792348	1487.8216 1495.4498 1499.8843
H,0,-3.0944324806,-1.8353416345,0.6744506237	1508.8787 1736.9258 2274.0303
H,0,-3.215559872,-0.667112373,1.9735419536	3045.0821 3056.7141 3058.9918
C,0,-3.3052070067,1.0894019536,-0.6602531496	3061.3131 3069.662 3084.606
H,0,-2.7748908778,1.8298280563,-1.2443999589	3099.2051 3101.7782 3112.7187
H,0,-4.3858041593,1.1085288461,-0.7123451482	3128.5285 3135.2964 3139.1961
O,0,1.4868306745,-0.5645032118,1.3060013489	3149.8824 3160.2695 3230.1867
O,0,1.5363118429,-0.2119179306,-1.1207883149	
O,0,1.2889383114,-1.9866401207,0.1185764955	
UM06-2X/6-311++G(2df,2p): E = -615.8863058 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.174165 Hartree	
TS-SOZ2-decomposition 0,1	
C,0,-0.4363571516,1.3650316114,-0.226932467	-1389.5867 62.7182 84.4819
C,0,0.9228534319,1.6072524611,0.428300987	126.769 186.033 193.0698
C,0,1.9583923329,0.5328475106,0.1255690043	202.3521 215.8573 232.6909
C,0,0.7277721865,-1.452599549,0.1328081893	262.583 293.7706 319.0487
C,0,-0.7296090401,-1.1895746305,-0.2220016165	352.1604 401.6878 413.5718
C,0,-1.2276172128,0.1665806302,0.3219138832	440.2549 466.2285 496.2996
H,0,1.3357382172,2.5467208791,0.0501984746	515.635 556.2731 594.6792
H,0,0.8235849529,1.7116923935,1.5095376497	629.1941 688.6433 694.2415
H,0,-1.0972421648,0.1423644972,1.4081629826	744.5226 797.9904 852.0752
H,0,-0.2918426598,1.252642333,-1.3033208823	887.572 910.3353 928.624
H,0,1.0212102565,-2.6445913573,0.0529879283	950.7133 953.1086 958.1756

H,0,-1.3488899148,-1.9939478578,0.1765846119	990.1353 1004.914 1021.7613
H,0,-0.8159927251,-1.2157916577,-1.3091528108	1040.5186 1055.9634 1074.9977
H,0,-1.0403452489,2.2607750666,-0.0774355006	1096.7111 1129.3298 1173.5263
C,0,3.2954657137,0.6539829023,0.8070856218	1219.6045 1223.8026 1270.1845
H,0,3.1804566371,0.8026307927,1.8784730865	1276.0682 1312.3983 1332.1383
H,0,3.8724032344,-0.2479789767,0.6186783316	1346.9972 1371.5709 1379.2592
H,0,3.8248553513,1.5070335487,0.3802905616	1396.7837 1409.1134 1417.886
C,0,-2.7160205764,0.2496199747,0.0399583712	1428.7391 1456.7755 1462.7302
C,0,-3.5969314766,-0.4797327866,1.0156306862	1476.2887 1477.1633 1485.6894
H,0,-4.6411469455,-0.4477943294,0.7114834166	1488.062 1490.2078 1498.8586
H,0,-3.3026303695,-1.5264040633,1.1166581488	1511.0551 1736.6093 2291.2357
H,0,-3.5102322667,-0.0322925344,2.008236044	3044.5406 3046.8289 3055.5617
C,0,-3.2195681587,0.9010886055,-1.0014683358	3059.4764 3066.0522 3069.8547
H,0,-2.5947918101,1.4402153891,-1.700642838	3098.4866 3099.7259 3112.1507
H,0,-4.285673292,0.9157759231,-1.1862724708	3121.342 3138.181 3143.7838
O,0,1.5892008706,-1.6930633434,-0.8538105776	3152.822 3160.865 3233.7145
O,0,1.949484678,0.1035529727,-1.0974735105	
O,0,1.2590346503,-0.7855122354,1.0975066408	
UM06-2X/6-311++G(2df,2p): E = -615.8882834 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1760949 Hartree	
PRC5 0,1	
C,0,-0.9487826191,2.0943201981,0.0044399651	28.9459 42.6562 48.5801
C,0,-2.4035956806,1.9599366834,-0.4315294899	82.6995 87.6621 126.419
C,0,-3.0249609933,0.6599930265,0.0119239738	129.8929 144.7482 171.2253
C,0,-2.2809865031,-0.35329567,0.4447540101	195.5822 215.2581 240.7609
C,0,-0.7782110394,-0.3417585344,0.498358445	266.861 312.0043 331.2142
C,0,-0.1773474349,0.818355687,-0.3108043809	357.0241 443.8871 451.8903
H,0,-2.9953187832,2.7904390429,-0.0369299043	498.3146 532.7294 561.8782
H,0,-2.4778634865,2.0344757177,-1.5224858356	653.3168 740.5531 784.4738
H,0,-0.3379029896,0.5863662139,-1.3708713813	797.7952 825.1701 828.3094
H,0,-0.9107634449,2.2786735263,1.0821347022	915.3225 938.1762 939.4797
H,0,-2.7738334852,-1.2624441264,0.7746802328	960.5026 983.0229 1009.7033
H,0,-0.4005329936,-1.2960013146,0.1256210063	1023.1264 1042.2737 1052.5223
H,0,-0.4384595284,-0.2657795571,1.5378933096	1065.039 1085.7043 1112.3544
H,0,-0.4868170001,2.9527139748,-0.4871846007	1150.8127 1176.5149 1188.1198
C,0,-4.5207283852,0.586924416,-0.0707883008	1234.0828 1276.8884 1285.5696
H,0,-4.8590534312,0.8005505598,-1.0877968727	1324.547 1339.3478 1346.0384
H,0,-4.8921133862,-0.3953610315,0.2157310852	1354.2206 1367.2969 1380.0997
H,0,-4.9811705712,1.3351704422,0.5784677951	1408.0586 1412.3061 1417.1478
C,0,1.3156613018,0.9071366331,-0.0905388681	1421.8248 1454.6311 1480.5273
C,0,2.1211971271,-0.2407554061,-0.6315592016	1482.6481 1485.3142 1489.2018
H,0,3.1883421022,-0.0392066896,-0.5614793713	1495.6664 1497.0121 1502.5816
H,0,1.9098476692,-1.1601212529,-0.0818514311	1712.0848 1761.6838 3014.0081
H,0,1.871399824,-0.4228152096,-1.6784594103	3025.5789 3027.2242 3033.6987
C,0,1.9015513133,1.90450661,0.5710848015	3039.1907 3045.8929 3079.2431
H,0,1.3443837113,2.737078763,0.9796788295	3082.302 3083.9847 3088.3047
H,0,2.971271957,1.9083250475,0.733916138	3106.7303 3123.4076 3141.4217
O,0,1.8749864978,3.2639441371,-2.2523916278	3143.5368 3156.1544 3237.3755
O,0,1.4418713586,2.1667894212,-2.6147300745	
O,0,2.9812745731,3.2935621915,-1.7135125532	
UM06-2X/6-311++G(2df,2p): E = -615.7746438 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0735988 Hartree	
