

## **Substituent effects on the stability of extended benzylic carbocations: a computational study of conjugation**

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### **Supporting Information**

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**Table S1. Calculated Energies**

Molecule	Energy <sup>a</sup>
1	-614.90602
1 <sup>+</sup>	-614.06963
2	-654.01020
2 <sup>+</sup>	-653.16851
3	-654.00715
3 <sup>+</sup>	-653.16475
4	-768.49957
4 <sup>+</sup>	-767.65485
5	-271.43834
5 <sup>+</sup>	-270.54466
6	-425.03383
6 <sup>+</sup>	-424.15872
7	-425.03572
7 <sup>+</sup>	-424.15814
8	-539.52105
8 <sup>+</sup>	-538.66795
9	-539.52203
9 <sup>+</sup>	-538.65044
10	-539.52340
10 <sup>+</sup>	-538.67157
11	-539.52366
11 <sup>+</sup>	-538.65945
12	-539.52262
12 <sup>+</sup>	-538.65265
13	-539.52289
13 <sup>+</sup>	-538.66233
14	-539.51811

<b>14<sup>+</sup></b>	-538.65408
<b>15</b>	-539.52006
<b>15<sup>+</sup></b>	-538.65520
<b>16</b>	-539.52662
<b>16<sup>+</sup></b>	-538.65874
<b>17</b>	-539.52581
<b>17<sup>+</sup></b>	-538.65447
<b>18</b>	-539.52582
<b>18<sup>+</sup></b>	-538.65240
<b>19</b>	-539.52423
<b>19<sup>+</sup></b>	-538.66469
<b>20</b>	-539.52447
<b>20<sup>+</sup></b>	-538.65126
<b>21</b>	-539.52499
<b>21<sup>+</sup></b>	-538.66159
<b>22</b>	-654.01285
<b>22<sup>+</sup></b>	-653.17123
<b>23</b>	-654.00445
<b>23<sup>+</sup></b>	-653.15819
<b>24</b>	-654.00662
<b>24<sup>+</sup></b>	-653.15182
<b>25</b>	-654.01030
<b>25<sup>+</sup></b>	-653.17635
<b>26</b>	-768.50056
<b>26<sup>+</sup></b>	-767.66970
<b>27</b>	-768.47924
<b>27<sup>+</sup></b>	-767.63973
<b>28</b>	-768.48826
<b>28<sup>+</sup></b>	-767.66433

<b>29</b>	-768.49978
<b>29<sup>+</sup></b>	-767.67434
<b>30</b>	-654.00875
<b>30<sup>+</sup></b>	-653.15794
<b>31</b>	-654.01544
<b>31<sup>+</sup></b>	-653.16336
<b>32</b>	-768.50504
<b>32<sup>+</sup></b>	-767.66412
<b>33</b>	-882.97992
<b>33<sup>+</sup></b>	-882.16192
<b>34</b>	-882.98162
<b>34<sup>+</sup></b>	-882.14752
<b>35</b>	-997.45038
<b>35<sup>+</sup></b>	-996.62077
<b>36</b>	-1226.41026
<b>36<sup>+</sup></b>	-1225.58272
<b>37</b>	-1226.41023
<b>37<sup>+</sup></b>	-1225.57016

<sup>a</sup> B3LYP/6-31G(d) + zpve in Hartrees

**Table S2** GAUSSIAN 98 Archive entries

**1**

```
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1830132282,-0.4002728583,-0.1458643444\C,-0.4919633679,0.0870981218,-1
.2632631181\C,0.8295389822,0.5272181479,-1.0586443884\O,1.4746001222,0
.9986244356,-2.1706242104\C,2.809504118,1.4540852033,-2.0376763132\O,-
2.4641218495,-0.812726963,-0.4026158812\C,-3.2438498801,-1.3250150634,
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,-0.0192682305,2.4806145937\C,0.7125326335,-0.5074144921,3.629290637\H
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9731468344\H,3.1154937975,1.7763738102,-3.0350866984\H,3.4783328513,0.
