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Supplementary material on the calculations

Structure 19

Zero-point correction=	0.100498 (Hartree/Particle)
Thermal correction to Energy=	0.105049
Thermal correction to Enthalpy=	0.105993
Thermal correction to Gibbs Free Energy=	0.073965
Sum of electronic and zero-point Energies=	-192.704110
Sum of electronic and thermal Energies=	-192.699559
Sum of electronic and thermal Enthalpies=	-192.698615
Sum of electronic and thermal Free Energies=	-192.730644

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\05-Mar-1996\
1\\#MP2=(FULL) 6-31G* FREQ, IOP(7/33=1)\\\\1,1\C\C
,1,R2\C,2,R3,1,A3\O,2,R4,3,A4,1,D4,0\H,2,R5,3,A5,1,D5,0\H,1,R6,2,A6,3,
D6,0\H,1,R7,2,A7,3,D7,0\H,4,R8,2,A8,3,D8,0\H,3,R9,2,A9,1,D9,0\H,3,R10,
2,A10,1,D10,0\H,3,R11,2,A11,1,D11,0\\R2=1.46034718\R3=1.48802808\R4=1.
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0930279\R10=1.09537284\R11=1.09179718\A3=123.1725035\A4=116.0485629\A5
=117.96584273\A6=120.71574929\A7=119.57942679\A8=110.4815283\A9=112.38
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Structure 21

Zero-point correction=	0.100445 (Hartree/Particle)
Thermal correction to Energy=	0.105023
Thermal correction to Enthalpy=	0.105967
Thermal correction to Gibbs Free Energy=	0.073875
Sum of electronic and zero-point Energies=	-192.704413
Sum of electronic and thermal Energies=	-192.699836
Sum of electronic and thermal Enthalpies=	-192.698892
Sum of electronic and thermal Free Energies=	-192.730983

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\08-Apr-1996\
0\\#MP2=(FULL) 6-31G* FREQ IOP(7/33=1) GEOM=CHECKPOINT\\
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.00567633,0.00943029,-0.00183357,-0.00460740,-0.00062626,0.00058515,0.

00167634,0.00027055,0.00141733,-0.00137090,-0.00028588,0.06687688,-0.0
0371731,0.01032481,0.01709184,0.01236115,-0.06502935,-0.05326606,-0.00
168224,-0.00505286,-0.00066970,-0.00054728,-0.01645889,-0.02946187,0.0
0029155,0.00062226,0.00042105,-0.00015566,0.00039926,-0.00084595,0.001
01191,0.00185095,-0.00192064,-0.00497851,0.07403107,0.00108849,-0.0032
4479,-0.00715191,0.05835282,-0.07047080,-0.33398182,0.00435095,-0.0017
7725,-0.01307286,-0.00205541,0.00743898,0.00955398,-0.00101554,-0.0015
1103,0.00050664,0.00019421,0.00032322,0.00109966,-0.00025671,-0.001603
63,0.00087781,-0.06187623,0.06960143,0.34057375,-0.06569771,0.06506540
,-0.00403833,0.00831045,-0.02406634,0.00087900,0.00212158,-0.00024733,
-0.00062941,-0.00519214,-0.00554091,0.00358184,-0.00027688,-0.00004698
,-0.00018906,-0.00003224,0.00012898,0.00010254,-0.00082428,-0.00121858
,-0.00101109,0.00051721,0.00109523,-0.00001701,0.06747956,0.06616700,-
0.30963974,0.02480421,0.00332079,-0.01951192,0.00191576,-0.00032467,-0
.00030441,-0.00075635,-0.00173508,0.00291610,0.00181609,-0.00015978,-0
.00016023,0.00005121,0.00003111,-0.00001781,0.00008703,-0.00039451,-0.
00005526,-0.00037654,-0.00032621,0.00059425,-0.00004621,-0.06826935,0.
33525331,-0.00395160,0.02599552,-0.05042353,-0.00556418,0.01318667,-0.
00266277,-0.00070540,-0.00005734,0.00014541,0.00243529,0.00292206,-0.0
0151143,0.00010899,-0.00014518,0.00011704,0.00002911,-0.00005549,0.000
03521,0.00003436,0.00049444,0.00068236,-0.00001447,-0.00111676,0.00017
744,0.00470615,-0.02911884,0.05018259,-0.06187384,0.01568582,0.0409780
9,-0.00714972,0.01242424,0.02689421,0.00132476,0.00107776,0.00181286,0
.00098982,0.00019363,-0.00159503,-0.00053704,-0.00059306,-0.00045009,-
0.00001178,0.00037006,-0.00032804,0.00019741,0.00019834,0.00002325,-0.
00282855,-0.00350346,0.00121869,-0.00191198,0.00227269,0.00622661,0.06
372087,0.01941799,-0.09174922,-0.10365952,-0.00608696,0.00318398,0.020
37407,0.00016546,0.00154472,0.00043109,0.00121770,0.00125977,0.0002517
9,0.00010885,0.00013131,-0.00037875,0.00004573,0.00006653,0.00001112,0
.00021049,0.00015244,0.00018976,-0.00321602,-0.00128200,0.00118887,0.0
0494782,-0.00912049,-0.03071238,-0.01638574,0.09529933,0.04336557,-0.1
0100999,-0.28933391,0.00323755,-0.00336171,-0.01375607,-0.00080392,-0.
00083952,0.00107120,-0.00057684,-0.00032163,-0.00001619,0.00017509,0.0
0050945,0.00037686,-0.00001017,-0.00017616,0.00015412,-0.00041743,0.00
000593,0.00003490,0.00173213,0.00078820,0.00076803,-0.00187484,0.00276
233,0.00538809,-0.04984843,0.10827573,0.30858879,-0.24537078,0.0163549
8,-0.13236249,-0.02315830,0.00097875,-0.01545598,-0.00252730,0.0001475
9,0.00350394,0.00211500,0.00015346,-0.00001431,-0.00001007,0.00011585,
0.00020212,-0.00000637,-0.00095746,-0.00050215,-0.00004037,0.00006341,
-0.00016190,0.00101681,-0.00017539,0.00001573,-0.00449356,-0.00058199,
-0.00330487,0.00808005,-0.00042533,0.00502130,0.26439488,0.01956485,-0
.04934076,0.01085255,-0.01839976,-0.00412116,-0.01012964,-0.00463437,-
0.00021008,0.00189984,0.00193369,0.00276332,-0.00079483,0.00022870,0.0
0024331,0.00019721,-0.00020363,-0.00106770,-0.00022608,-0.00020222,0.0
0032782,0.00016949,0.00097486,0.00000050,0.00010121,0.02815205,0.00004
619,0.01860730,-0.01174028,0.00051364,-0.00663264,-0.01567388,0.050844
92,-0.13540502,0.01167054,-0.14893709,0.01804059,-0.00225237,0.0126846
3,0.00255631,0.00110674,-0.00215123,-0.00203214,0.00031175,-0.00002882
,0.00025790,0.00028410,0.00005630,0.00033982,0.00065526,0.00057671,0.0
0002306,0.00000039,0.00018647,-0.00039722,-0.00062153,0.00064927,-0.00
150978,-0.00113870,-0.00213041,-0.02493213,0.00402823,-0.01327583,0.14
305861,-0.01404440,0.15236999\\-0.00003921,0.00004029,0.00002658,0.000
13467,-0.00023556,-0.00003627,-0.00006072,0.00005639,0.00000693,-0.000
00911,0.00010120,-0.00000827,0.00000524,-0.00000841,-0.00000856,-0.000
01324,-0.00000041,-0.00000828,-0.00000266,0.00001849,0.00002314,-0.000

00858,0.00002285,0.00000432,-0.00002044,0.00000220,-0.00000856,0.00001
072,-0.00001234,-0.00000149,0.00000335,0.00001530,0.00001047\\\@

Structure 28

Zero-point correction=   0.094906 (Hartree/Particle)
Thermal correction to Energy=   0.100703
Thermal correction to Enthalpy=   0.101647
Thermal correction to Gibbs Free Energy=   0.066054
Sum of electronic and zero-point Energies=   -192.689837
Sum of electronic and thermal Energies=   -192.684040
Sum of electronic and thermal Enthalpies=   -192.683096
Sum of electronic and thermal Free Energies=   -192.718689