PRC6 0,1	
C,0,-0.8664512861,2.0626259006,-0.009070499	32.5247 49.3974 54.6172
C,0,-2.3188389464,1.9633956133,-0.462218124	77.0605 88.8374 113.524

C,0,-2.9839891545,0.6874575937,-0.012354501	123.9075 162.9704 176.8035
C,0,-2.2771744801,-0.3414050161,0.4452732322	189.9387 214.6021 231.7815
C,0,-0.7755308381,-0.3742001036,0.5199720214	267.5322 312.2864 333.9982
C,0,-0.130711427,0.7591988361,-0.2933483678	358.3159 442.4846 451.1538
H,0,-2.8917591196,2.8143913316,-0.0839013168	498.2934 532.3739 559.1978
H,0,-2.3783143684,2.0283959236,-1.5547180839	653.417 723.761 784.1953
H,0,-0.28198383,0.5184882378,-1.3532910616	798.3286 826.9426 828.1508
H,0,-0.8387853123,2.2617165678,1.0665672864	916.8583 937.2527 940.5065
H,0,-2.8012187131,-1.2315426423,0.7790654097	946.7568 983.3552 1008.7221
H,0,-0.4222305175,-1.3431286342,0.1609942107	1022.2833 1044.6685 1052.6826
H,0,-0.4473274772,-0.2981198514,1.5633444928	1061.6091 1085.4144 1113.664
H,0,-0.3674006874,2.8928420869,-0.5102451509	1150.043 1176.8343 1187.1829
C,0,-4.4798057233,0.6553380747,-0.1184218916	1232.2843 1279.6321 1285.8454
H,0,-4.7947812895,0.8449661487,-1.1475839882	1325.9361 1339.1523 1345.3515
H,0,-4.8855844387,-0.3053064382,0.1940543515	1352.96 1367.229 1377.5525
H,0,-4.9279034809,1.4385748314,0.4973814283	1406.2248 1409.6089 1418.1692
C,0,1.3600222867,0.8117658719,-0.0579645819	1421.3355 1456.5466 1480.3583
C,0,2.1350167059,-0.3901097163,-0.5269887479	1483.2397 1485.1985 1490.3424
H,0,3.2082565997,-0.2194318199,-0.4622182447	1496.3978 1498.8112 1508.14
H,0,1.8969654023,-1.2663224291,0.0792198014	1717.0949 1761.3398 3014.729
H,0,1.8808553572,-0.6358675622,-1.5598371338	3022.0223 3025.9679 3032.7923
C,0,1.9673632814,1.8250092855,0.5592646119	3039.9699 3044.5224 3071.2775
H,0,1.4290651168,2.6853873524,0.9306680728	3087.2055 3088.7372 3099.1629
H,0,3.0374579641,1.8113777638,0.7258372573	3102.8561 3126.1708 3133.9729
O,0,2.3449935836,2.9033511674,-2.362069009	3143.887 3149.6746 3235.1853
O,0,1.433344586,2.1015420088,-2.5795874473	
O,0,2.1380495361,3.7945278273,-1.537544017	
UM06-2X/6-311++G(2df,2p): E = -615.7751026 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0738582 Hartree	
TS5	
0,1	
C,0,-0.9531200634,2.082140184,-0.1100913496	-314.4925 51.0102 63.5835
C,0,-2.4177088304,1.9330525687,-0.5055931677	72.858 117.197 175.6296
C,0,-3.0317804129,0.6626969664,0.0260967557	186.6855 198.2759 206.576
C,0,-2.2816028269,-0.3304574829,0.4947536533	215.7491 227.6505 270.1926
C,0,-0.7778526453,-0.3265241135,0.5062479787	307.238 333.9315 366.8817
C,0,-0.2016740901,0.7835982509,-0.3863378357	441.0329 450.7668 474.0762
H,0,-2.9951377104,2.7866483631,-0.1408517672	496.1443 534.9249 568.0435
H,0,-2.5188519371,1.9496401887,-1.5963782216	656.3522 778.9356 793.9988
H,0,-0.3971493284,0.4964610289,-1.4244775764	794.5118 816.4067 827.3494
H,0,-0.8969754602,2.3097938346,0.9583327203	908.4192 936.2177 937.9958
H,0,-2.7696019449,-1.2166118864,0.8879952319	965.0276 980.1347 1014.1075
H,0,-0.4125600577,-1.3005803678,0.1730704983	1017.9678 1036.4908 1052.4171
H,0,-0.4082395704,-0.1967549222,1.5305645865	1058.4214 1080.4748 1108.8933
H,0,-0.4979617048,2.9170221048,-0.6456307003	1146.8847 1177.9716 1186.7774
C,0,-4.5295465211,0.5952759446,-0.0109408695	1211.8739 1230.7988 1277.7437
H,0,-4.8936224254,0.7357250499,-1.0316954104	1285.2341 1292.8487 1322.828
H,0,-4.8991293119,-0.3598512799,0.357768666	1337.3333 1349.1445 1368.3424
H,0,-4.9671315773,1.3935151072,0.5927994054	1405.6709 1410.2749 1417.8577
C,0,1.2973304376,0.8710669262,-0.2110667823	1419.1449 1440.2218 1479.1449
C,0,2.0936508053,-0.3191576592,-0.6629552594	1480.951 1486.4602 1488.8923
H,0,3.144696915,-0.0588911416,-0.7723319864	1492.0492 1495.3647 1502.2691
H,0,2.0125152428,-1.1296102379,0.0647688767	1608.9376 1757.8147 3013.2487
H,0,1.726720788,-0.6915036517,-1.6194512364	3031.35 3034.6241 3035.4553
C,0,1.8898023117,1.8281273412,0.5605570897	3047.222 3048.5639 3065.8074
H,0,1.3169103668,2.6014854549,1.0508638016	3067.9479 3086.691 3110.885
H,0,2.9227063618,1.7225420432,0.8588659664	3113.7157 3129.9741 3133.6293

O,0,1.7592880431,3.0924640575,-1.8181808901 O,0,1.673903141,1.9011687318,-2.2247715059 O,0,2.6645639654,3.2581996365,-0.9628205616	3142.0837 3173.3202 3265.7363
UM06-2X/6-311++G(2df,2p): E = -615.7684469 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.0682093 Hartree	