6538505881,-1.6941903832\H,2.8808627592,2.302926708,-1.3448359343\H,-4
.2104942476,-1.5860655702,0.2268548634\H,-2.7917091044,-2.2246062211,1
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0.7749891199,-2.6024133787\H,-1.5035208922,-0.8678481401,-2.9162673052
\H,-0.4695750543,0.5015929508,-3.3749707851\H,1.4259675655,-0.42149649
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1<sup>+</sup>

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2

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Supplementary Material for Organic & Biomolecular Chemistry  
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2<sup>+</sup>

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### 3

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3<sup>+</sup>

1\1\MF (MLIB83-EXE) -BOSON\Freq\RB3LYP\6-31G(d)\C13H13O2(1+)\THEIS\11-May-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\and et na ftalen derivat\1,1\C, -2.5055452704, -0.0432215657, -0.9353576415\C, -2.3917821598, -0.9574559338, 0.1142837467\C, -1.1787957223, -1.1388309775, 0.7895887373\C, -0.0306264454, -0.3881321083, 0.4148659063\C, -0.1802086511, 0.5383551999, -0.6625930615\C, -1.4119709604, 0.7049060988, -1.3288822714\C, 1.2832170796, -0.5091225253, 1.0634484977\C, 2.3576977294, 0.3208497173, 0.5719210819\C, 2.2175278031, 1.2063282005, -0.4574839551\C, 0.9530779682, 1.3274975795, -1.0861087971\C, 1.6142685784, -1.3350708003, 2.1018535435\O, -1.0391303236, -2.015440567, 1.8079148579\C, -2.1606638613, -2.8027253536, 2.2342365795\O, 0.7306993816, 2.1543875107, -2.0821933551\C, 1.7710335442, 3.0094455656, -2.6136789983\H, -3.4592536888, 0.0749184435, -1.4393313661\H, -3.2613047997, -1.5331757676, 0.4058888149\H, -1.4895252809, 1.4159655297, -2.1411099577\H, 3.3248456225, 0.2252044234, 1.0569570082\H, 3.0585064672, 1.8038244508, -0.7850367574\H, 0.9101001791, -2.0076699797, 2.5658055174\H, 2.6294056931, -1.3240979706, 2.4887223607\H, -1.7872023503, -3.4151180941, 3.0546013205\H, -2.5146577612, -3.4497463857, 1.4250871445\H, -2.9732153675, -2.1632701331, 2.5941795625\H, 1.2894641879, 3.5672105495, -3.4146243169\H, 2.5883157384, 2.4041813394, -3.0136592223\H, 2.1285911025, 3.6932594627, -1.8398123394\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-653.3961094\RMSD=4.763e-09\RMSF=1.846e-05\Dipole=0.9365604, 0.3977428, -0.0689751\DipoleDeriv=0.2710002, -0.1165766, 0.2601127, 0.1086654, -0.1413625, 0.1263291, 0.0123772, 0.0379187, -0.1021731, 0.2204293, 0.1756882, -0.0627925, -0.0971285, -0.0521058, -0.1035387, 0.2371948, 0.0034752, -0.0223706, -0.522774, -0.143907, -0.1127037, 0.2046946, 0.7734965, -0.5855038, -0.4958543, -0.72208

08, 0.7670573, 0.0081169, -0.2151467, 0.2428535, 0.2453353, -0.002257, 0.0900388, -0.2633278, -0.0905533, -0.0116313, -0.5577101, -0.4559355, 0.2873171, -0.4896193, -0.3493756, 0.1787204, 0.3244286, 0.1919098, -0.0958721, -0.0959475, 0.2486836, -0.2774792, -0.0919647, -0.0085544, -0.1209547, 0.0970357, 0.0126159, -0.0615441, 0.2281218, 0.0034619, 0.0703896, 0.0556315, -0.4323323, 0.5402617, 0.0126731, 0.5200052, -0.5278999, 0.0717446, 0.1514738, -0.1475033, -0.1992723, 0.4821654, -0.5830636, 0.238405, -0.4454243, 0.6066259, -0.4137001, 0.4419719, -0.5758171, 0.2742409, -0.3400334, 0.2779987, -0.3914156, 0.3437661, -0.716536, 1.2006632, -0.2345279, 0.6125551, 0.506871, 1.1815311, -0.7743174, -0.2027821, -1.0651228, 1.3877548, 0.0681102, -0.0802468, 0.1469755, 0.0682887, 0.1768394, -0.2572255, -0.0157836, -0.3160095, 