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\20-Mar-1996\
0\\#N GEOM=ALLCHECK GUESS=READ TEST RMP2(FULL)/6-31G(D) FREQ\\
\\1,1\C,-0.9293417178,0.0176796795,-1.2569415812\C,-0.9284169115,0.00
3512314,0.1729426165\C,0.2879122071,0.0074555811,0.9504205589\O,1.4036
589323,-0.012228071,0.1270814545\H,0.1796755463,0.9183361785,1.5894550
14\H,0.2163120827,-0.8256445498,1.6813921327\H,-1.8634655371,-0.028860
8813,0.7360522812\H,-1.8992422567,0.1721579548,-1.7216718004\H,-0.1263
629618,0.6613003027,-1.6423757832\H,-0.5368594704,-0.9943796612,-1.516
5543731\H,2.219749672,0.023029777,0.6585213273\\Version=SGI-G94RevB.3\
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.8032746,-0.0403872,0.6891708\DipoleDeriv=-0.0439382,0.0059765,0.44165
72,-0.0994336,-0.2293627,-0.39499,0.0410138,-0.1360044,-0.8154796,0.45
34287,0.0358743,0.3421601,0.0634169,0.2572606,0.1059804,0.3195723,0.13
12759,1.3297896,0.5263593,-0.0442987,-0.4738182,-0.1223051,0.1244194,-
0.0947183,-0.8549305,-0.0657301,-0.5362468,-0.8964902,0.0102584,0.0914
567,0.0115135,-0.499584,0.0207906,0.2919903,0.0163729,-0.2615225,-0.03
2135,0.0216606,-0.0349488,0.0838181,0.1212293,0.0232367,0.1419765,-0.0
069652,0.2263075,0.0049275,-0.0260323,-0.0066797,-0.0287637,0.1185774,
0.0270048,0.1586812,0.0217032,0.2254182,0.1350135,-0.0024876,-0.002153
9,0.0205172,0.13581,0.0063685,-0.0054649,0.0034292,0.08586,0.0894064,0
.0035075,0.007288,0.0116921,0.1520824,0.0575051,0.0120772,0.003288,0.1
139295,0.1362134,-0.0156887,-0.1834688,0.0018982,0.197349,0.0697445,-0
.0368411,-0.0295503,0.2090982,0.178755,0.010995,-0.1868094,0.0554855,0
.2086523,0.1830424,-0.0467725,0.0693652,0.1739595,0.4484595,0.0002349,
0.0053169,0.0021609,0.4135662,-0.0039647,-0.0213022,-0.0071845,0.24888
65\Polar=37.1041888,0.1197147,24.3999137,4.6507822,1.034508,42.1558271
\PG=C01 [X(C3H7O1)]\NImag=0\\0.64614467,0.00236226,0.43166310,0.068080
05,-0.05367611,0.57697917,-0.11739995,0.00241975,0.00695113,0.68615521
,-0.00230617,-0.07343588,0.01683465,0.00345459,0.24283244,-0.03459629,
0.03763365,-0.30775935,-0.04222673,-0.02131084,0.65005860,0.00703143,-
0.00218042,-0.00765948,-0.24603736,0.00229980,-0.10036035,0.61582313,-
0.00413093,0.02496947,-0.00565306,0.00709273,-0.07701367,0.01479659,-0
.00789022,0.45262830,-0.01402903,-0.01473275,-0.03499830,-0.06409509,0
.01016763,-0.10631013,-0.01334540,-0.02466199,0.52399996,0.00302934,-0
.00137671,0.00000474,-0.05754951,0.00211407,0.03469142,-0.23354996,0.0
0271083,0.11119836,0.66994445,-0.00086133,-0.00442823,0.00147619,-0.00
137356,0.00456864,-0.00143754,0.00092531,-0.05552974,-0.00026007,0.010
63756,0.04481503,-0.00563436,0.00341222,0.00342971,-0.02013282,-0.0017
2722,0.00378329,0.07559083,0.00096629,-0.15957090,0.08338456,0.0140201
1,0.37354591,-0.00105020,0.00433595,-0.00534256,0.00640499,-0.02234958
,-0.00683355,-0.04886379,-0.00893048,-0.00584418,-0.01321206,0.0231018

5,0.02676750,0.05180528,-0.00186756,-0.00149693,0.00293728,-0.00084124
,-0.00924707,-0.00501201,0.00570606,-0.18546946,-0.10625905,0.00607888
,0.00515283,-0.00049418,-0.00575483,0.21457448,-0.00526458,0.00399807,
0.00238331,-0.00706235,-0.01966909,-0.02338019,0.01249936,-0.11676619,
-0.10416726,0.01038242,-0.01293833,-0.01469638,-0.01424924,0.12387656,
0.12975013,0.00007456,-0.00753241,-0.00272904,0.00386415,0.02346625,-0
.01470432,-0.05090651,0.00834537,-0.00241983,-0.01145835,-0.02068779,0
.02759039,0.00339834,-0.00432025,0.00271735,0.05538675,0.00026837,-0.0
0303677,-0.00114637,-0.00213233,-0.00401864,-0.00298994,-0.00006851,-0
.17283521,0.12433535,-0.00477937,0.00596580,-0.00235882,0.00582363,-0.
02578045,0.01801022,0.00123250,0.19722088,-0.00423284,0.00207291,0.003
47724,-0.00795550,0.01485129,-0.02543381,0.00960633,0.12868906,-0.1344
7506,0.01043373,0.01142262,-0.01608131,0.00344227,-0.01441911,0.008604
93,-0.01130421,-0.13631692,0.16295855,0.00797371,0.00072981,-0.0036042
4,-0.27917729,-0.00824984,0.12435158,-0.01445250,-0.00006641,0.0188076
4,-0.00328354,-0.00033804,-0.00487755,0.00076637,-0.00064782,-0.000253
90,0.00063355,0.00056857,-0.00019787,0.28673455,0.00705953,0.02894748,
-0.00203651,-0.00769241,-0.06608704,0.00415146,-0.00007988,0.00806724,
0.00166206,0.00000831,0.00284115,-0.00037267,-0.00034983,0.00148452,0.
00314646,0.00042685,0.00085172,-0.00319779,0.00811931,0.02917540,0.024
63225,0.00474046,-0.00776549,0.12732523,0.00330793,-0.14300717,-0.0161
0512,0.00025333,0.01525032,-0.00456322,-0.00011677,-0.00319695,0.00098
752,-0.00048593,0.00053865,0.00065487,0.00055221,0.00031304,-0.1336189
3,-0.00586045,0.14152345,-0.30062514,0.03793813,-0.11354397,0.00815071
,-0.00236461,0.00375875,-0.00029487,0.00303248,0.00275356,-0.00025333,
-0.00015576,-0.00109009,0.00081462,-0.00008998,0.00037441,-0.00024485,
-0.00014279,-0.00027264,0.00088795,-0.00120433,0.00012334,0.31136713,0
.03586165,-0.05560146,0.02427093,-0.00295175,-0.00441883,-0.00611229,-
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00170316,-0.00038639,0.00064961,-0.00111492,-0.00024490,-0.00114592,0.
00011966,-0.00291876,0.00000311,-0.04180928,0.05364668,-0.10695631,0.0
2241946,-0.10526027,-0.03646715,0.00612343,-0.01739436,0.00358407,-0.0
0101214,-0.00476337,0.00123740,0.00023116,0.00125405,-0.00094935,0.000
17869,-0.00059747,-0.00047138,0.00000136,-0.00055243,-0.00005018,-0.00
098782,0.00184215,0.11993899,-0.02077016,0.11424426,-0.19023378,-0.120
09192,0.05339134,0.00310344,0.00283037,0.01726270,0.00033731,-0.001144
84,-0.00749808,-0.00201458,0.00155008,0.00042527,-0.00148215,0.0010689
5,0.00105847,-0.00138943,0.00008281,0.00141008,0.00044637,-0.00416764,
0.00030548,-0.01177125,-0.01478318,0.01070523,0.20201216,-0.12027125,-
0.12542072,0.06888233,0.00351584,-0.00222659,-0.01020881,-0.00087585,0
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.00005622,-0.00063993,0.00044655,0.00020599,-0.00049593,0.00021786,-0.
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609790,0.06202480,0.06667071,-0.07837665,0.02671075,0.02321182,-0.0163
0705,0.00135153,-0.00550278,-0.00066192,-0.00007519,0.00048966,0.00017
040,-0.00150708,0.00064039,-0.00046931,0.00150737,0.00038414,0.0008189
0,-0.00145371,-0.00239976,-0.00460465,-0.00811519,-0.01050178,0.006390
52,-0.07589386,-0.06531649,0.08707541,-0.05511357,0.08292688,0.0032317
6,-0.00216111,0.00147917,0.01607169,0.00061982,0.00154081,-0.00760281,
-0.00039312,0.00026437,0.00191849,-0.00112104,0.00059009,0.00162229,-0
.00154786,-0.00040570,0.00075795,0.00004056,-0.00206418,0.00115577,-0.
00805026,0.02332378,0.00942949,0.00103786,-0.01975234,-0.00409010,0.06
672975,0.08357580,-0.22254314,-0.05165959,-0.00188738,-0.01025513,-0.0
0976807,0.00121433,0.00296712,0.00442768,0.00099663,-0.00006229,-0.000
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9281,-0.00046773,-0.00333485,-0.00047231,-0.00156582,-0.00273237,-0.00
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14809,-0.07278079,-0.05160707,0.01175388,-0.03181958,-0.00950928,-0.00
091774,0.00780057,-0.00439720,-0.00008007,-0.00096414,0.00067846,0.002
19026,-0.00034161,0.00162033,-0.00230153,-0.00103332,0.00016654,-0.000
19397,0.00587013,-0.00181516,-0.00377154,0.01317213,0.00459805,-0.0010
3232,0.01305305,0.00554281,-0.02265745,0.06658600,0.05466779,0.0001689
1,0.00046868,0.00122028,-0.00535329,-0.00037403,0.00258511,-0.02970670
,-0.00055934,-0.01792514,-0.35125934,-0.01306270,-0.18394223,0.0025396
3,0.00007770,-0.00182423,0.00218966,-0.00044717,-0.00168728,-0.0005697
4,-0.00005573,-0.00089720,0.00001929,-0.00003405,-0.00000082,-0.000045
94,0.00008032,-0.00045932,-0.00004101,-0.00038163,-0.00013760,0.382058
53,0.00030964,0.00038308,-0.00022973,0.00039577,-0.00069823,0.00025781
,0.00131595,-0.00672100,0.00021747,-0.01630381,-0.00241546,-0.01116971
,0.00063938,0.00153632,0.00069325,-0.00061591,0.00132160,-0.00066740,0
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0035701,0.00010764,-0.00054313,0.00021431,0.00010812,0.00045756,0.0142
8794,0.00432148,-0.00117177,0.00024218,-0.00050230,0.00519864,0.000029
98,-0.00474055,0.03575597,0.00109033,0.01009385,-0.24661417,-0.0119228
9,-0.18931629,0.00133843,-0.00062101,0.00041325,0.00146033,0.00056209,
0.00020341,0.00109113,0.00002489,0.00092181,-0.00015562,-0.00011250,0.
00023886,-0.00013429,-0.00056065,0.00042154,0.00016292,0.00033157,0.00
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002,-0.00000032,0.00000009,-0.00000021,-0.00000002,-0.00000013,0.00000
025,-0.00000006,0.00000014,0.00000002,0.00000007,-0.00000005,0.,0.0000
0010,0.00000010,-0.00000003,0.00000005,-0.00000008,0.00000006,0.000000
01,0.,0.00000010,-0.00000001,-0.00000030,-0.00000012,0.00000010,0.,-0.
00000006,-0.00000002,-0.00000007,-0.00000002\\\@