TS6 0,1 C,0,-0.9214462307,2.0778949809,-0.0736936225 C,0,-2.3838165122,1.9505635888,-0.4841156618 C,0,-3.0151240837,0.673073532,0.0100219056 C,0,-2.2808852346,-0.3375352593,0.4668797445 C,0,-0.7773221142,-0.3463886712,0.5007880063 C,0,-0.1841313119,0.7756571968,-0.3634724061 H,0,-2.9579690777,2.7999459541,-0.1045160915 H,0,-2.475624688,1.9938611753,-1.5750898165 H,0,-0.3726427462,0.5104613864,-1.4098926668 H,0,-0.8730956114,2.2869133241,0.999170106 H,0,-2.7824171959,-1.2285328613,0.8310783571 H,0,-0.4136541688,-1.3174106755,0.1561847795 H,0,-0.422256777,-0.2374763244,1.5325992611 H,0,-0.4405133105,2.9060350318,-0.5960076953 C,0,-4.5126377649,0.6180617975,-0.0516286409 H,0,-4.8591504232,0.7834916955,-1.0747878316 H,0,-4.8958845201,-0.3416057288,0.2905914904 H,0,-4.9535285682,1.4069068806,0.5619431717 C,0,1.3111953775,0.8509019059,-0.1855103477 C,0,2.1027993634,-0.3570208675,-0.6084998467 H,0,3.1432693681,-0.0930586009,-0.7974466348 H,0,2.0891562147,-1.1139486318,0.1792024686 H,0,1.6869358199,-0.8042233069,-1.5104777909 C,0,1.9122334006,1.8286068721,0.5513126144 H,0,1.3434692661,2.6139792428,1.0243769576 H,0,2.9513330763,1.7379092341,0.8370889006 O,0,2.6111399715,2.4995428171,-1.9714578738 O,0,1.5282121988,1.902153674,-2.2139961745 O,0,2.5237375227,3.3100615376,-1.0154538019	-309.7349 52.6335 58.9587 67.8957 120.1244 164.3473 180.214 196.6277 205.1139 213.7081 218.6295 269.1944 304.1592 332.0465 366.8443 444.0858 453.0162 477.7794 484.1118 532.6949 572.4494 657.6159 779.7835 791.8877 798.1661 822.6082 830.7037 907.2101 936.3919 940.1488 966.072 981.634 1012.9291 1020.6283 1037.9228 1050.6025 1056.7474 1081.4742 1110.9255 1148.7914 1179.8266 1187.4048 1215.4781 1234.5635 1277.4202 1287.5076 1291.2364 1328.222 1336.6591 1350.9394 1369.9176 1405.2857 1409.8875 1416.8752 1423.0693 1437.8568 1480.26 1481.2071 1484.8918 1488.3116 1492.8571 1494.8278 1504.178 1609.6911 1758.9309 3011.9349 3027.1371 3032.0409 3036.5973 3042.5207 3045.8821 3066.7622 3068.3011 3086.9314 3110.2425 3113.4386 3125.8404 3134.9285 3144.0905 3165.2002 3263.6957
UM06-2X/6-311++G(2df,2p): E = -615.7692612 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.068763 Hartree	
POZ5 0,1 C,0,-0.9937699397,2.1151838252,-0.488870265 C,0,-2.4752988348,1.8488173465,-0.731562516 C,0,-2.997622222,0.6909761268,0.0783122202 C,0,-2.1756474431,-0.1848639918,0.6480058103 C,0,-0.6774188933,-0.1593510409,0.5137792935 C,0,-0.2058403973,0.8086535286,-0.5759021933 H,0,-3.0605333058,2.7415560755,-0.4963181944 H,0,-2.6541784327,1.6489071108,-1.7940659592 H,0,-0.4368018442,0.3565546477,-1.547322906 H,0,-0.87422272,2.55767254,0.5036196926 H,0,-2.595006749,-0.9930856628,1.2383366027 H,0,-0.3286316768,-1.1707075936,0.2942562291 H,0,-0.2283495088,0.1078464964,1.4790374908 H,0,-0.6127900942,2.8357554557,-1.2106313922 C,0,-4.4893018341,0.5903374207,0.1951253791 H,0,-4.9480885227,0.5468755883,-0.7956273188 H,0,-4.7920818144,-0.2937437939,0.7533127645	60.6752 79.7011 103.5586 159.4729 168.8657 193.9992 240.6085 251.7646 283.2772 294.0111 312.2647 359.3694 391.1185 430.6815 448.8274 499.8962 517.8988 547.3477 605.9569 722.3554 748.9895 783.5078 816.6381 821.5798 861.8957 903.3069 933.2801 938.0119 944.65 980.6979 988.3676 1003.6497 1025.8325 1041.9208 1051.5007 1076.4578 1081.8998 1107.9348 1142.8111 1166.7154 1180.4811 1192.6517 1203.9411 1243.4966 1266.8962 1278.1567 1293.4316 1333.5262 1344.2209 1349.2168 1369.2517

H,0,-4.8978998061,1.4728441411,0.6923879153	1386.6817 1407.2575 1412.3424
C,0,1.3161878098,1.0001021441,-0.54992614	1417.9157 1421.0045 1481.5032
C,0,2.0733642192,-0.2743788925,-0.8853854856	1485.2461 1488.0294 1494.6821
H,0,3.14357699,-0.0724523448,-0.8831006257	1497.2461 1499.0702 1500.9786
H,0,1.8598726303,-1.0557737527,-0.1578995132	1518.4429 1765.6908 3007.7754
H,0,1.7884124782,-0.634247292,-1.873888536	3030.4186 3032.9692 3035.0976
C,0,1.8422576831,1.6645501836,0.7500523873	3050.0454 3059.689 3080.5096
H,0,1.0322700449,2.0371373268,1.3774939561	3083.4125 3086.4627 3087.9498
H,0,2.495512659,1.0084766116,1.3214638355	3117.6426 3130.3779 3137.1716
O,0,1.8949663458,3.1607659996,-0.8374842572	3145.8259 3146.042 3147.9684
O,0,1.7153681043,1.9562079631,-1.5475279953	
O,0,2.6357679245,2.7349959928,0.2801693009	
UM06-2X/6-311++G(2df,2p): E = -615.8802494 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.8802494 Hartree	
POZ6	
0,1	
C,0,-0.9441724796,2.1064212605,-0.3818069024	60.1437 74.5257 101.3249
C,0,-2.4309238184,1.9098278018,-0.6545726095	165.7599 187.6961 211.022
C,0,-2.9912133316,0.700449957,0.0488665678	251.8761 273.3641 289.097
C,0,-2.1981888925,-0.2421398896,0.5496870487	298.4562 316.5844 357.079
C,0,-0.6981805736,-0.2456173692,0.4316140236	383.9771 443.0295 453.3563
C,0,-0.1975931278,0.7882315214,-0.5785722893	476.8332 520.5106 559.8418
H,0,-2.9913633398,2.7950952627,-0.3431317684	607.7582 704.1308 760.1114
H,0,-2.6084370673,1.8100178084,-1.7311981526	781.3205 819.9095 827.5531
H,0,-0.4366685115,0.418361108,-1.5828092012	863.865 904.2513 933.8478
H,0,-0.8222104413,2.4458041276,0.6509195613	937.6591 947.4943 980.2871
H,0,-2.6446403266,-1.0855052929,1.0663344119	993.8607 1014.8731 1031.7064
H,0,-0.3682348984,-1.2458491905,0.1431355178	1040.6777 1050.0141 1073.4827
H,0,-0.2498103436,-0.0563880324,1.4158725381	1084.4472 1106.4135 1135.7138
H,0,-0.5284170445,2.8780931684,-1.0272359473	1157.5112 1179.3698 1193.859
C,0,-4.4861528784,0.6302112893,0.144308959	1201.0354 1241.6628 1259.8213
H,0,-4.9357211423,0.6825964814,-0.8501453494	1288.489 1312.859 1334.6871
H,0,-4.8176207538,-0.2888761892,0.6240618215	1338.4615 1345.841 1380.7481
H,0,-4.8765996735,1.4785152906,0.7109034542	1387.0519 1405.6072 1409.7945