0.2599738, -0.5034853, -0.2518914, 0.1898455, -0.5361035, -1.0269144, 0.6095916, 0.5021637, 0.7209439, -0.8767839, 0.6517536, 0.4510511, -0.3622974, 0.3101746, 0.6350995, -0.2347847, -0.2075068, -0.1796621, 0.427085, -0.4461703, -0.032829, -0.0434277, -0.4826208, -1.2655084, 0.9340599, 0.4511722, 1.1105242, -1.2875576, 0.4700155, 0.4403068, -0.4079528, 0.2568399, 0.7302755, -0.3984461, -0.2062435, -0.326316, 0.5540252, 0.0056838, -0.0002085, -0.0467127, -0.0014657, 0.0992558, 0.0281145, -0.0453093, 0.0286211, 0.0761105, 0.0534344, -0.0547272, 0.0302604, -0.0513029, 0.0779389, 0.0367031, 0.0264701, 0.035346, 0.1011874, 0.1040277, -0.0191747, 0.0135997, -0.0007338, 0.0781656, 0.049143, -0.0066483, 0.0419062, 0.0744478, 0.0355326, -0.0109168, -0.0189095, 0.0148498, 0.0890527, 0.0336426, -0.0471978, 0.0235241, 0.0699314, 0.0556446, -0.0430712, 0.0129478, -0.0425956, 0.0850383, 0.0475736, 0.0123242, 0.0472896, 0.0962407, 0.0995166, 0.0140348, -0.0274163, -0.0225101, 0.1197477, 0.0024123, 0.0127263, 0.0170119, 0.1162763, -0.0057093, -0.0208077, -0.0260494, -0.0502376, 0.1037931, -0.0029367, 0.0060507, 0.0087263, 0.1118254, 0.0466355, 0.0350108, -0.058313, -0.0182903, 0.0327221, 0.063564, 0.0003134, 0.084498, 0.004203, -0.0175143, -0.1017422, 0.057275, -0.0256731, -0.002379, -0.0071764, -0.0468222, -0.0923257, -0.0530044, -0.0688589, -0.0393801, 0.1028654, 0.0741377, -0.0529225, -0.0221235, -0.0014752, -0.0112386, 0.0489006, 0.0443931, 0.016733, -0.0435153, -0.0176227, 0.0551704, 0.0518656, -0.0057994, 0.0652739, 0.0346777, -0.0216516, -0.0508183, 0.1086997, 0.0440638, -0.0559206, 0.0044645, 0.0154851, 0.0115662, 0.0623566, 0.018692, -0.1065135, 0.0751974, -0.0366567, 0.0093629, 0.015593, -0.0126498, -0.0561842, -0.0433146, Polar=179.3711716, 27.9039302, 135.6778645, 17.2994086, -75.4954578, 146.8750032, PG=C01 [X(C13H13O2)] \NImag=0\\

#### 4

1\1\MF (MLIB83-EXE) -MESON\Freq\RB3LYP\6-31G(d) \C14H16O3\THEIS\04-May-2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Naftalenderivat\0, 1\C, 0.2432806538, 0.4136579621, -0.5315023843\C, -0.8226185311, -0.0471854623, 0.3038255017\C, -0.5119030816, -0.7860555519, 1.4798452409\C, 0.8005414592, -1.0404158437, 1.812307793\C, 1.8903851751, -0.5961231538, 0.9939694294\C, 1.5875210199, 0.101141671, -0.1568653985\O, 2.6068096993, 0.5586494182, -0.9763587813\C, 3.0030028232, -0.3684437201, -1.9872307843\O, 1.1942337911, -1.7301310154, 2.9249766242\C, 0.1923582361, -2.2075524969, 3.8072948712\C, 3.3068833633, -0.8882063027, 1.4158222616\C, -0.0711772288, 1.1721776597, -1.6821048345\C, -1.3788759975, 1.4564787376, -2.0209361652\C, -2.4350825865, 0.9841973271, -1.2024916364\C, -2.1545324053, 0.2507001185, -0.0621209362\O, -3.7589956656, 1.2127547723, -1.4616296194\C, -4.1050092336, 1.9718634118, -2.6076716979\H, -1.3283407787, -1.1308242979, 2.1039224611\H, 3.7801913607, 0.127465734, -2.5741914814\H, 2.1607762594, -0.6284289467, -2.6414910933\H, 3.4101977762, -1.2889305493, -1.5489736655\H, 0.7216784573, -2.7150100421, 4.6160793612\H, -0.4774431735, -2.919204741, 3.3068060984\H, -0.4040136166, -1.3839804291, 4.2214751393\H, 3.5309207298, -1.9613054938, 1.3628617972\H, 3.4699279173, -0.5888385485, 2.4566760266\H, 4.01263

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4<sup>+</sup>

1\1\MF (MLIB83-EXE) -NEUTRON\Freq\RB3LYP\6-31G(d)\C14H15O3(1+)\THEIS\04-  
May-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Naftal