Structure 26

Zero-point correction=   0.100143 (Hartree/Particle)
Thermal correction to Energy=   0.105280
Thermal correction to Enthalpy=   0.106224
Thermal correction to Gibbs Free Energy=   0.072436
Sum of electronic and zero-point Energies=   -192.731246
Sum of electronic and thermal Energies=   -192.726108
Sum of electronic and thermal Enthalpies=   -192.725164
Sum of electronic and thermal Free Energies=   -192.758953

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\05-Mar-1996\
1\\#MP2=(FULL) 6-31G* FREQ, IOP(7/33=1)\\\1,1\C\
C,1,R2\C,2,R3,1,A3\O,3,R4,2,A4,1,D4,0\H,3,R5,2,A5,1,D5,0\H,2,R6,3,A6,1
,D6,0\H,2,R7,3,A7,1,D7,0\H,1,R8,2,A8,3,D8,0\H,1,R9,2,A9,3,D9,0\H,1,R10
,2,A10,3,D10,0\H,4,R11,3,A11,2,D11,0\\R2=1.56045062\R3=1.44915591\R4=1
.27330299\R5=1.09343409\R6=1.09578213\R7=1.09116291\R8=1.09051367\R9=1
.09134952\R10=1.09047769\R11=0.98879241\A3=106.96313318\A4=119.7326185
2\A5=121.63083115\A6=108.5809687\A7=110.60552005\A8=106.95907538\A9=11
1.96196755\A10=110.98547322\A11=114.41330388\D4=-106.215177\D5=70.2489
741\D6=-117.02589108\D7=121.47351281\D8=-178.01742855\D9=-59.48689118\
D10=63.58859209\D11=176.61278108\\\Version=SGI-G94RevB.3\HF=-192.262787
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63471,0.6309042\DipoleDeriv=-0.1744864,0.0358868,-0.1850431,-0.0288979
,0.0721943,-0.0007017,0.2352562,-0.0475832,0.403223,-0.3509871,0.10424
96,-0.2152951,0.0472844,-0.0722338,-0.0075754,-0.4218051,0.1132631,-0.

5194681,1.188023,-0.2846198,0.604373,-0.4032544,0.8042601,-0.3714363,0.4176556,-0.2667934,0.6280745,-0.6527246,0.3045001,-0.3419794,0.513948 2,-0.5747685,0.383608,-0.2731899,0.1994948,-0.4173031,0.0533932,-0.018 3801,-0.0113124,0.0133679,0.0965416,0.0177952,-0.0047542,0.0090351,0.1 347038,0.1172353,-0.0186728,-0.0183991,-0.0614961,0.0939522,-0.0508525 ,0.0413306,-0.0325652,0.1451485,0.0941777,0.0164902,-0.0233335,-0.0005 501,0.0668858,0.0353639,0.0129495,0.0265562,0.081921,0.06078,0.0011256 ,0.0208977,-0.0011968,0.1243415,-0.006861,-0.0560488,0.0122592,0.00722 14,0.0654041,-0.0753768,0.0422313,-0.0532281,0.006263,0.0279154,0.0041 702,-0.0188313,0.0430544,0.067229,0.0627804,0.0288647,0.0423004,0.0060 606,-0.0293538,-0.0216037,0.0196079,0.0238365,0.5319558,-0.1279833,0.0 989958,-0.0682775,0.3765032,0.0020983,0.0660397,-0.0144433,0.4695882\P olar=36.9880425,-3.2341464,31.4346967,7.4157662,-3.841629,32.8107188\P G=C01 [X(C3H7O1)]\NImag=0\\0.60548953,-0.00034420,0.62736907,-0.011607 29,0.00034975,0.43153433,-0.06680242,-0.00864549,0.02620507,0.59009190 ,-0.00994519,-0.07638479,0.00130673,0.02480912,0.65587972,-0.01204830, -0.00103163,-0.14410821,-0.04093828,-0.02527520,0.39397365,0.00347512, 0.00487888,-0.03336679,-0.27604278,-0.03585027,-0.01105164,0.70559878, -0.00223538,-0.00476318,0.01027362,-0.02274069,-0.10075202,-0.01235258 ,0.00310360,0.80133430,-0.02563075,0.00154636,-0.02549857,-0.04195268, -0.00710964,-0.07472682,0.12257059,-0.18869000,0.31571416,-0.00729620, 0.00046789,0.00997318,-0.01992272,0.04897586,-0.03047880,-0.19997695,0 .16850819,-0.09222955,0.64052320,0.00486819,0.00103897,-0.01269990,0.0 2102993,-0.00169526,0.02033432,0.10287012,-0.45398566,0.15568569,-0.12 847954,0.52327604,-0.00314838,-0.00037651,0.00415309,-0.01475608,0.017 98035,-0.00957891,-0.07038605,0.17256696,-0.13120879,0.19009266,-0.188 53743,0.16444324,0.00046294,0.00009986,-0.00036682,-0.00706204,-0.0232 5722,0.00609189,-0.18023348,-0.14345106,0.01822116,0.01556159,0.024055 18,-0.01124741,0.17009206,0.00075246,0.00038504,0.00024231,0.00211456, 0.00765119,0.00214072,-0.12854980,-0.23623970,0.02369487,-0.01255473,- 0.02526675,0.01520308,0.13956775,0.25229267,0.00319434,0.00042799,0.00 267086,-0.00851137,-0.00647210,0.01299968,0.01725558,0.02077841,-0.071 85231,0.00073068,0.02379227,0.02150748,-0.01114988,-0.03955208,0.03976 713,0.00341894,-0.00258394,-0.00011242,-0.10698568,0.09719163,0.039626 73,-0.01333500,0.03263549,0.01248720,-0.00681499,-0.00073281,-0.001585 39,0.00148350,-0.00134349,-0.00186449,0.11184430,0.00110062,0.00051372 ,0.00179762,0.09547897,-0.25110631,-0.07309807,0.00373117,-0.00266876, 0.00464699,-0.00142369,0.00302986,-0.00358729,0.00020969,0.00039551,0. 00090694,-0.11127242,0.26473479,0.01597849,-0.02851113,-0.01931691,0.0 4275307,-0.07194377,-0.05704688,-0.01003261,0.01438175,-0.00048325,-0. 00233750,-0.00167068,-0.00004947,0.00033297,-0.00033623,-0.00021457,-0 .03844986,0.07741041,0.07722680,0.00303483,0.00330363,-0.00031508,-0.1 2092941,-0.10402143,0.04794894,-0.02108793,-0.03265796,0.01299023,0.00 352728,0.00069976,0.00085874,-0.00390539,0.00127609,-0.00261337,0.0094 5632,0.01229297,-0.00708955,0.12870965,0.00152472,0.00299205,-0.001999 33,-0.10937093,-0.24097584,0.08295366,0.00026742,0.00187991,-0.0021930 6,0.00120402,-0.00041286,-0.00032022,0.00053428,0.00122087,0.00193961, -0.01388514,-0.01627813,0.00952706,0.11907468,0.25023850,0.01534173,0. 02615902,-0.01403688,0.05332512,0.08460484,-0.08159961,-0.01038519,-0. 01264218,0.00272191,0.00200864,-0.00090021,-0.00066978,-0.00314830,0.0 0141706,0.00131126,-0.00646701,-0.00800589,0.00304322,-0.05035125,-0.0 8880520,0.09213454,-0.32047924,0.00954046,-0.08074257,0.00308105,0.000 76497,0.00459613,-0.00121577,0.00138171,0.00001719,0.00122430,-0.00157 802,0.00048083,0.00018696,-0.00003026,-0.00027700,0.00036549,-0.000466 83,-0.00016519,0.00024191,0.00016615,-0.00007147,0.33926628,0.01027572

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20,0.00000105,-0.00000131,0.00000091,0.00001099,0.00000296,0.00000183\
\\@

Structure 27

Zero-point correction=   0.099633 (Hartree/Particle)
Thermal correction to Energy=   0.104682
Thermal correction to Enthalpy=   0.105626
Thermal correction to Gibbs Free Energy=   0.072286
Sum of electronic and zero-point Energies=   -192.732682
Sum of electronic and thermal Energies=   -192.727633
Sum of electronic and thermal Enthalpies=   -192.726689
Sum of electronic and thermal Free Energies=   -192.760028