C,0,1.326031333,0.9420092614,-0.5370096724	1414.8492 1419.2605 1482.4984
C,0,2.0709031713,-0.3729847225,-0.6955576814	1485.8508 1487.7215 1494.4066
H,0,3.1253998645,-0.1667160361,-0.8754950534	1496.431 1497.4725 1501.5537
H,0,1.9881144013,-0.9816294678,0.2054839318	1520.8648 1761.8102 3004.1086
H,0,1.6732323084,-0.939673135,-1.5370579105	3028.6182 3030.6807 3036.054
C,0,1.862490003,1.7428099758,0.6803842677	3047.9889 3048.5091 3072.9328
H,0,1.119674473,1.917562962,1.45468627	3084.5571 3087.3481 3087.9286
H,0,2.7456698204,1.2594243108,1.1027324971	3116.689 3124.7083 3135.4692
O,0,2.7033055295,2.6199207267,-1.1283854928	3139.7907 3148.8351 3162.8272
O,0,1.6597817719,1.8156477846,-1.6277042229	
O,0,2.2026838283,2.9983736866,0.1322094031	
UM06-2X/6-311++G(2df,2p): E = -615.8812454 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1603711 Hartree	
TS_POZ5_CH_2OO-AMCH	
0,1	
C,0,0.6502193422,-1.1407175056,-0.1090558588	-556.5698 58.4828 62.8862
C,0,2.1349971972,-1.2192363431,-0.4484983181	95.864 169.3295 177.6831
C,0,2.9135711806,-0.0379905859,0.0721343341	192.2012 213.2341 234.121
C,0,2.3078123528,1.0703653211,0.4886822564	272.1259 279.7112 302.3879
C,0,0.8183776969,1.2919870015,0.4518007333	318.7759 350.7608 418.0778
C,0,0.1210674441,0.253527268,-0.4264349462	455.6286 485.4049 518.4197
H,0,2.5671902095,-2.137626369,-0.0428211385	522.0081 558.8692 570.7474
H,0,2.2708416943,-1.2823139839,-1.5338556854	631.5257 666.7471 778.9012

H,0,0.4061682153,0.4749201039,-1.4634670384	799.6697 820.7236 866.4081
H,0,0.5312976289,-1.3514985229,0.9583812212	917.8907 935.3968 939.2054
H,0,2.9109129509,1.8864418706,0.873113723	971.4336 985.4702 1014.6856
H,0,0.6194971873,2.3002754756,0.0823536803	1041.4764 1051.8027 1074.2026
H,0,0.4291657543,1.2628964332,1.4765894441	1095.4444 1115.1352 1146.1323
H,0,0.0789280101,-1.8912433362,-0.6512729405	1157.9425 1174.41 1183.8129
C,0,4.4054799203,-0.1913614236,0.0838493167	1201.1876 1245.0409 1276.068
H,0,4.7747477379,-0.4117877933,-0.9207262586	1285.1839 1305.8362 1325.7617
H,0,4.9008638709,0.7089823244,0.4424885717	1334.8672 1344.235 1383.89
H,0,4.7026136447,-1.028797219,0.7189711857	1391.0761 1394.5765 1406.8023
C,0,-1.4245703931,0.338472395,-0.4665131304	1421.6054 1465.3302 1480.6797
C,0,-2.0012446684,1.6979935568,-0.8649635852	1484.0317 1486.9376 1489.6787
H,0,-3.0855789268,1.6633305916,-0.7821197958	1497.4055 1497.8175 1503.7666
H,0,-1.6156669211,2.5169991183,-0.2599736679	1512.2301 1760.2017 3006.0177
H,0,-1.7441843511,1.892145758,-1.9074669204	3020.7654 3024.4222 3038.9867
C,0,-1.9070469744,0.2262647022,1.3749022482	3040.2147 3051.8776 3074.0124
H,0,-1.1823181517,-0.521533843,1.6714562677	3078.5006 3095.4863 3123.4976
H,0,-1.8864074828,1.2067552945,1.8327779495	3125.3433 3126.9661 3131.0193
O,0,-3.1278069523,-1.3622741117,0.6020672875	3144.1713 3149.3638 3252.4629
O,0,-2.0261849693,-0.6789779831,-0.9329312594	
O,0,-3.1325410871,-0.2113413045,1.1983669243	
UM06-2X/6-311++G(2df,2p): E = -615.8361843 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1297996 Hartree	
TS_POZ5_CH_2O-Syn-2c 0,1	
C,0,0.5207173105,-1.0398279205,0.2749279149	-541.8622 42.3714 83.9769
C,0,1.969113627,-1.3107706124,-0.1182774442	160.8145 172.0858 174.8875
C,0,2.8560187155,-0.1043540129,0.0261612902	242.2856 250.2638 278.0808
C,0,2.3399367276,1.1110193654,0.1739022047	284.1354 288.921 310.2991
C,0,0.8675223295,1.4182065599,0.1519426148	321.5372 359.0101 403.357
C,0,0.0379672281,0.2520940741,-0.3994301919	435.6023 442.1792 500.2398
H,0,2.3683413204,-2.122909867,0.4947891713	537.4314 557.2258 586.3138
H,0,2.0188918577,-1.6708681686,-1.1522724298	653.1524 679.7491 786.0125
H,0,0.2543872982,0.1550366378,-1.4734844607	796.8767 824.5914 887.2246
H,0,0.4667462937,-0.9156729048,1.3600287243	922.1146 939.2112 941.9805
H,0,3.0055528119,1.958226962,0.3019981253	990.5893 995.5552 1005.6372
H,0,0.7120752278,2.3198299746,-0.4419089704	1042.427 1048.8246 1078.3492
H,0,0.5270329451,1.6621985251,1.1664981167	1108.5244 1131.3482 1161.9805
H,0,-0.1088407121,-1.8803893534,0.0136485251	1180.4062 1191.0613 1224.9464
C,0,4.3334313377,-0.3563501065,-0.0054961265	1236.7943 1246.0269 1276.7211
H,0,4.6133503227,-0.8693651849,-0.9286592066	1281.6992 1312.576 1323.8672
H,0,4.9017019068,0.5696659017,0.060166589	1340.7079 1347.1774 1367.8296
H,0,4.6314496788,-1.0073251806,0.8193062615	1398.0523 1410.5919 1418.6139
C,0,-1.4570544106,0.5898212765,-0.3805772541	1420.4967 1426.775 1477.1162
C,0,-1.8620421877,2.0365384452,-0.4840309788	1481.4269 1483.9193 1492.212
H,0,-2.940356106,2.1044328131,-0.6058466135	1496.2249 1499.9268 1505.8653
H,0,-1.5705641005,2.5763452853,0.4144814279	1560.0162 1767.9682 2984.8055
H,0,-1.3783390663,2.5132279887,-1.3371385585	2994.3269 3009.1087 3030.976
C,0,-2.1643361404,-0.1221165714,1.2033504955	3034.3035 3049.6911 3056.7785
H,0,-1.3112973448,0.1917418859,1.8227066079	3065.0889 3068.9652 3083.2692
H,0,-3.0636780637,0.4969635401,1.3131749952	3086.9579 3127.2885 3138.9596