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, -0.8524504,0.9786411,0.1535577,0.292988,0.4274772,0.2839225,-0.119371  
1,0.7152457,-0.2490646,1.7954463,-1.5613632,0.1359555,-0.8403709,-0.12  
3665,-0.4039776,-0.2027863,-0.6485211,0.0174144,-0.8450382,1.0377669,-  
0.2312699,0.4666441,-0.4163549,0.3836114,-0.1746568,0.1023247,-0.01825  
51,0.2887059,-1.4510658,-0.8604896,0.3883317,-0.8668309,-0.9076865,0.3  
372205,0.3570633,0.3097326,-0.5695879,0.9052899,0.4162335,-0.1334873,0  
.2932777,0.5062523,-0.0479227,0.3457615,0.2570712,0.1626389,0.0566684,  
0.072811,0.0261143,0.0823602,-0.0020084,-0.0383144,-0.0641557,-0.11621  
86,0.4441831,-0.0640177,0.0929759,-0.2577175,-0.0510774,0.0389036,-0.3  
306983,0.2406375,-0.0314998,0.5791751,-0.2163805,0.0851772,-0.4267512,  
0.0510062,-0.0518874,-0.1494347,-0.3936493,-0.0850772,-0.6781169,0.795  
5039,0.4547982,-0.5055095,0.3514191,0.7511843,-0.9226512,0.034454,-0.5  
84846,2.4416368,-0.3761564,-0.3062764,0.787562,-0.2496891,-0.5986139,0  
.789993,0.5317897,0.6030844,-1.1653215,-0.4115959,-0.0406365,-0.212708  
4,-0.0745046,-0.4510668,0.4910456,-0.1047311,0.5935674,-2.6388026,0.37  
16078,-0.1362844,0.6779454,0.0149451,0.236704,0.2595649,0.1428833,-0.1  
213896,1.0824177,0.0338781,-0.0649225,-0.0250336,-0.0503576,0.1072781,  
0.0027588,-0.062472,-0.017137,0.0446694,-0.000356,-0.0006809,-0.060147  
5,-0.0242639,0.0419581,-0.041391,-0.064773,-0.032371,0.0325177,-0.0153  
723,0.0221924,-0.0278567,0.051167,0.0453844,0.040514,0.088242,-0.01933  
7,-0.0558759,-0.0276214,-0.0659985,-0.0027496,0.0642932,-0.0651884,0.0  
782779,0.0084644,0.0442899,0.0450228,0.0199692,-0.0573038,0.0212188,-0  
.0651365,0.0506356,0.03329,0.0516436,0.0530969,0.0230858,-0.0451904,0.  
0207835,0.0740503,0.0004619,0.0068625,-0.0288799,-0.0628384,-0.1364305  
,0.0127704,-0.0238818,-0.0283163,0.0074867,0.063676,-0.060988,0.036227  
9,-0.1262149,-0.027987,0.0625416,0.0850462,-0.0184233,-0.0215607,-0.02  
99175,0.1129435,-0.0195793,-0.0121112,-0.0092571,0.1376463,0.0577577,-  
0.0406608,-0.0127515,-0.0279617,0.0926109,0.0067646,-0.013751,-0.00140  
34,0.1350896,0.0543189,-0.0299273,-0.0162597,-0.0230186,0.1034664,-0.0

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00341,-0.0466349,-0.0232509,0.0569468,0.0781027,-0.0433504,0.0078247,-  
0.0480586,0.0978654,0.0206746,0.0067536,0.0254219,0.0712201,0.0344324,  
-0.0516604,-0.0660244,-0.0617596,0.0993583,-0.0159907,-0.0344635,0.004  
4794,0.0432185,0.0712167,-0.0255296,0.0153055,-0.0215654,0.075614,0.05  
01708,-0.0015308,0.040093,-0.0484391,-0.0529123,0.0633501,-0.1109371,0  
.0280482,0.0572991,-0.0951255,0.0620677,-0.0366593,-0.0255706,0.033356  
8,0.0453914,-0.1378608,0.000853,-0.0632223,-0.0924512,-0.0253972,0.049  
7261,0.006457\Polar=154.8871362,50.9506661,119.4853593,-3.7687031,-63.  
6783351,282.9544631\PG=C01 [X(C14H15O3)]\NImag=1\

5

1\1\MF(MLIB83-EXE)-MESON\Freq\RB3LYP\6-31G(d)\C7H8\THEIS\15-May-2004\0  
\# B3LYP/6-31\* OPT=(CALCALL,NORAMAN)\toluen\0,1\C,1.1118481888,-0.4  
107414274,0.2803363512\C,1.2265973285,-0.3979476153,-1.110380115\C,0.1  
505208234,0.0125303188,-1.8990638962\C,-1.0388890737,0.4077867205,-1.2  
846253018\C,-1.1479256321,0.3929612218,0.106529362\C,-0.0746016922,-0.  
0127946344,0.910800334\C,-0.1849472357,0.0029778795,2.4183556719\H,1.9  
545688384,-0.7360139333,0.8869325326\H,2.1560839177,-0.7131992031,-1.5  
778465393\H,0.236566433,0.0201879588,-2.9823953862\H,-1.8855361986,0.7  
242294233,-1.888700231\H,-2.0802931435,0.6990108935,0.5765976945\H,-1.  