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\05-Mar-1996\
1\\#MP2=(FULL) 6-31G* FREQ, IOP(7/33=1)\\
\\1,1\C\C,1,R2\C,2,R3,1,A3\O,1,R4,2,A4,3,D4,0\H,1,R5,2,A5,
3,D5,0\H,2,R6,3,A6,1,D6,0\H,2,R7,3,A7,1,D7,0\H,3,R8,2,A8,1,D8,0\H,3,R9
,2,A9,1,D9,0\H,3,R10,2,A10,1,D10,0\H,4,R11,1,A11,2,D11,0\\R2=1.4527833
5\R3=1.52113101\R4=1.27212033\R5=1.09355045\R6=1.10459777\R7=1.1045837
\R8=1.0900716\R9=1.0910124\R10=1.09101144\R11=0.98928861\A3=116.313909
44\A4=119.83235074\A5=121.5994484\A6=113.13152846\A7=113.13543444\A8=1
08.94220233\A9=111.3164668\A10=111.31645208\A11=114.38568216\D4=-0.007
86483\D5=179.99439435\D6=-121.91003111\D7=121.92121493\D8=180.00066419
\D9=-60.7733722\D10=60.77475651\D11=-179.99702883\\Version=SGI-G94RevB
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531,-0.0000444,-0.5245336,0.0541505,-0.0000047,0.0569076,-0.0000116,0.
0316966,0.0000411,0.0070548,0.0000025,0.0030302,-0.576317,-0.0000368,0
.5834052,-0.0000467,-0.2035958,0.0000867,0.3517157,0.0000341,-0.762450
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5123,-0.0000008,0.0270569,0.1155651,0.033213,-0.164338,0.0459501,0.125
7773,0.0302198,-0.0471157,0.0251454,0.1090965,0.115534,-0.0332145,-0.1
64345,-0.0459664,0.1257824,-0.0301068,-0.0471363,-0.025132,0.1091226,0
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0.0348448,0.024175,-0.0640553,0.0715469,0.0404931,-0.0193342,-0.020977
6,-0.0433053,0.0036642,0.03484,0.0241736,0.064054,0.0715596,0.3631925,
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56,40.1950613\PG=C01 [X(C3H7O1)]\NImag=0\\0.86293306,0.00007913,0.2235
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03849,-0.00065653,0.00006608,-0.00314001,-0.00006794,-0.00147504,0.000
52894,-0.00017984,0.00014237,0.01780045,-0.02907511,-0.00550651,-0.037
55738,0.06533807,0.07205094,-0.00016582,-0.00076071,0.00223153,-0.0176
5008,-0.02478264,0.00687625,-0.12836218,-0.11929445,0.03712474,0.00073
835,-0.00023297,-0.00094988,-0.00001865,0.00056572,0.00006716,0.000560
99,-0.00043085,0.00064019,-0.00454617,0.00071870,-0.00338294,-0.001905
25,-0.00271668,0.00050332,0.01150574,0.01549045,-0.00557156,0.13961436
,-0.00086201,0.00008916,0.00083907,0.00291969,0.00352362,-0.00178156,-

0.12154704,-0.24522563,0.05948791,0.00035744,0.00019353,-0.00005359,0.
00008019,-0.00017996,-0.00013201,-0.00011339,0.00047971,-0.00036019,0.
00099818,0.00111917,0.00059948,0.00193418,0.00131622,-0.00134797,-0.01
548993,-0.01947552,0.00812316,0.13150945,0.25816645,-0.00208018,-0.001
51242,0.00217263,-0.00945980,-0.01539293,0.00192248,0.03865609,0.06075
729,-0.07024907,0.00068080,-0.00049617,-0.00067714,0.00003837,0.000656
41,0.00006594,0.00052913,0.00017984,0.00014251,-0.00313966,0.00006846,
-0.00147490,0.01780018,0.02907551,-0.00550596,-0.00557183,-0.00812380,
0.00163668,-0.03755455,-0.06533509,0.07204826,-0.00326026,-0.00000214,
0.05374034,-0.00535397,-0.00000271,-0.00085972,0.00025972,-0.00000009,
-0.00113979,-0.04928681,0.00000142,-0.08750833,0.00051106,0.00000093,0
.00128243,-0.00001508,-0.00003275,0.00084288,-0.00001505,0.00003307,0.
00084393,0.00000757,0.00000004,-0.00009826,0.00022862,-0.00021315,0.00
010149,0.00022870,0.00021324,0.00010144,0.05669550,0.00000067,-0.00212
844,0.00000732,-0.00000162,0.01711559,-0.00000086,0.,-0.00013513,-0.00
000055,-0.00000135,-0.03007165,0.00000837,0.00000109,-0.00786276,-0.00
000029,0.00001096,-0.00080924,0.00319541,-0.00001189,-0.00080912,-0.00
319401,-0.00000005,0.00006423,-0.00000001,0.00006609,-0.00000684,-0.00
012285,-0.00006601,-0.00000674,0.00012290,0.00000213,0.02465009,-0.003
85180,-0.00000032,-0.02510611,-0.00034527,0.00000314,0.00540651,-0.000
08800,-0.00000020,0.00031928,-0.02973465,0.00001471,-0.44038642,-0.001
69083,-0.00000064,0.00406156,0.00141415,0.00008201,-0.00032695,0.00141
409,-0.00008334,-0.00032783,0.00015716,0.00000002,0.00009082,0.0000158
0,0.00003923,-0.00008141,0.00001575,-0.00003920,-0.00008143,0.03269361
,-0.00001541,0.45643197\\0.00025774,0.00000051,-0.00010275,-0.00022835
,-0.00000621,0.00013742,-0.00004435,0.00000165,-0.00009563,-0.00008303
,-0.00000015,0.00027033,-0.00005854,0.00000007,0.00003457,0.00007850,0
.00003833,0.00000543,0.00007772,-0.00003479,0.00000607,-0.00003200,-0.
00000001,0.00000937,0.00001053,-0.00003383,-0.00001276,0.00001025,0.00
003387,-0.00001229,0.00001155,0.00000055,-0.00023975\\\@

Structure 20

1	2	3
?A	?A	?A

Frequencies --   -970.7313   227.5551   362.8248

Zero-point correction=   0.098068 (Hartree/Particle)
Thermal correction to Energy=   0.102603
Thermal correction to Enthalpy=   0.103548
Thermal correction to Gibbs Free Energy=   0.071544
Sum of electronic and zero-point Energies=   -192.677689
Sum of electronic and thermal Energies=   -192.673153
Sum of electronic and thermal Enthalpies=   -192.672209
Sum of electronic and thermal Free Energies= -192.704213

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\09-Apr-1996\
0\\#MP2=(FULL) 6-31G* FREQ IOP(7/33=1) GEOM=CHECKPOINT\\
\\1,1\C,-0.4476726399,-0.34402
42586,-1.4591264752\C,-0.4484408025,-0.341638325,0.0264804744\C,0.8090
476274,-0.3478361141,0.8371275502\O,0.0776182282,0.8983398301,0.681158
6518\H,1.7628227722,-0.3470219941,0.3188657028\H,0.7929392793,-0.72773
94956,1.8534747177\H,0.0709299321,1.8554480602,0.9070899259\H,-1.35155
22894,-0.6583449909,0.541914178\H,-0.5680438934,-1.3826399487,-1.78564
78298\H,0.486692321,0.04682555,-1.863846628\H,-1.2923390575,0.22774636