O,0,-2.0701708962,-1.4172455112,-1.0144338202	3145.2371 3161.7881 3190.919
O,0,-2.2694373136,-0.1424479766,-1.1487493859	
O,0,-2.3056964272,-1.3582420346,0.9687328369	
UM06-2X/6-311++G(2df,2p): E = -615.8387887 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.130348 Hartree	
TS_POZ6_CH_2O-Anti-2c	

0,1			
C,0,0.6495850198,-1.1664488965,-0.1727870603	-553.2621	60.9813	64.7612
C,0,2.1325339429,-1.2150408075,-0.5277932284	147.4877	159.2432	174.8053
C,0,2.9241644559,-0.0775736859,0.0627828425	192.3321	204.5687	233.5822
C,0,2.3276050688,0.987459688,0.5883510022	277.0188	295.5502	308.3125
C,0,0.8377995548,1.1933368986,0.625774211	345.5736	357.159	402.7015
C,0,0.1172467066,0.2556931982,-0.3501642215	435.7249	461.6477	481.7472
H,0,2.5629883073,-2.1614637466,-0.1909132265	522.7941	565.0413	596.7787
H,0,2.2589539486,-1.2053667271,-1.6162850618	634.2295	739.3736	781.6315
H,0,0.3749586005,0.5890410418,-1.3647071336	808.1901	824.4407	896.2547
H,0,0.5104750313,-1.4698517346,0.8683794212	900.5429	938.5859	940.3019
H,0,2.935745042,1.7741323221,1.0219754239	987.6902	995.0114	1029.8209
H,0,0.613919698,2.2358662787,0.3918095995	1043.6317	1050.4456	1077.5046
H,0,0.47417105,1.0230907967,1.6441031311	1106.8539	1140.1272	1149.1201
H,0,0.0947860977,-1.8719134772,-0.7874721997	1182.6322	1190.9945	1216.1953
C,0,4.4157690974,-0.2238025763,0.0139009698	1239.4414	1248.6832	1278.1774
H,0,4.7535194213,-0.3621878483,-1.0159304663	1293.5679	1325.1645	1333.3431
H,0,4.9196298652,0.6476791193,0.4276587152	1345.6607	1356.4882	1376.0055
H,0,4.7345479591,-1.1067460295,0.5722006264	1404.3561	1409.2863	1418.1436
C,0,-1.3905422135,0.3717262708,-0.2495963967	1419.4888	1427.9332	1475.6482
C,0,-2.0315497436,1.6439198653,-0.7411166022	1480.693	1484.4503	1488.4164
H,0,-3.0311875556,1.7654094392,-0.3365124516	1496.2594	1502.4466	1505.9589
H,0,-1.4149308595,2.4977968046,-0.472382999	1558.4059	1766.6076	2985.2485
H,0,-2.1042890787,1.5871532284,-1.82987752	3006.5304	3032.5798	3037.3726
C,0,-2.0258696173,0.260712684,1.523839963	3039.8744	3050.1514	3054.6088
H,0,-1.3216969237,-0.4531854723,1.9691383702	3067.988	3077.4294	3091.0932
H,0,-1.821803251,1.3163538725,1.7475308205	3092.6288	3123.0475	3129.8015
O,0,-3.2993689359,-0.6575896694,-0.4991837051	3137.5569	3152.2877	3175.616
O,0,-2.007622596,-0.7582872432,-0.6072950058			
O,0,-3.2372422123,-0.0859781637,1.3859232319			
UM06-2X/6-311++G(2df,2p): E = -615.842455 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1343081 Hartree			
TS_POZ6_CH_2OO-AMCH			
0,1			
C,0,0.5089910024,-1.0642687723,-0.0316948971	-545.8437	69.1023	88.2743
C,0,1.9711116494,-1.2910682532,-0.3974920201	100.8436	163.8677	176.1787
C,0,2.8556879521,-0.1497671021,0.0368542618	196.7081	237.551	276.5204
C,0,2.3521400596,1.0286968531,0.3933115541	292.3929	294.5547	303.9404
C,0,0.8875241167,1.375962869,0.3578715228	324.4326	356.5256	408.2379
C,0,0.0856301037,0.3438590982,-0.4327528117	452.7675	495.7783	519.7167
H,0,2.3363249694,-2.2165063559,0.0554154679	528.8847	552.9346	583.9978
H,0,2.0744500516,-1.4284997129,-1.4795451472	634.2636	661.2631	784.5873
H,0,0.3517311885,0.4727672641,-1.4897690525	815.3501	830.3393	904.0503
H,0,0.3974369267,-1.1837754226,1.0500407193	911.6427	937.8342	945.5795
H,0,3.0298542557,1.8126503677,0.7155456996	976.9404	989.8175	1015.4936
H,0,0.7704818579,2.3682440263,-0.0836087086	1045.21	1051.3802	1078.1207
H,0,0.5086789036,1.4620323399,1.3838723245	1094.2033	1118.1276	1143.0503
H,0,-0.1384608405,-1.7986338289,-0.5102274636	1163.166	1180.1419	1191.7209
C,0,4.3300497064,-0.4249416558,0.0351121264	1209.7554	1247.083	1283.1311
H,0,4.6581064925,-0.7433570302,-0.9573733924	1290.6423	1309.7064	1326.3151
H,0,4.9046255184,0.4542653621,0.3211146015	1336.3394	1346.7019	1386.0949
H,0,4.5730973074,-1.2382000754,0.7225775083	1391.6654	1405.6934	1410.4626
C,0,-1.4428210388,0.5556745978,-0.421634902	1419.7735	1465.5298	1480.5816
C,0,-1.9112412857,2.0130194266,-0.4891452727	1481.9058	1484.8801	1496.2976
H,0,-2.994277356,2.0330014253,-0.5874948806	1497.367	1498.4766	1505.6214
H,0,-1.6068378797,2.5979750321,0.3786771607	1518.348	1765.2779	3008.0828
H,0,-1.4745210463,2.4738856699,-1.3765911329	3023.7389	3028.9751	3036.5211

C,0,-2.0200067449,0.1271450617,1.3477543567 H,0,-1.2594451755,0.3739517618,2.0774809961 H,0,-2.937815095,0.701177299,1.3176258013 O,0,-3.0359656614,-1.4312251565,0.2732321688 O,0,-2.123501979,-0.281928678,-1.093704064 O,0,-2.1590271795,-1.1690834208,1.1910630056	3049.0159 3049.9195 3066.6596 3080.9626 3092.9417 3119.3238 3122.3643 3124.415 3144.8721 3151.7757 3153.9337 3270.3512
UM06-2X/6-311++G(2df,2p): E = -615.8366381 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1293502 Hartree	