215047071,-0.1713387843,2.7474405801\H,0.1277595163,0.9718433509,2.830  
729163\H,0.4502814655,-0.7633544868,2.8755277499\Version=HP-PARisc-HP  
UX-G98RevA.11.3\HF=-271.5666503\RMSD=5.725e-09\RMSF=2.253e-07\Dipole=-  
0.0049257,0.0132033,0.1249795\DipoleDeriv=0.0451343,-0.0626284,0.12678  
6,-0.0614199,-0.104052,-0.0508192,0.0845953,-0.0310939,-0.1131198,0.09  
39999,-0.0723744,-0.0750025,-0.0703876,-0.0770572,0.0168107,-0.0508857  
,0.0145543,0.0037046,-0.101345,-0.0066304,-0.0163875,-0.0066494,-0.120  
0533,-0.0051286,-0.0164694,-0.0053776,0.0890139,0.0777662,-0.0614695,0  
.0819118,-0.0625771,-0.0816628,-0.0388404,0.0618576,-0.0251486,0.02453  
04,0.072042,-0.0688821,-0.1016381,-0.0694366,-0.1023789,0.0305409,-0.0  
564269,0.0193166,-0.1416925,-0.0725015,0.0194472,-0.0046385,0.0145393,  
-0.0218344,0.0788794,-0.0273171,0.015076,0.345028,0.1193103,-0.0016213  
, -0.0286083,0.0060129,0.113453,-0.0977396,0.0066572,0.0015097,0.038155  
3,-0.0406675,0.0534718,-0.0772595,0.0563413,0.0802496,0.0360522,-0.091  
1394,0.0389613,-0.0102431,-0.0738033,0.062273,0.0770305,0.0644589,0.08  
65705,-0.0212925,0.0692023,-0.0206906,0.0144858,0.0623417,0.0169758,0.  
0159475,0.0169126,0.1059824,0.0041543,0.0156558,0.0033333,-0.1306063,-  
0.051085,0.0588149,-0.0850284,0.0563557,0.0878087,0.0363433,-0.0784661  
,0.0321842,-0.0094711,-0.0691719,0.0568206,0.0718387,0.0537056,0.08359  
99,-0.0179581,0.0845818,-0.0240576,0.0149117,-0.1142666,-0.0331387,0.0  
921105,-0.0224133,0.0647406,0.0244741,0.0176029,0.0072256,-0.0111965,0  
.0585819,-0.0536511,-0.0174001,-0.051483,-0.0867681,-0.0844291,-0.0073  
597,-0.0561881,-0.0877258,-0.0063356,0.0925928,-0.0596621,0.0760407,-0  
.0285981,0.0889525,-0.0120887,0.0303954,-0.0257744\Polar=73.5774687,-1  
5.0937453,36.16329,-1.3186427,-1.1181859,90.8142828\PG=C01 [X(C7H8)]\N  
Imag=0\

5<sup>+</sup>

1\1\MF(MLIB83-EXE)-PROTON\Freq\RB3LYP\6-31G(d)\C7H7(1+)\THEIS\15-May-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\toluen\1,1  
\C,-1.2468837037,-0.2361758005,-0.0868917235\C,-1.2334257624,1.0587214  
628,0.3783653367\C,0.0038937329,1.6967000574,0.6095799846\C,1.23827482  
06,1.0522757713,0.3805769917\C,1.2457758696,-0.2425894342,-0.084906380  
7\C,-0.0021355893,-0.9253464795,-0.3323609788\C,-0.0050931188,-2.21460  
08062,-0.7966467675\H,-2.1826884228,-0.7549066094,-0.2747690441\H,-2.1  
596670811,1.5905366454,0.5681588932\H,0.0062139033,2.7196329428,0.9775

812807\H,2.1669472994,1.5792182524,0.5720681818\H,2.1791673392,-0.76618  
72699,-0.2712728112\H,0.9203185194,-2.7535292994,-0.9881036845\H,-0.93  
27291035,-2.7486732878,-0.9899615914\\Version=HP-PARisc-HPUX-G98RevA.1  
1.3\HF=-270.6622707\RMSD=2.605e-09\RMSF=8.281e-05\Dipole=-0.0013566,-0  
.5949887,-0.2136462\DipoleDeriv=0.0435912,-0.2792753,-0.1004944,0.3262  
754,0.5577012,0.1929278,0.1172587,0.1918162,0.0916994,-0.16358,-0.4259  
109,-0.1532747,-0.5487458,-0.4769923,-0.1438535,-0.197403,-0.1436292,-  
0.1313334,0.6080487,-0.0005024,0.000662,-0.0005433,0.4394393,0.1210918  
,0.0006932,0.1211796,0.145867,-0.1591151,0.4244506,0.1525502,0.5473353  
, -0.4820218,-0.1437549,0.1966288,-0.1438434,-0.1307175,0.04336,0.28163  