42,-1.8480085776\\Version=SGI-G94RevB.3\HF=-192.2046202\MP2=-192.77575
63\RMSD=7.946e-09\RMSF=2.203e-05\Dipole=0.1688382,0.4432783,0.6394273\
DipoleDeriv=-0.0458098,-0.0233526,-0.0411001,-0.0181027,-0.0817164,-0.
0530127,-0.0310522,-0.0771507,-0.1881121,0.3334332,0.0854482,0.0849321
,0.2568482,0.7609022,0.4085031,0.1517193,0.2693988,0.7354809,0.3144689
,-0.109522,0.0005433,-0.2962548,0.5804119,-0.1343145,-0.0604417,0.0048
529,0.2287483,-0.3887324,0.0346746,0.0230117,0.0164917,-1.4975747,-0.3
890468,0.0326718,-0.2713746,-0.6136131,0.0954795,0.0183869,0.004641,-0
.0069647,0.0877812,0.0368545,0.023043,0.023862,0.0695724,0.0735636,0.0
205017,0.0074039,0.0174716,0.1090139,-0.0216949,0.0037367,0.0156525,0.
0769931,0.3530846,-0.0149891,-0.1225336,0.0140831,0.7128467,0.0903612,
-0.0899459,0.0535885,0.4443731,0.0735421,-0.0196807,-0.0035919,0.01156
35,0.0882338,-0.0310149,0.0049586,-0.0089359,0.0167679,0.1336072,-0.00
39429,0.0166951,-0.0042075,0.0513514,0.0297531,-0.0070571,0.0155412,0.
089435,-0.001703,-0.0389255,0.0207927,-0.0420279,0.0947218,0.0308835,-
0.0289974,-0.0104066,0.0742126,0.0590662,0.0514012,0.0092058,0.0510995
,0.0940283,0.0327285,0.0013649,-0.0150282,0.0661418\Polar=31.0043649,0
.136641,29.3799395,3.464584,1.3298753,33.376426\PG=C01 [X(C3H7O1)]\NIm
ag=1\\0.63557022,0.00660385,0.59839187,-0.00833409,-0.02301167,0.53448
855,-0.09983088,0.00695071,0.00867903,0.65001160,-0.00244152,-0.072823
60,0.01740287,0.11372241,0.26094975,0.01381063,0.03116033,-0.25481378,
-0.01964897,-0.04615242,0.60642600,0.00360684,-0.00420443,-0.00035632,
-0.22030053,-0.02371080,-0.09140390,0.66786134,0.00031566,-0.00794328,
-0.00226817,0.00384395,0.01818833,0.02882253,-0.05523792,0.30739382,-0
.02804807,0.01520311,-0.01050229,-0.08256452,0.00532198,-0.13172004,-0
.04368124,-0.13583918,0.65686402,0.00024527,-0.00982941,-0.00453392,-0
.05064978,-0.03480895,-0.02601818,-0.08997417,0.06927420,-0.01911856,0
.15718181,-0.00359247,-0.01245041,-0.01102068,-0.05891064,-0.11299971,
-0.04462022,0.10733691,-0.18689842,0.03349371,-0.05978597,0.78899147,-
0.00652945,-0.03880330,-0.00983115,-0.03265984,-0.03821117,-0.04272678
,-0.00907413,0.00499586,-0.03640318,0.11123371,0.16036694,0.06890954,0
.00143439,-0.00098103,0.00088890,-0.01527306,0.00166031,0.01150672,-0.
28813847,-0.00145260,0.13161276,-0.00508271,0.00087415,-0.00166865,0.3
0124523,0.00146684,0.00075380,0.00067554,-0.01033664,-0.00613107,0.009
82257,-0.01775566,-0.04813423,0.00724753,0.03490834,-0.00839884,-0.009
48997,-0.00115812,0.05207292,0.00001076,-0.00115696,0.00145250,-0.0183
1068,0.00039401,0.01168377,0.13641829,0.00836679,-0.13686099,-0.004817
65,-0.00103730,0.00204349,-0.13680816,-0.00825053,0.13012400,-0.003000
87,0.00169706,-0.00012051,0.00249102,0.01042283,-0.02037665,-0.0601492
3,-0.00312440,0.02019931,-0.00378286,0.00591554,-0.01280406,0.00543173
,-0.00983999,0.02352205,0.05744072,-0.00294183,0.00220591,-0.00019392,
0.00701382,0.00056270,-0.01574926,-0.00911400,-0.08111945,0.09066586,0
.00899473,-0.01609592,0.02695498,-0.00056040,0.00557185,-0.00084681,-0
.00329500,0.08809291,-0.00182837,0.00115759,-0.00006069,0.00485651,0.0
0366282,-0.00957971,0.01013576,0.10361025,-0.33516028,-0.00039088,-0.0
0481308,0.00976056,-0.00319409,0.00336975,-0.00580567,-0.00986767,-0.1
0647429,0.33867081,0.00019764,-0.00117404,-0.00102623,-0.00333400,0.01
421180,0.01663842,0.00315525,-0.00622614,0.01023702,-0.00873803,0.0021
3294,-0.04562412,0.00059036,0.00411775,0.00171807,0.00033226,-0.000294
86,-0.00000047,0.00637756,-0.00069486,0.00360829,-0.00090986,0.0016067
0,-0.00955799,0.00296139,-0.00702467,-0.00508406,-0.00184936,0.0153254
8,-0.44223596,-0.11112292,-0.00051863,0.00261856,0.00026265,-0.0008451
3,0.00096668,-0.00009163,-0.00869345,0.44886081,0.00064799,-0.00615775
,-0.00160844,0.01126562,0.01291456,-0.00671922,0.01022693,-0.00191010,
-0.00903243,-0.04202391,-0.12104189,0.00690839,-0.00018218,-0.00186654

,-0.00066082,0.00070950,0.00532928,0.00143549,0.01926601,0.10899331,0.01097764,0.00632021,0.00204824,-0.00276551,-0.26610763,-0.07577719,0.11967388,-0.01750570,-0.00767316,0.01139138,0.00047710,0.00262565,-0.00236717,-0.00073103,-0.00163827,-0.00206919,0.00082590,0.00046044,0.00026290,0.00123955,0.00042297,-0.00026490,0.27416385,0.00235593,0.00630065,-0.00049792,-0.06117478,-0.07051901,0.04582928,0.01204477,0.00145934,-0.01136196,-0.02679192,-0.01778708,0.00057103,0.00168922,0.00167874,0.00172082,-0.00100185,0.00024091,-0.00005935,-0.00526946,0.00110125,0.00302481,0.07962733,0.07571555,0.02607619,0.00998538,-0.00938053,0.13045980,0.04355348,-0.13124936,-0.01571670,-0.00732903,0.00592155,-0.01424015,-0.00637873,0.00214940,-0.00116158,-0.00156860,-0.00142750,-0.00013826,0.00098131,0.00092587,-0.00035134,0.00064898,0.00058719,-0.12316816,-0.03917555,0.13576472,-0.05005769,-0.02980397,-0.00681796,-0.00240388,-0.00131981,-0.00171639,-0.00022518,-0.00041098,0.00014916,0.00053513,0.00166713,-0.00046231,-0.00001450,-0.00014368,-0.00009227,0.00009307,-0.00005110,0.00001646,0.00013391,0.00017322,0.00013444,-0.00000166,-0.00040120,-0.00014765,0.05020667,-0.03002688,-0.30126276,-0.07725618,-0.00076974,-0.00362061,-0.00334509,-0.00050167,0.00021468,-0.00083710,0.00133800,0.00525450,0.00249742,0.00009505,-0.00011267,-0.00008835,0.00002672,-0.00008418,0.00001047,0.00062162,-0.00011953,0.00094855,-0.00023534,0.00031132,-0.00042712,0.03203803,0.32283959,-0.00771885,-0.07834494,-0.07536487,-0.00272623,-0.03351946,-0.00753030,-0.00050705,-0.00174365,0.00147201,-0.00158268,-0.00285468,-0.00718602,-0.00026088,0.00024719,-0.00016594,0.00008671,0.00010654,0.00001097,-0.00053512,0.00142396,-0.00173086,0.00052341,0.00138999,0.00100399,0.01013498,0.08737521,0.08012307,-0.26748533,-0.08955154,0.08946506,0.00254381,0.00201941,-0.00162171,0.00138788,-0.00005982,-0.00080708,0.00003774,0.00087456,-0.00010769,0.00014392,0.00028366,0.00014512,-0.00000368,-0.00004525,-0.00005981,-0.00009041,-0.00009234,0.00031365,0.00093053,-0.00046978,-0.00124718,-0.00157388,0.00117054,0.00033365,0.28181780,-0.08851826,-0.08767078,0.04063374,0.00138003,-0.00281394,-0.00420021,-0.00058703,0.00089525,0.00021299,0.00116189,0.00046516,0.00071127,0.00017906,0.00009301,0.00047422,0.00015821,-0.00009324,-0.00008662,0.00046186,-0.00005606,-0.00026510,-0.00002570,0.00156869,-0.00059771,-0.02698244,-0.00850336,0.01318829,0.09700175,0.08853966,0.08566718,0.03711431,-0.08890636,0.03283508,0.01487088,-0.01770076,0.00181766,0.00112294,0.00130712,-0.00007407,-0.00112073,0.00368157,-0.00090617,-0.00019404,-0.00033844,-0.00012508,0.00027531,0.00025576,-0.00003679,-0.00019245,-0.00048621,-0.00165745,-0.00067440,-0.00541573,-0.01075852,-0.00314094,0.00467649,-0.09619715,-0.04170924,0.09759282,-0.22699980,0.11824455,-0.07507845,0.00285335,-0.00397849,-0.00084384,0.00028198,0.00075121,0.00062983,-0.00024950,0.00086219,0.00006371,0.00039414,0.00009577,0.00028366,0.00032194,-0.00016656,0.00006966,0.00013592,0.00034070,-0.00009315,0.00038888,-0.00060827,-0.00036497,0.00330799,-0.00375633,0.00225206,-0.01770838,0.01577062,-0.01056468,0.23727348,0.11747354,-0.12910967,0.05644624,-0.00332583,-0.00123485,-0.00452891,-0.00124551,0.00102802,-0.00225759,0.00021360,0.00215521,0.00152989,0.00017297,-0.00001208,0.00016146,-0.00011401,-0.00024818,-0.00028592,0.00011198,-0.00010199,0.00003087,0.00016504,-0.00007035,0.00030758,0.02523481,-0.01491698,0.01273155,-0.01113119,0.00757562,-0.00635164,-0.12755539,0.13493526,-0.07375392,0.05285391,-0.08547295,-0.03218580,0.01976244,-0.01606982,0.00214069,0.00217176,-0.00588549,0.00156629,-0.00097335,0.00269419,0.00017333,0.00000711,-0.00004439,-0.00108533,-0.00104901,-0.00045312,-0.00028546,-0.00012407,0.00032928,0.00044081,-0.00076676,0.00112038,0.00956007,-0.00573687,0.00469146,0.00978314,-0.00836163,0.00533374,0.0836461

7,-0.05778354,0.09375673\\0.00000945,0.00001117,-0.00000745,0.00000825
,0.00003384,-0.00002472,0.00005493,0.00002051,0.00002461,-0.00006311,0
.00000158,0.00003241,-0.00001022,-0.00001163,-0.00001434,-0.00003244,-
0.00001218,-0.00000674,0.00002868,-0.00000421,-0.00002257,0.00001251,-
0.00001215,0.00001266,0.00000434,0.00000256,-0.00001512,0.00000224,-0.
00002142,0.00000300,-0.00001464,-0.00000808,0.00001826\\\@

Structure 22

	1	2	3
	?A	?A	?A
Frequencies --	-379.7971	113.5852	266.5041

Zero-point correction=   0.096066 (Hartree/Particle)
Thermal correction to Energy=   0.101108
Thermal correction to Enthalpy=   0.102052
Thermal correction to Gibbs Free Energy=   0.068666
Sum of electronic and zero-point Energies=   -192.671516
Sum of electronic and thermal Energies=   -192.666474
Sum of electronic and thermal Enthalpies=   -192.665530
Sum of electronic and thermal Free Energies=   -192.698916