TS_POZ5_POZ6 0,1 C,0,0.6186814892,-1.089688059,0.0906997317 C,0,2.0761433665,-1.251396758,-0.3243696065 C,0,2.9052792513,-0.042742629,0.0295767357 C,0,2.3406827676,1.118784726,0.3472688079 C,0,0.8589166043,1.3803951393,0.3293174326 C,0,0.0960604229,0.2647060394,-0.3880356589 H,0,2.5098500156,-2.1332527936,0.1541838229 H,0,2.1467130421,-1.4327047183,-1.4026713433 H,0,0.3207080114,0.3452198904,-1.4578809727 H,0,0.5661557772,-1.134698198,1.181918638 H,0,2.9760432812,1.9545770599,0.6216316335 H,0,0.6763512374,2.3398942915,-0.1576870944 H,0,0.4867282326,1.4870193218,1.3565454062 H,0,0.0075478485,-1.8999967043,-0.3048522233 C,0,4.3922021453,-0.2352251067,0.0020937659 H,0,4.7145047522,-0.5845016245,-0.9818319824 H,0,4.9221672719,0.687691965,0.2300349708 H,0,4.6964072706,-0.9982475775,0.7220675878 C,0,-1.4208579562,0.4381397552,-0.2687905442 C,0,-1.9073983259,1.7990741268,-0.7504781609 H,0,-2.9940929878,1.798527607,-0.8079452991 H,0,-1.5952489875,2.5930802887,-0.0730456665 H,0,-1.5038328878,2.0059000234,-1.7413136731 C,0,-2.0337315043,0.0736228829,1.0812048902 H,0,-1.5647346626,-0.8083010097,1.5194934264 H,0,-2.0583942508,0.900528247,1.7877894356 O,0,-3.2942707061,-0.8625457741,-0.5312957356 O,0,-1.9987860822,-0.5893787663,-1.0720811031 O,0,-3.3702437067,-0.1888754754,0.725038949	-139.2161 50.2159 79.3771 134.0503 180.0608 186.1275 239.2927 258.6788 261.3016 289.1774 295.9691 326.3169 376.1089 397.8908 446.8905 473.3718 511.9168 534.1158 605.9474 720.6076 748.4389 787.5603 811.1329 829.0957 865.6105 913.9604 935.9135 942.0655 950.6579 968.3928 989.9689 993.074 1029.5107 1040.7855 1051.1451 1075.8349 1097.4475 1110.5563 1148.6129 1159.9413 1177.0089 1188.9589 1213.3451 1249.9139 1273.3284 1279.1498 1291.9778 1333.6762 1338.5089 1348.1346 1382.0048 1387.6433 1404.8168 1413.8936 1417.96 1419.5481 1480.7274 1486.8954 1488.6457 1493.6557 1496.4571 1500.8627 1508.6107 1511.3291 1762.773 3005.5888 3029.0052 3031.6522 3036.0285 3047.1227 3064.1443 3072.9399 3079.8682 3088.5119 3097.7428 3121.8971 3133.3468 3143.3796 3147.8173 3148.8151 3168.1407
UM06-2X/6-311++G(2df,2p): E = -615.8752338 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -615.1542666 Hartree	
Anti-2c 0,1 C,0,0.8096572581,-1.2600536999,0.0475796495 C,0,2.323193197,-1.3051041041,-0.13252851 C,0,2.9870911833,0.0272779797,0.1074528051 C,0,2.2887797391,1.1564990312,0.1763651007 C,0,0.7989810425,1.2459159687,-0.0047584449 C,0,0.2417443896,-0.0331728454,-0.6564445946 H,0,2.7556569188,-2.0445311818,0.5458064868 H,0,2.5763863304,-1.6475667896,-1.1422396822 H,0,0.5647028972,-0.0346738319,-1.7047645742 H,0,0.5627593365,-1.1999682248,1.1095960058 H,0,2.8083441189,2.0884486282,0.3720585642 H,0,0.5526399645,2.1185811053,-0.6127881009 H,0,0.3099085531,1.3978867764,0.9635734349 H,0,0.3470544006,-2.1702324196,-0.3327643758	52.9535 76.1691 125.0075 160.6272 171.7741 203.174 244.3935 284.4215 303.4784 324.4951 353.5704 396.1723 438.0682 466.7637 523.3438 551.8204 609.6816 706.8801 779.0619 809.8896 823.9067 904.756 927.9937 938.5428 968.5979 992.7992 1019.068 1039.8762 1048.1506 1059.4058 1082.1398 1106.5223 1143.5058 1175.9798 1187.8195 1223.6818 1271.6172 1291.3119 1317.0741 1339.7769 1355.0572 1363.0194

C,0,4.4784946443,-0.0057408422,0.259148759	1393.4627 1408.4381 1420.9535
H,0,4.9426639108,-0.4669630581,-0.6157566846	1424.1172 1441.6331 1478.5508
H,0,4.8929409405,0.9929027603,0.3832917461	1481.5497 1483.6625 1490.5323
H,0,4.7637449189,-0.6098226612,1.1230881128	1495.798 1508.6398 1641.2897
C,0,-1.2491371624,0.0258323318,-0.6649357839	1766.2976 3026.6343 3027.4773
C,0,-2.021817076,1.0090438865,-1.4461924614	3036.5372 3039.0311 3046.1764
H,0,-2.6191878845,1.6104214123,-0.756823787	3064.4724 3076.6368 3079.7775
H,0,-1.3750309883,1.6303255441,-2.0580069462	3091.2032 3098.8387 3130.4458
H,0,-2.7518934158,0.4662218,-2.0504683205	3130.9003 3153.4782 3170.1805
O,0,-3.2230310373,-0.7180865073,0.087916673	
O,0,-1.8574351797,-0.7917800583,0.0584269284	
UM06-2X/6-311++G(2df,2p): E = -501.4215164 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -500.8206828 Hartree	
Syn-2c 0,1	
C,0,0.3905084037,-0.8017662515,0.2377227847	69.7392 80.0255 136.6909
C,0,1.8329984538,-1.2142895519,-0.0246741625	176.2402 194.1596 195.6221
C,0,2.7912539361,-0.0508767876,-0.0098480245	255.5625 266.9007 298.6076
C,0,2.3689695425,1.2092354215,-0.0619984043	309.3008 343.5394 413.2239
C,0,0.9248451994,1.6178140994,-0.1731419676	435.4878 470.3521 519.3688
C,0,0.0595142934,0.4416557392,-0.6141935192	604.8971 624.6881 650.0353
H,0,2.1506235853,-1.948616068,0.7202173373	777.0865 798.0473 824.8771
H,0,1.9013504354,-1.7206313161,-0.9932367991	913.4467 934.3772 936.4733
H,0,0.2634859132,0.1736183646,-1.6553258078	956.9154 976.7095 1030.1265
H,0,0.265654,-0.5427896798,1.2933104453	1039.6808 1051.2703 1057.1589
H,0,3.0990649434,2.0107717787,-0.0318776591	1079.2614 1102.3156 1141.5261
H,0,0.833245243,2.442347577,-0.8845732728	1174.7697 1186.8133 1242.1634
H,0,0.582347917,2.0073876097,0.7916730696	1282.7711 1294.4299 1309.7344
H,0,-0.2952330317,-1.6094296125,-0.0101196911	1334.2015 1342.7367 1365.5151
C,0,4.2465592963,-0.406036674,0.0587771493	1402.3605 1407.1031 1422.6436
H,0,4.5160182369,-1.0752539765,-0.7616544125	1427.7115 1464.6421 1471.752
H,0,4.8795686984,0.4777025862,0.0045697717	1475.0037 1485.0847 1487.1977
H,0,4.4705805307,-0.9377028557,0.9862345789	1496.8059 1499.294 1637.3682