57,0.101367,-0.3239103,0.5579131,0.1919115,-0.116364,0.1929008,0.09168  
51,-0.0942127,-0.0020403,-0.0009762,-0.0020706,-1.0132584,-0.3831581,-  
0.0009621,-0.3830594,-0.0857508,0.2559134,0.0009692,0.0007027,0.001016  
3,0.751879,0.2510033,0.0007351,0.2499852,0.144344,0.0762668,-0.0016071  
, -0.0006449,-0.0322122,0.0610357,-0.0228701,-0.0116267,-0.0227352,0.11  
62707,0.0590917,0.0140827,0.0049139,0.0107149,0.0911291,-0.0180807,0.0  
037714,-0.0180851,0.135005,0.0996193,-0.000038,-0.0000429,-0.0000434,0  
.0791335,-0.0125905,-0.0000387,-0.0128024,0.1097377,0.0589863,-0.01387  
92,-0.005143,-0.0105259,0.0912736,-0.0180797,-0.0039549,-0.0181008,0.1  
349832,0.0764226,0.0015582,0.0004697,0.0322038,0.0608487,-0.0228307,0.  
0113757,-0.0227851,0.1162884,0.0476859,-0.0157014,-0.0057092,-0.028844  
9,0.1410786,0.0041304,-0.0105305,0.0045468,0.1309237,0.0479219,0.01625  
82,0.0056197,0.0293508,0.1408409,0.0041535,0.010417,0.0046119,0.130997  
5\Polar=73.6456523,0.0423926,99.3755609,0.1054326,27.3370507,33.177089  
9\PG=C01 [X(C7H7)]\NImag=0\

## 6

1\1\MF(MLIB83-EXE)-BOSON\Freq\RB3LYP\6-31G(d)\C11H10\THEIS\15-May-2004  
\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\1-methylnaftal  
en\0,1\C,-2.5647854337,0.066821731,-1.0576090921\C,-2.5727894015,0.11  
02433048,0.3559643326\C,-1.3890870351,0.0859866307,1.0613363763\C,-0.1  
344612363,0.0172298679,0.3953685145\C,-0.1309190963,-0.0266076736,-1.0  
38953014\C,-1.3686475116,-0.0000604269,-1.7354340505\C,1.1134805071,-0  
.0094275171,1.1018909593\C,2.287903786,-0.0767269082,0.3790301029\C,2.  
2921819942,-0.1199360455,-1.0358252847\C,1.1079643774,-0.0954380954,-1  
.7316953598\C,1.1486539991,0.0349649177,2.6112258662\H,-3.503628248,0.  
0863916625,-1.6045394311\H,-3.5192084836,0.1630739249,0.8876670467\H,-  
1.413846071,0.1200905954,2.1459398893\H,-1.3533466782,-0.0337699332,-2  
.8225323047\H,3.2367250975,-0.0973124214,0.9101556941\H,3.2395393188,-  
0.1726555301,-1.5657562393\H,1.1004109744,-0.1282795128,-2.8186718511\  
H,2.1796995284,0.006070148,2.9760174923\H,0.6142217447,-0.8138078861,3  
.056660873\H,0.6824631216,0.9479002412,3.0032627271\\Version=HP-PARisc  
-HPUX-G98RevA.11.3\HF=-425.2096906\RMSD=2.712e-09\RMSF=6.175e-06\Dipol  
e=0.0057266,0.0032694,0.116111\DipoleDeriv=0.0312861,-0.0012182,0.1489  
549,-0.0026899,-0.1177531,-0.0016317,0.099198,0.0002762,0.0168312,0.03  
91942,-0.0101907,-0.1369901,-0.0088025,-0.1152776,0.0107039,-0.0909331  
,0.0089369,0.0618849,-0.067905,-0.0026118,-0.0033194,-0.0043741,-0.132  
6821,0.0066718,-0.0611582,0.008848,0.0792976,0.1120742,-0.0036981,-0.0  
139017,-0.0027926,0.0271913,-0.0070961,0.0172738,-0.0082866,-0.2234261  
,0.0966999,-0.0014844,0.000995,-0.002664,0.0569383,-0.0066903,-0.03800  
63,-0.0051751,-0.1610028,-0.0320658,-0.0050111,-0.0363717,-0.0022849,-  
0.1326957,0.010185,0.0531637,0.0067604,0.1559692,-0.0510142,-0.0004497  
, -0.032546,0.0030787,-0.0371546,0.0117667,0.082676,0.0073267,0.3093908  
,0.0304609,-0.0010377,0.1792283,-0.0046513,-0.1370756,-0.004793,0.0628  
815,-0.0003254,-0.0678943,0.0501395,-0.0103965,-0.1448217,-0.0081349,-