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\29-Feb-1996\
1\\#MP2=(FULL) 6-31G* FREQ, IOP(7/33=1)\\\\1,1\
C\C,1,R2\C,2,R3,1,A3\O,1,R4,2,A4,3,D4,0\H,2,R5,3,A5,1,D5,0\H,1,R6,2,A6
,3,D6,0\H,1,R7,2,A7,3,D7,0\H,4,R8,2,A8,3,D8,0\H,3,R9,2,A9,1,D9,0\H,3,R
10,2,A10,1,D10,0\H,3,R11,2,A11,1,D11,0\\R2=1.48501982\R3=1.43337788\R4
=1.42376768\R5=1.09351421\R6=1.09064622\R7=1.09918853\R8=0.97595184\R9
=1.08700674\R10=1.10353686\R11=1.10878615\A3=123.72002016\A4=100.36992
823\A5=116.95510046\A6=112.52246158\A7=110.22022212\A8=118.54763267\A9
=115.70372806\A10=108.11320381\A11=106.62794465\D4=-58.54474006\D5=185
.43511792\D6=185.30127264\D7=62.9505171\D8=45.64907118\D9=-9.19046059\
D10=-136.94532011\D11=114.0931027\\Version=SGI-G94RevB.3\HF=-192.20859
63\MP2=-192.7675821\RMSD=4.999e-09\RMSF=1.395e-05\Dipole=-0.0186708,-0
.9599378,0.8235819\DipoleDeriv=0.305734,0.1148088,0.1607822,0.1223381,
0.2769016,0.0085625,0.0209349,-0.1340252,0.027336,0.6135098,0.065381,0
.2782484,-0.0024165,0.3109787,-0.0579729,0.195038,-0.0816674,1.1482348
,-0.2448975,-0.0519992,-0.3560726,-0.1529606,-0.2308592,-0.2511655,-0.
4580836,0.0189327,-0.7974192,-0.4755703,-0.2963626,0.1286143,-0.151255
3,-0.417431,0.1240852,0.0032505,0.1670116,-0.7540242,0.1015465,0.00255
84,-0.0139099,0.0170153,0.1544847,-0.0234634,-0.010709,0.0081965,0.082
8087,0.0328674,-0.0205144,0.0009239,-0.0057407,0.0890974,0.0180541,0.0
023425,0.0098453,0.0906956,0.0749501,0.0342829,0.0026929,0.0074831,0.0
587559,0.0580185,-0.0049663,0.0283401,0.1318657,0.3234787,0.1046461,-0
.1083854,0.0525858,0.2497648,-0.0150645,-0.027247,-0.0090942,0.3724997
,0.0986661,0.0084803,0.0110462,0.0188827,0.1228507,0.0145949,0.0595131
,-0.0124841,0.0709049,0.0664488,-0.0220385,-0.018701,0.0073446,0.19191
54,0.0484423,0.1175189,-0.0058583,0.3159905,0.1032665,0.0607573,-0.085
2389,0.0867235,0.1935409,0.0759087,0.1024079,0.010803,0.3111074\Polar=
33.6633224,1.3606908,27.3506543,2.090399,-2.4655804,41.5996903\PG=C01
[X(C3H7O1)]\NImag=1\\0.63976411,-0.06811008,0.47942642,0.06237124,0.04
316274,0.49894258,-0.09886033,0.02507135,-0.00892131,0.68228506,0.0215
0078,-0.05600310,-0.02214845,-0.02830710,0.24733431,-0.03303169,-0.025
71556,-0.23654602,-0.00618296,0.03027700,0.57643910,0.00973997,0.00558
265,-0.00151644,-0.27971225,0.00273045,-0.09118220,0.66005536,-0.01578

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21,-0.00001658,0.00000156,0.00000922,-0.00000112,-0.00000892,0.0000083
0\\\@

Structure 23

1	2	3
?A	?A	?A

Frequencies --   -240.0595   105.0590   209.7472

Zero-point correction=   0.095411 (Hartree/Particle)
Thermal correction to Energy=   0.100651
Thermal correction to Enthalpy=   0.101595
Thermal correction to Gibbs Free Energy= 0.067769
Sum of electronic and zero-point Energies=   -192.674593
Sum of electronic and thermal Energies=   -192.669354
Sum of electronic and thermal Enthalpies=   -192.668410
Sum of electronic and thermal Free Energies=   -192.702236

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\12-Apr-1996\
0\\#MP2=(FULL) 6-31G* FREQ IOP(7/33=1)\\\\1
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468472,-0.6668337893\C,0.4217006891,-0.5338796532,0.6523434691\O,1.288
5980122,0.5699376471,0.9029343458\H,-0.3630561637,-0.6723219829,1.4017
712164\H,0.98913493,-1.4729074732,0.5595835367\H,0.6525890628,0.197796
9606,-1.3689045102\H,-1.6770787554,-0.0604093193,-2.0997818337\H,-2.18
88409581,-0.575380539,-0.4093615176\H,-1.6305639814,1.0761284505,-0.77
41116564\H,0.9858807717,1.0424256124,1.7003698327\\Version=SGI-G94RevB
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7943,-0.1021138,-0.5956206,-0.0962808,-0.3361915,-0.1344723,-0.640155,
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8,-0.00282298,-0.02497295,-0.03190601,-0.07566020,0.07749131,0.1589080
8,0.00098762,-0.00135054,-0.00028633,0.00020958,0.00061471,0.00053194,
-0.00001137,-0.00099490,-0.00022123,0.00025383,-0.00004830,-0.00004165
,0.00027735,-0.00047425,-0.00013303,-0.00178278,-0.00031083,-0.0010877
9,0.07814844,0.00125595,-0.00294459,-0.00083515,-0.00392159,-0.0021352
1,0.00042768,0.01075221,-0.01634212,-0.02738994,0.04259807,-0.12472341

,-0.16960456,0.00062101,0.00215552,0.00080792,-0.00389385,-0.00407643,
-0.00278913,0.00006217,0.00060911,-0.00016289,-0.00024130,0.00013170,-
0.00006720,-0.00016906,0.00020501,0.00004863,0.00098318,0.00056828,0.0
0044245,-0.04804681,0.14655213,0.00039452,0.00037845,0.00051023,-0.002
03437,-0.00260658,-0.00401393,0.00592370,0.00925427,-0.00388740,0.1223
0686,-0.21125997,-0.33561781,0.00160409,0.00225870,0.00310317,0.001208
72,0.00322010,0.00100938,-0.00009288,-0.00061424,0.00021004,0.00011216
,0.00010779,-0.00008575,-0.00014698,0.00005246,0.00015353,-0.00069461,
0.00008682,-0.00030482,-0.12858121,0.19912219,0.33892336\\-0.00000178,
-0.00000147,0.00000990,0.00000410,0.00000261,-0.00000013,0.00000206,-0
.00001147,-0.00000678,0.00000411,0.00000849,0.00000024,0.00000390,0.00
000017,0.00000393,-0.00000712,0.00000031,0.00000303,-0.00000153,0.0000
0095,-0.00000046,0.00000052,0.00000125,-0.00000284,0.00000134,0.000000
72,-0.00000144,-0.00000008,0.00000076,-0.00000392,-0.00000551,-0.00000
233,-0.00000153\\\@

Structure 24

	1	2	3	
	?A	?A	?A	
Frequencies --	-345.5184	154.4025	176.1907	

Zero-point correction=	0.095523 (Hartree/Particle)
Thermal correction to Energy=	0.100707
Thermal correction to Enthalpy=	0.101651
Thermal correction to Gibbs Free Energy=	0.068071
Sum of electronic and zero-point Energies=	-192.673418
Sum of electronic and thermal Energies=	-192.668235
Sum of electronic and thermal Enthalpies=	-192.667291
Sum of electronic and thermal Free Energies=	-192.700871

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\02-Apr-1996\
0\\#MP2=(FULL) 6-31G* FREQ, IOP(7/33=1)\\\\1,1\
C,-0.5131620057,-0.2968683014,-0.8494013447\C,-0.5138423186,-0.2897028
718,0.6380667992\C,0.6947762623,-0.2918516517,1.3930897384\O,0.2956913
956,0.8379699472,-1.143602372\H,-1.4608135664,-0.2922677342,1.18523905
95\H,-1.5222617198,-0.243507138,-1.2635245707\H,-0.0296585352,-1.21355
29904,-1.2170408507\H,-0.2628019014,1.5370692955,-1.5312681172\H,1.602
6891983,-0.1138552382,0.8210891088\H,0.6669957995,-1.3661082228,1.7265
145489\H,0.6336879326,0.2589994006,2.3372786403\\\Version=SGI-G94RevB.3
\HF=-192.2097157\MP2=-192.7689419\RMSD=4.070e-09\RMSF=6.308e-07\Dipole
=-0.9742789,-0.5019919,0.8907281\DipoleDeriv=0.2329209,0.1054762,0.088
429,0.0469798,0.2943634,0.0812891,0.0043739,-0.1841813,0.1431839,0.626
7036,-0.0855629,0.3029531,-0.1027348,0.3838759,-0.2736788,0.2424544,-0
.1754442,0.9829647,-0.3240706,0.1587041,-0.3192383,0.3639951,-0.299844
2,0.3594286,-0.3696798,0.1493473,-0.59386,-0.3022419,-0.141588,-0.0061
696,-0.0874679,-0.648925,0.1331307,0.0113896,0.2299285,-0.7311685,0.09
71107,-0.0017361,-0.0088803,0.0250322,0.1753481,-0.0506733,-0.0098026,
0.0077319,0.079704,0.0097648,-0.0307308,-0.0079331,-0.001181,0.0619282
,0.0511131,0.0030889,0.0304504,0.0632592,0.0844917,0.0337439,-0.008648
9,0.0243581,0.0532958,0.0615671,-0.0211965,0.0172071,0.128265,0.237931
1,-0.0199944,0.0382614,0.0121584,0.4151091,-0.0720492,-0.0142443,-0.01
63798,0.3335395,0.1663003,-0.0052297,0.0139661,-0.0484827,0.1543961,-0
.0571048,0.0166901,-0.0125773,0.0910692,0.0788329,-0.0360089,-0.083080
6,-0.1787816,0.2112924,-0.1477457,0.0463067,-0.0281469,0.2602698,0.092