C,0,-1.3984294554,0.6936580917,-0.5442469448	1761.3462 3025.0145 3026.9081
C,0,-2.02985773,1.7472529045,0.292721756	3043.1374 3044.3376 3048.609
H,0,-3.1110749993,1.7045001441,0.2004491839	3058.9634 3066.2122 3072.8305
H,0,-1.7427206768,1.6058263617,1.3367791784	3097.8263 3109.1471 3116.4521
H,0,-1.6683008104,2.7312628736,-0.0088944168	3137.5585 3151.6364 3167.7002
O,0,-1.6827212945,-1.0377095224,-1.9601163086	
O,0,-2.1921526302,-0.029689256,-1.1890388642	
UM06-2X/6-311++G(2df,2p): E = -501.4206353 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -500.819936 Hartree	
TS_ Anti-2c_dioxirane3 0,1	
C,0,-0.2995047927,-1.1691370914,0.3038982226	-491.4528 47.737 68.5126
C,0,-1.7934856472,-1.1101815185,0.599144557	122.5633 171.7847 187.5398
C,0,-2.4863462549,0.0257476692,-0.1096294691	237.5061 240.9121 289.2423
C,0,-1.8039193005,1.0195821204,-0.6691156032	307.293 338.6957 385.8888
C,0,-0.3083476786,1.1573397611,-0.6368201914	438.3341 461.7287 513.468
C,0,0.3062752557,0.2306246156,0.4401227668	568.6176 581.3782 650.8451
H,0,-2.2637425565,-2.0516696728,0.3046213866	775.4898 817.9624 819.5144
H,0,-1.9674541253,-1.0163461671,1.6769298179	841.6863 905.5197 932.1066
H,0,0.0825003657,0.6460843408,1.4254752693	946.0685 983.1235 991.0615
H,0,-0.1316390611,-1.5200284472,-0.7149319196	1008.1903 1040.9421 1051.5702
H,0,-2.3434989723,1.8036613691,-1.189739413	1075.8887 1103.0116 1121.345
H,0,-0.0339687382,2.1937787611,-0.4317817177	1173.5114 1187.8506 1211.191
H,0,0.1318148526,0.9114471621,-1.6078354596	1258.956 1281.8834 1319.9624

H,0,0.1966650151,-1.8709190117,0.9750440452	1339.0113 1353.1187 1364.1243
C,0,-3.9838620522,-0.0419960472,-0.141783072	1398.5279 1410.329 1421.0471
H,0,-4.3873005613,-0.1082820361,0.8715044318	1426.5279 1443.3155 1466.4561
H,0,-4.4153095963,0.8311784969,-0.6275063995	1478.9726 1485.7684 1487.7902
H,0,-4.3179454826,-0.9351352541,-0.6742239509	1495.9243 1505.9885 1596.8519
C,0,1.7735755416,0.253403598,0.2088912201	1767.3381 3032.063 3033.0462
C,0,2.645833552,1.0930789843,1.0705111267	3036.6451 3048.4967 3062.7153
H,0,2.389210643,2.1455809584,0.9383731567	3068.8325 3072.5277 3090.2842
H,0,2.4310904217,0.8379367236,2.1126955164	3097.6201 3112.723 3117.2048
H,0,3.6891946071,0.9476234593,0.8190633512	3133.1613 3145.1278 3193.4601
O,0,2.9069756985,0.5775910478,-1.4059651558	
O,0,2.2193783466,-0.5184361316,-0.6973457964	
UM06-2X/6-311++G(2df,2p): E = -501.3857048 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -500.7882949 Hartree	
TS_ Anti-2c-H-shift 0,1	
C,0,-0.3004084354,-1.1324449173,0.0422157872	-1598.2873 35.5703 74.3254
C,0,-1.7776905976,-1.1651896463,0.4197890424	129.5302 162.1458 174.1885
C,0,-2.5294004426,0.0646842939,-0.0232915313	244.6808 290.1383 303.1694
C,0,-1.9003416478,1.1634511987,-0.4292947897	323.4831 394.8536 439.3834
C,0,-0.4064834051,1.3237224247,-0.4606239658	474.1156 518.4238 537.0546
C,0,0.2868266749,0.2352792602,0.3762331428	579.258 629.356 742.2102
H,0,-2.2530842636,-2.0478240062,-0.0150522449	777.8103 797.5866 824.4178
H,0,-1.8897923083,-1.2741316485,1.5045053963	849.5437 890.618 936.6899
H,0,0.0986843528,0.4627245349,1.4317458036	941.7187 964.5161 983.6102
H,0,-0.1872514738,-1.3115739268,-1.029197755	1011.5866 1040.8333 1049.7071
H,0,-2.4855312949,2.0158187265,-0.757995321	1065.0071 1085.886 1106.9802
H,0,-0.1260549927,2.3099979398,-0.0865337376	1143.9317 1173.3101 1186.6786
H,0,-0.0423191047,1.2726082469,-1.4924766132	1232.8971 1282.214 1296.8072
H,0,0.2471319082,-1.9225631211,0.5551379644	1315.3006 1340.8464 1348.4324
C,0,-4.024898832,-0.0330636562,0.0283683131	1360.9053 1390.5694 1409.7376
H,0,-4.3570344882,-0.2987701277,1.0347373507	1420.2665 1429.5319 1479.6816
H,0,-4.4999373754,0.9042552477,-0.2548660945	1483.3371 1487.9955 1496.3683
H,0,-4.3827517132,-0.8193833143,-0.6398145643	1506.4996 1522.187 1557.4417
C,0,1.7622505169,0.3342895951,0.1890019553	1765.3952 1899.8924 3027.3428
C,0,2.6470466573,1.2706326509,0.763506038	3028.1597 3037.4886 3043.4762
H,0,3.2387365723,1.844977459,0.0521653185	3063.3651 3075.7248 3082.1405
H,0,2.2524334125,1.8573176863,1.581593137	3092.8105 3102.5197 3128
H,0,3.5796559032,0.3450087993,0.6583580971	3129.4306 3162.1338 3204.2209
O,0,3.7048274623,-0.5046053123,-0.4113057061	
O,0,2.321735615,-0.6284981474,-0.4571134035	
UM06-2X/6-311++G(2df,2p): E = -501.3968883 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -500.7958486 Hartree	
VHP4 0,1	
C,0,-0.2715260376,-1.0842056993,0.301929823	56.0784 66.0951 100.6137
C,0,-1.7637299702,-1.094146753,0.6162155947	169.048 180.7912 185.6455
C,0,-2.5138870687,0.0134667289,-0.0797471976	206.5463 239.8908 280.0776
C,0,-1.8830456538,1.0411188362,-0.6400897871	323.0334 342.4264 382.4845
C,0,-0.3932738756,1.240123182,-0.6172293039	440.7814 492.648 519.9806
C,0,0.2810770558,0.3396324731,0.4249394258	596.9423 659.8711 702.4128
H,0,-2.2003651295,-2.0547346784,0.3296821364	753.5204 776.4512 817.6898
H,0,-1.9241924306,-1.0068313156,1.6969897432	822.9314 881.5892 928.4023