0.104373,0.0108429,-0.0708691,0.0080156,0.0683913,-0.0628691,-0.002732  
7,0.0117059,-0.0050076,-0.1427409,0.0072153,-0.0631241,0.0100632,0.107  
0717,0.0930059,0.0019277,0.0433733,0.0012429,0.1090008,-0.0036416,0.02  
09832,-0.0027536,0.0446149,-0.0893989,0.0052818,-0.0850149,0.0051064,0  
.1142694,0.0001325,-0.0902467,0.0003413,0.0113721,-0.0934901,0.0102668  
,0.0750932,0.0106565,0.1122252,-0.00594,0.0877842,-0.0064317,0.0132184  
,0.0700054,0.0009962,-0.0111816,0.0020534,0.1044567,-0.0058315,0.02296  
52,-0.0071175,-0.0995175,0.0513674,0.0032468,0.0344677,0.0015092,0.107  
962,-0.0082266,-0.0225118,-0.006043,-0.1184189,-0.0853408,0.0048822,-0  
.0825525,0.0041935,0.1058707,-0.0000366,-0.1068044,0.00088,-0.0007568,  
-0.0912309,0.0105244,0.0864434,0.0104188,0.1126916,-0.0065857,0.082665  
3,-0.0064274,0.0068023,0.0510486,0.0011552,-0.0366286,0.0029486,0.1096  
307,-0.0055218,0.0226858,-0.00779,-0.117214,-0.1221442,0.0039792,-0.11  
83123,0.0069505,0.0730796,0.0028571,-0.0203787,-0.0009389,0.0163286,0.  
0294551,-0.0856188,0.065914,-0.0646026,-0.0478449,0.0668212,0.0092753,  
0.0394145,-0.0547519,0.0407218,0.0821894,0.0554649,0.0578459,-0.065719  
1,-0.0712016,0.0024805,-0.0395735,-0.0481906\Polar=160.7223548,-4.4716  
547,42.3314134,3.5826019,2.529916,129.7170064\PG=C01 [X(C11H10)]\Nimag  
=0\

6<sup>+</sup>

1\1\MF (MLIB83-EXE) -BOSON\Freq\RB3LYP\6-31G(d)\C11H9(1+)\THEIS\15-May-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\l-methylnaf  
t\1,1\C,-2.5633693056,0.1422031538,-1.0422070587\C,-2.5889802906,-0.0  
217682189,0.3543483778\C,-1.4122074438,-0.1180572267,1.0965816983\C,-0  
.1666461102,-0.0534637669,0.4657245631\C,-0.1359617554,0.1139629254,-0  
.9605522036\C,-1.3489615643,0.2095558841,-1.6944760918\C,1.12136978,-0  
.1463317227,1.1715860222\C,2.3441185867,-0.0660676097,0.4090479871\C,2  
.3364574507,0.0946204726,-0.9572163011\C,1.1041826995,0.1828081961,-1.  
6270621758\C,1.238733607,-0.3061113565,2.5223362483\H,-3.4923042429,0.  
2146585858,-1.5979041722\H,-3.5434398821,-0.0749773194,0.869381189\H,-  
1.4862582826,-0.2438120562,2.1712852494\H,-1.3040875532,0.335917778,-2  
.7723093214\H,3.2862062221,-0.1363445708,0.9453243076\H,3.2642866734,0  
.1531630509,-1.5156179907\H,1.101192698,0.3098429437,-2.7074240563\H,2  
.2168428985,-0.3686519132,2.9904210897\H,0.385147544,-0.3779008824,3.1  
881773092\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-424.323708\RMSD=5.4  
36e-09\RMSF=2.438e-06\Dipole=0.6808587,-0.0535948,0.4112308\DipoleDeri  
v=0.0629208,-0.047684,0.3969648,-0.0378017,-0.0724354,0.0302481,0.3129  
41,0.0309005,-0.3524225,0.3569721,-0.013263,0.0891407,-0.0097332,0.001  
7374,-0.0538701,0.0591648,-0.053652,0.4477906,-0.7087174,0.052015,-0.4  
022984,0.0170194,-0.0932442,-0.0204865,-0.1047321,-0.0227643,0.1050181  
,0.3042645,-0.037555,0.3035732,0.059743,0.0620639,0.000182,-0.5240976,  
0.0065417,0.0410987,-0.8726665,-0.0028303,0.0836691,-0.0641041,0.03688  
11,0.0289441,0.6048608,0.0249403,-0.2118401,0.3223024,0.0345333,-0.318  
4536,-0.0203758,-0.052031,-0.0346854,0.1486071,-0.038272,0.2595753,0.0  
776943,-0.0215329,0.1809031,0.027935,0.0296362,0.1185348,-0.2395784,0.  