2563,0.0229265,-0.0096587,-0.0538755,0.1991602,-0.0852768,0.0906197,-0
.0179355,0.2427732\Polar=32.7145829,-0.0590527,29.4334992,4.2594689,-4
.2519626,38.6473227\PG=C01 [X(C3H7O1)]\NImag=1\\0.62093995,-0.06448535
,0.48128864,0.08377537,0.01833497,0.49893041,-0.10126504,0.02215662,-0
.00601259,0.69276032,0.01979136,-0.05300751,-0.02347222,0.00945942,0.2
4126820,-0.02986495,-0.02502510,-0.23152650,-0.01176051,0.03192336,0.5
7726583,0.00941762,0.00129167,-0.00522818,-0.29272566,-0.01698611,-0.0
9211872,0.65748060,-0.02154476,0.01225838,0.00078316,-0.02427818,-0.05
314219,-0.04277845,0.06242570,0.41445163,-0.02811201,0.01156434,-0.013
67711,-0.08879587,-0.02261083,-0.15108134,-0.04163950,0.05889542,0.600
50672,-0.13273124,-0.05411265,-0.02631468,-0.00565441,-0.00733396,0.02
488613,-0.00092033,0.00709521,-0.00047491,0.34621968,-0.08886324,-0.18
393311,0.02841830,-0.01915953,-0.03198406,0.02497217,0.00084957,0.0035
5021,0.00241098,-0.08069567,0.50787708,0.01478513,0.08743836,-0.056487
86,0.02175934,0.02111810,-0.00596749,-0.00381504,0.00876564,-0.0067704
1,0.09963472,-0.22418511,0.13091670,0.00632432,-0.00171043,-0.00361602
,-0.27812244,0.00191112,0.12172087,-0.01775793,-0.00262217,0.01520915,
0.00068267,0.00035077,-0.00000878,0.28780200,0.00141616,0.03415229,0.0
1485820,-0.00538999,-0.07521134,-0.00546433,0.00628819,0.01235436,-0.0
0632915,0.00199259,0.00217528,-0.01129812,0.00061979,0.02377741,0.0227
1830,-0.00613233,-0.00500015,0.12760244,0.00350933,-0.13991094,-0.0204
2380,-0.00252057,0.01435590,0.00076466,0.00372826,-0.00187498,-0.12939
868,0.00041794,0.13672924,-0.29551946,0.02006802,-0.10108465,0.0057425
5,-0.00043397,0.00460088,0.00041082,0.00157642,0.00126731,-0.01409626,
-0.00664074,-0.00291855,0.00080403,-0.00105691,-0.00011684,0.31302930,
0.02496320,-0.05765755,0.01323176,0.00062902,-0.00168434,-0.00318560,-
0.00025213,0.00244572,0.00095217,-0.03237934,-0.00687744,-0.01005706,0
.00018525,-0.00110770,0.00034080,-0.01498103,0.06188940,-0.09663260,0.
00969429,-0.09470342,-0.03648446,0.00568987,-0.01719819,0.00288951,-0.
00316339,-0.00534680,0.01372793,0.00206745,0.00463990,0.00005723,-0.00
077586,0.00147736,0.10522812,-0.01134834,0.10191657,-0.10991249,0.1103
2523,0.03936857,0.00037166,-0.00061325,0.00016149,0.00083509,0.0018554
0,-0.00120937,0.00813897,-0.02620777,-0.00137362,0.00042644,-0.0002713
5,-0.00004582,-0.01147833,0.02418789,0.01163506,0.11306039,0.10247463,
-0.20793026,-0.06437306,-0.00150425,0.00059588,-0.00908912,0.00121454,
-0.00108041,0.00207125,0.00470906,-0.03203202,-0.00284309,-0.00050187,
-0.00447614,0.00023628,0.00066753,0.00001852,-0.00178477,-0.10547130,0
.24706301,0.04017350,-0.08792701,-0.08822146,0.02108324,-0.02871012,-0
.01642171,-0.00025505,0.00581159,0.00243821,-0.00562860,0.01400770,0.0
0976847,-0.00095548,0.00350616,-0.00398053,-0.00697522,0.01195103,0.00
708085,-0.04742912,0.08057986,0.08944541,0.00581545,-0.03516478,0.0192
2055,-0.00202525,-0.00384757,-0.00461916,0.00028782,-0.00114905,0.0012
9912,-0.20272823,0.22070596,-0.12726620,-0.00003580,0.00176623,0.00059
799,0.00075525,-0.00230878,0.00044976,-0.00081494,-0.00195722,0.000617
22,0.19757365,0.02098267,-0.02139207,0.01353011,-0.00105062,-0.0029958
8,0.00166585,-0.00056936,0.00099734,-0.00144241,0.16202539,-0.25893465
,0.13292986,0.00012015,-0.00131300,-0.00009188,0.00071429,0.00313763,-
0.00132565,-0.00326812,-0.00383731,0.00262579,-0.17889002,0.28456649,-
0.00448827,-0.00008066,-0.00853920,0.00031921,0.00514652,-0.00056764,-
0.00046530,0.00100827,-0.00105660,-0.10353571,0.14929960,-0.07558780,0
.00028505,-0.00111986,-0.00044342,-0.00040238,-0.00156756,0.00247504,-
0.00161681,-0.00423580,0.00123884,0.10991692,-0.14823013,0.08323752,0.
00004232,0.00060502,0.00102433,-0.02543559,-0.00392788,0.01380972,-0.2
5675236,-0.04560841,0.12999843,0.00103458,-0.00011635,0.00039370,-0.00
182422,-0.00162046,-0.00317139,0.00017406,-0.00003667,0.00023215,-0.00

012540,-0.00007697,-0.00028586,0.00037665,0.00036813,0.00022701,0.2758
5213,0.00055549,-0.00319602,-0.00088982,0.00722429,-0.00208435,0.00146
781,-0.04591221,-0.05573453,0.01917745,-0.00081699,-0.00064644,0.00114
876,0.00119545,0.00697735,0.00049338,-0.00003726,-0.00028781,0.0000865
3,-0.00001296,0.00015888,-0.00088742,0.00000339,-0.00001692,-0.0000068
0,0.04688000,0.05466318,-0.00040871,-0.00002868,0.00072198,-0.01998469
,-0.00501281,0.01791724,0.13560110,0.02091382,-0.14492590,-0.00059271,
0.00063207,-0.00220032,-0.00340932,0.00218963,-0.00258845,0.00027335,0
.00002932,0.00008952,0.00033868,-0.00024584,0.00007461,0.00026930,0.00
023149,-0.00026642,-0.13890721,-0.02612963,0.14455731,0.00347122,-0.00
221381,-0.00184075,0.00191789,0.02046309,0.00111815,-0.04105761,0.0187
1930,-0.00888264,-0.00095958,-0.00164490,-0.00037414,0.00062523,-0.004
59261,0.00127003,-0.00026329,-0.00017316,0.00031783,-0.00076448,0.0006
6089,-0.00113424,0.00031776,-0.00018374,0.00015933,0.00303639,-0.02410
535,0.00782331,0.03219250,0.00242903,-0.00270203,-0.00136050,0.0063136
7,-0.01941785,0.01204973,-0.00816362,-0.22978658,0.06675288,-0.0003655
2,0.00068522,-0.00128527,0.00069347,0.00363873,0.00018090,0.00008104,0
.00018559,0.00033400,-0.00037145,0.00132264,-0.00105194,0.00042000,-0.
00017191,-0.00014821,0.00221405,-0.00399448,-0.00048104,-0.00501262,0.
26885373,0.00176820,-0.00364129,-0.00127558,-0.00330513,0.01752477,-0.
01153417,0.00259286,0.08259829,-0.04316090,-0.00217155,-0.00086776,0.0
0063767,0.00001571,-0.00005017,0.00047343,-0.00020157,-0.00050751,0.00
016157,-0.00012532,-0.00005540,-0.00138030,-0.00004954,-0.00007848,-0.
00052649,-0.00124613,0.01221842,-0.00527046,-0.00063846,-0.08075476,0.
05791918,-0.00658266,0.00324045,0.00070805,0.00443598,-0.01848226,-0.0
2793390,-0.05921806,0.00353053,0.02134029,0.00101414,0.00142190,-0.000
81656,0.00107569,0.00084836,0.00020310,0.00044132,0.00016575,-0.001420
52,0.00026310,-0.00021503,0.00078961,0.00047765,-0.00024878,-0.0003990
4,0.00362143,0.01502616,0.01899690,0.00148396,0.00176195,0.00336092,0.
05298744,0.00228079,0.00211926,0.00093910,0.00559956,-0.00233657,0.013
46369,-0.00018624,-0.10631392,-0.13144211,-0.00011812,0.00011992,-0.00
173208,-0.00024152,-0.00096725,-0.00016211,0.00004261,-0.00006202,0.00
052587,-0.00015232,0.00019722,0.00009436,0.00042185,-0.00003971,-0.000
06537,0.00131954,0.00416114,0.00790167,-0.00191710,-0.01861307,-0.0263
8610,-0.00704904,0.12173499,-0.00371396,-0.00419690,-0.00022112,-0.004
42099,-0.00510597,-0.02097509,0.02286212,-0.13031376,-0.25128177,-0.00
029529,-0.00048366,0.00292613,0.00010029,0.00406556,0.00076254,0.00032
956,0.00016099,-0.00059240,0.00029625,-0.00026032,-0.00004240,-0.00043
595,0.00018545,0.00003619,-0.00207476,-0.00667868,-0.00810912,0.002181
58,0.00576420,0.00395606,-0.01482884,0.13686308,0.27354097\\0.00000019
,0.00000095,-0.00000010,0.00000012,-0.00000062,0.00000178,-0.00000056,
-0.00000170,-0.00000148,0.00000012,0.00000015,-0.00000036,-0.00000010,
-0.00000042,-0.00000005,0.00000001,0.00000003,0.00000007,-0.00000007,0
.00000013,0.,0.00000010,-0.00000003,-0.00000011,0.00000062,-0.00000007
,0.00000014,0.00000009,0.00000012,0.00000019,-0.00000050,0.00000146,-0
.00000007\\\@