H,0,0.0319985348,0.7183497968,1.4193114912	936.6948 944.6502 975.967
H,0,-0.1086323812,-1.4386510668,-0.7181100872	998.1 1039.2437 1048.7184
H,0,-2.467948612,1.8018108814,-1.1471504083	1069.1551 1083.4732 1106.0949
H,0,-0.1616883699,2.2849550339,-0.399616611	1138.7201 1173.6241 1184.4985

H,0,0.0278952269,1.033460863,-1.6053791948	1238.1371 1279.1344 1301.2361
H,0,0.2667740961,-1.7570476161,0.9712890733	1316.2572 1323.8875 1341.5654
C,0,-4.0079469307,-0.1206041666,-0.0943491494	1367.9807 1392.0294 1404.3689
H,0,-4.3972719845,-0.1973119741,0.9239311054	1417.1991 1429.585 1449.7079
H,0,-4.4831083031,0.7292761853,-0.5808598467	1481.0034 1483.5628 1485.7266
H,0,-4.3089707261,-1.0318063523,-0.6164304909	1496.5909 1501.8603 1744.0629
C,0,1.7776585711,0.3892110948,0.315034557	1762.8404 3027.0005 3033.1268
C,0,2.6086164744,0.8736904345,1.2273981771	3037.2738 3049.5012 3056.4191
H,0,3.6743101642,0.9071144412,1.0758110569	3066.9793 3076.0866 3087.3383
H,0,2.1966636877,1.2680663725,2.1426274104	3102.203 3126.9089 3148.9085
H,0,3.8287775281,-0.9638572234,-0.8123749042	3194.4771 3289.2395 3819.493
O,0,3.5442878647,-0.0837637413,-1.0895526235	
O,0,2.1522208997,-0.1496017469,-0.8892470698	
UM06-2X/6-311++G(2df,2p): E = -501.4508055 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -500.8452513 Hartree	
Dioxirane3 0,1	
C,0,-0.2075590784,-1.1734368912,0.1413342133	37.4621 82.3086 164.3046
C,0,-1.677652028,-1.1293294416,0.5424886985	187.6578 196.8412 226.3451
C,0,-2.3804438,0.1064919834,0.0422438079	255.7622 294.2137 318.6798
C,0,-1.7035110058,1.1603010179,-0.4036344021	344.0684 399.1007 424.8344
C,0,-0.2035250379,1.2646372892,-0.4177050518	449.6682 503.0803 519.9498
C,0,0.453865489,0.1702172885,0.4288639254	571.9484 643.5782 778.2175
H,0,-2.195995441,-2.0121009131,0.1592743576	793.7905 825.6338 859.7168
H,0,-1.778820081,-1.1775658495,1.6327585259	884.5675 936.697 944.9202
H,0,0.3009678416,0.4187053338,1.4861340353	967.0004 991.4383 1019.1367
H,0,-0.1253951762,-1.3798937137,-0.9277404887	1039.5395 1054.694 1068.1049
H,0,-2.2522227471,2.0193827959,-0.775454348	1103.9194 1116.9154 1152.2956
H,0,0.0880633935,2.2522904205,-0.0539027176	1177.1446 1190.4517 1222.0695
H,0,0.1665335833,1.1976780596,-1.4482691275	1261.4712 1283.7887 1323.9115
H,0,0.3140695761,-1.9736299172,0.663386874	1335.1562 1347.7564 1376.2201
C,0,-3.8791390678,0.0690843718,0.0806408347	1407.0717 1411.8269 1420.2192
H,0,-4.2310772637,-0.1368051616,1.0944524533	1424.5583 1452.5491 1481.1297
H,0,-4.3157813782,1.0095327985,-0.2507059914	1485.0219 1489.673 1492.1429
H,0,-4.2608699486,-0.7341812013,-0.5535705721	1498.717 1503.0785 1509.6393
C,0,1.9493705245,0.1487146869,0.2040967024	1766.8303 3012.697 3024.1727
C,0,2.7120421048,1.4244244299,0.4178916138	3031.3775 3046.2531 3066.8956
H,0,2.499346422,1.8294076665,1.4073914459	3068.9491 3072.4589 3085.4147
H,0,3.775277894,1.2200172025,0.3254724639	3100.9603 3120.7431 3137.5133
H,0,2.4230305751,2.166517491,-0.3249934336	3147.1844 3157.9513 3168.2875
O,0,2.4107224771,-0.6516272648,-0.8333156413	
O,0,2.6175735524,-1.0113888318,0.5712793323	
UM06-2X/6-311++G(2df,2p): E = -501.4583354 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -500.8536629 Hartree	
AMCH 0,1	
C,0,0.5171651919,-0.9999711033,-0.3332238607	60.1921 82.2107 164.6753
C,0,2.0054131465,-1.1769964116,-0.6108556466	173.9776 185.2757 197.3513
C,0,2.8556590029,-0.117140818,0.0422079399	266.4752 305.7978 329.698
C,0,2.3269546356,0.9987856473,0.5351194024	361.9986 438.8128 448.8452
C,0,0.8655568668,1.3487760765,0.4702912059	521.8239 563.0846 609.0625
C,0,0.1111979879,0.4534217149,-0.5234197962	658.4453 778.2797 804.6821
H,0,2.3375535278,-2.1601390363,-0.2671626521	819.3031 911.9046 925.216
H,0,2.1960322173,-1.1630308101,-1.6901580909	936.854 968.1296 997.5865
H,0,0.3905083724,0.7773527429,-1.5344797591	1021.0708 1047.3341 1052.0598
H,0,0.2919369523,-1.2903681253,0.6957932427	1086.462 1111.4324 1153.4009
H,0,2.978035138,1.7227999467,1.0141780963	1175.5682 1186.5485 1196.3308

H,0,0.7574625337,2.3998038753,0.1938080398 H,0,0.4155645625,1.2481084652,1.4653923962 H,0,-0.0803169409,-1.6461726356,-0.9746039427 C,0,4.3271496788,-0.4015641855,0.0958357126 H,0,4.7183026497,-0.586471443,-0.9075459238 H,0,4.8831287812,0.4245977201,0.5352895741 H,0,4.5233425138,-1.3028911826,0.6808743836 C,0,-1.3876575592,0.655886981,-0.3962061798 C,0,-1.9030819749,2.0690411817,-0.5544067574 H,0,-2.9739011116,2.0481988636,-0.7349919009 H,0,-1.7119261367,2.6216621061,0.3675721242 H,0,-1.3872982757,2.5912988645,-1.3599535022 O,0,-2.13559376,-0.2588654345,-0.1610081057	1256.6744 1281.0391 1312.6897 1329.5596 1344.9071 1368.104 1390.1296 1407.0482 1414.0941 1420.3762 1475.6609 1479.9746 1482.056 1485.7673 1488.8943 1496.4476 1501.9382 1768.0789 1842.7324 3014.3745 3021.6282 3025.3544 3039.6635 3059.4763 3061.258 3070.7575 3072.6299 3094.0408 3116.5434 3128.6887 3130.9538 3148.0851 3171.5818
UM06-2X/6-311++G(2df,2p): E = -426.3454185 Hartree RHF-UCCSD(T)-F12a/cc-pVDZ-F12 // M06-2X/6-311++G(2df,2p): E = -425.8087917 Hartree	