Structure 25

	?A	?A	?A	?A	?A
Frequencies ---	-202.2282	234.0467	269.6197	338.0039	413.3676

Zero-point correction=	0.095633 (Hartree/Particle)
Thermal correction to Energy=	0.100556
Thermal correction to Enthalpy=	0.101500

Thermal correction to Gibbs Free Energy=   0.068662
Sum of electronic and zero-point Energies=   -192.676459
Sum of electronic and thermal Energies=   -192.671537
Sum of electronic and thermal Enthalpies=   -192.670593
Sum of electronic and thermal Free Energies= -192.703430

1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\22-Feb-1996\
1\\#MP2=(FULL) 6-31G* FREQ,IOP(7/33=1) GUESS=READ\\
\\1,1\C\C,1,R2\C,2,R3,1,A3\O,3,R4,2,A4,1,D4,0\H,3,R5,2,A5,1,D5,0\H
,3,R6,2,A6,1,D6,0\H,2,R7,3,A7,1,D7,0\H,1,R8,2,A8,3,D8,0\H,1,R9,2,A9,3,
D9,0\H,1,R10,2,A10,3,D10,0\H,4,R11,3,A11,2,D11,0\\R2=1.4234213\R3=1.47
797396\R4=1.41761559\R5=1.09351043\R6=1.1017111\R7=1.09134977\R8=1.090
81637\R9=1.0913079\R10=1.12881517\R11=0.97573201\A3=125.20831204\A4=10
1.99051913\A5=112.47373545\A6=108.85980835\A7=115.08344073\A8=115.5097
9071\A9=115.54950907\A10=96.15766413\A11=110.67517619\D4=-117.81179624
\D5=-0.18745968\D6=120.03382189\D7=170.12856034\D8=-164.50721\D9=-25.5
2940439\D10=85.38533975\D11=248.19618891\\\Version=SGI-G94RevB.3\HF=-19
2.2122444\MP2=-192.7720926\RMSD=1.546e-09\RMSF=3.786e-05\Dipole=-0.696
8523,0.8516571,-0.3664906\DipoleDeriv=-0.0889417,0.0115385,0.0223089,-
0.1100287,-0.1853282,-0.7613673,-0.1022337,-0.2104316,-0.7069941,0.431
9902,0.0300043,0.2036189,0.0189499,0.2688428,0.1148551,0.3275579,0.089
4801,1.2908514,0.1068925,-0.0605767,-0.1279862,-0.0500515,0.3027006,-0
.1775925,-0.1822463,-0.2521489,0.1259703,-0.5174888,-0.0530934,-0.1173
768,0.006434,-0.474395,0.2558595,-0.1172322,0.3364672,-0.7084212,0.092
4615,-0.0058248,0.037965,0.0164978,0.0762936,0.035259,0.0530858,0.0353
411,0.0278484,0.1196075,0.0349386,0.0107203,0.0546604,0.0673044,0.0715
593,0.0146627,-0.0051001,0.1008697,0.1166576,0.0079385,-0.0070528,-0.0
12773,0.0964804,0.0006106,-0.0066152,-0.0001101,0.0748948,0.1208314,-0
.0007132,0.0684935,0.0158795,0.187345,0.1172786,0.0374586,0.0032376,0.
1551139,0.0722146,-0.0182331,-0.0663056,0.0015267,0.1640819,0.0994136,
-0.041502,-0.0077039,0.1616388,0.2106427,0.0060638,-0.0087693,0.045257
7,0.2245059,0.3045722,-0.0372135,0.0939963,0.0559986,0.3351324,0.04795
73,-0.0156159,0.0136472,0.2721686,-0.0604481,0.0542779,-0.0830277,0.42
22293\Polar=31.0592781,-0.1080619,27.6904227,4.5109554,-2.0959286,44.3
503319\PG=C01 [X(C3H7O1)]\NImag=1\\0.65629280,0.02524865,0.40137013,0.
00715464,-0.09790930,0.61539396,-0.11629864,-0.00619924,0.00941431,0.6
3608886,-0.00240410,-0.06488692,0.02696376,0.04535690,0.25255365,0.001
05656,0.05713863,-0.33724952,-0.04762618,-0.03521347,0.64609039,0.0055
7928,0.01092020,-0.00274212,-0.21881743,-0.01200395,-0.06185899,0.5977
2669,-0.01884027,0.03113129,-0.00582723,0.00336822,-0.06168487,-0.0218
2472,0.00520385,0.48173859,-0.02888181,0.00446448,-0.01844506,-0.05115
596,-0.02195945,-0.11536534,-0.08163279,0.04980568,0.54065941,0.001832
25,-0.01027190,-0.00174128,-0.00017067,0.02418260,-0.01070900,-0.05846
483,-0.01334523,0.01865161,0.06095100,0.00200900,0.00336702,-0.0004050
5,0.01222241,-0.03072231,0.02874401,-0.00873348,-0.20105528,0.03438115
,-0.00310634,0.31984967,0.00081411,-0.01541686,-0.00237434,-0.00836739
,0.03120058,-0.01742847,0.03067186,0.12966438,-0.12686893,-0.10707309,
-0.04221579,0.61629624,0.00330020,-0.00210105,0.00123551,-0.02817276,0
.00325795,0.01298096,-0.25191367,0.01005494,0.12642381,0.00668568,-0.0
0434172,-0.00014790,0.27059183,0.00082804,-0.00188950,-0.00017690,-0.0
0128267,0.00012163,-0.00257376,0.01240071,-0.04817782,-0.00932591,-0.0
02339653,-0.00735865,0.02556023,-0.00595417,0.05886759,-0.00057885,-0.0
0132518,0.00196066,-0.02631090,0.00215161,0.01008770,0.12820385,-0.007
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51996,0.00050273,-0.08610676,0.06612570,0.47755304\\-0.00005801,0.0000
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.00000136\\\@

Structure 29

1	2	3
?A	?A	?A

Frequencies --   -95.5704   164.3975   272.2193

Zero-point correction=   0.094600 (Hartree/Particle)
Thermal correction to Energy=   0.099692
Thermal correction to Enthalpy=   0.100637
Thermal correction to Gibbs Free Energy= 0.067442
Sum of electronic and zero-point Energies=   -192.684435
Sum of electronic and thermal Energies=   -192.679343
Sum of electronic and thermal Enthalpies=   -192.678399
Sum of electronic and thermal Free Energies=   -192.711593

Test job not archived.
1\1\ UOFC-OXYGEN\Freq\RMP2-FU\6-31G(d)\C3H7O1(1+)\JMCOXON\23-Mar-1996\
1\\# MP2=(FULL) 6-31G* FREQ, IOP(7/33=1)\\
\1,1\C\C,1,R2\C,2,R3,1,A3\O,3,R4,2,A4,1,D4,0\H,3,R5,2,A5,1,D5,0\H,3
,R6,2,A6,1,D6,0\H,2,R7,3,A7,1,D7,0\H,1,R8,2,A8,3,D8,0\H,1,R9,2,A9,3,D9
,0\H,1,R10,2,A10,3,D10,0\H,4,R11,3,A11,2,D11,0\\R2=1.43948254\R3=1.444
01879\R4=1.38856982\R5=1.11451764\R6=1.11451004\R7=1.09396554\R8=1.104
77639\R9=1.08864478\R10=1.10477149\R11=0.97423409\A3=124.64811653\A4=1
10.33480312\A5=105.62829793\A6=105.63220808\A7=116.52008128\A8=107.608
49016\A9=115.44875463\A10=107.61122233\A11=110.52921432\D4=-180.002427
52\D5=-54.54246213\D6=54.53354202\D7=-180.00030645\D8=-125.18852036\D9
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.00004018,0.21306868\\-0.00011391,0.00000031,-0.00003927,-0.00008976,-
0.00000044,-0.00020628,0.00008863,-0.00000012,-0.00020616,-0.00002448,
-0.00000095,0.00027187,-0.00004103,-0.00005005,0.00000213,-0.00004071,
0.00005023,0.00000198,0.00001408,0.00000031,0.00003183,0.00004927,0.00
002414,0.00000175,0.00001652,0.00000002,-0.00001074,0.00004917,-0.0000

2419,0.00000194,0.00009222,0.00000075,0.00015095\\\@