121723,-0.9757152,-0.0860702,0.0378869,-0.3147332,-0.0735232,0.0396773  
, -0.0937014,0.6327564,-0.1009641,0.845483,-0.3889769,0.0663646,-0.5460  
28,0.1153989,-0.1174515,0.0799198,-0.9631888,0.0831384,-0.751395,1.306  
8648,-0.0679409,0.4969967,-0.0080235,0.0747422,-0.0505846,-0.0125569,-  
0.0466771,0.4665923,0.1436596,-0.0045179,0.026636,-0.0082469,-0.029188  
7,-0.0731244,0.0583439,-0.0733671,0.5821897,0.0313065,0.0047539,-0.033  
7936,0.0050479,0.1320349,0.0083689,-0.0362986,0.0083884,0.0640705,0.03  
89588,-0.0032131,0.0328009,-0.0033834,0.1219508,0.0061227,0.0342599,0.  
0061107,0.0684215,0.0764179,0.0067399,-0.0545759,-0.000827,0.1166867,0  
.0172591,0.0097591,0.0167681,-0.0245745,0.0750014,-0.0058536,0.0529271



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, -0.0001493, 0.121512, 0.0126103, 0.0044167, 0.0129809, 0.0122806, 0.0695638  
, 0.001055, -0.0058575, 0.0056153, 0.11647, 0.0078241, -0.0446762, 0.0081253,  
0.05125, 0.0472349, -0.0014776, 0.0188726, -0.0010296, 0.1429528, 0.0077358,  
0.0150929, 0.0077613, 0.0768614, 0.0940493, 0.0046069, -0.038167, 0.0005835,  
0.1086794, 0.0083692, -0.0039497, 0.0081049, 0.0409748, 0.0423281, -0.000131  
1, 0.0069705, -0.003987, 0.1322213, 0.000492, 0.0397228, 0.0002438, 0.1275914  
, 0.0068915, -0.0019559, 0.0244524, -0.0001581, 0.1271048, -0.0001584, 0.0091  
531, -0.0000305, 0.1267491\Polar=166.8760213, -2.8485834, 36.4267355, 15.60  
58811, -13.4022325, 147.7992227\PG=C01 [X(C11H9)]\NImag=0\

7

1\1\MF(MLIB83-EXE)-MESON\Freq\RB3LYP\6-31G(d)\C11H10\THEIS\15-May-2004  
\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2-methylnaftal  
en\0,1\C,-2.8515068897,0.8765353066,-0.0215293681\C,-2.8500661078,-0.  
5398278158,-0.0068510455\C,-1.6607437143,-1.2340716802,0.0055291932\C,  
-0.4164094423,-0.5483614753,0.0038818235\C,-0.4191034395,0.8834141763,  
-0.010852416\C,-1.6618578352,1.5703380814,-0.0234323726\C,0.8284194033  
, -1.2346421911,0.0163039421\C,2.0320626256,-0.5612618621,0.0145972047\  
C,2.0137429179,0.862793034,-0.0000107633\C,0.8303823384,1.5612866499,-  
0.0123063297\C,3.3519331016,-1.2943400898,0.0277381663\H,-3.7965052002  
,1.4130337852,-0.031282359\H,-3.7945890579,-1.0774207153,-0.0054178581  
\H,-1.6579396396,-2.3217223557,0.0168045661\H,-1.6575137736,2.65803020  
24,-0.0346837549\H,0.8179260035,-2.3230405926,0.0273726606\H,2.9591959  
659,1.4010737065,-0.0013743049\H,0.8357720948,2.6490084547,-0.02337015  
58\H,3.9563420584,-1.0443199527,-0.8536668184\H,3.2076286289,-2.379135  
5656,0.0379481801\H,3.9485651711,-1.0266797702,0.9092616368\Version=H  
P-PARisc-HPUX-G98RevA.11.3\HF=-425.2111927\RMSD=2.169e-09\RMSF=4.470e-  
05\Dipole=0.1608451,-0.0325168,0.0010076\DipoleDeriv=0.0022797,-0.1382  
368,0.001992,-0.0948371,0.0123735,-0.0018102,0.001559,-0.0019989,-0.12  
15522,0.0352375,0.1272342,-0.0006501,0.0958033,0.0506982,-0.0013245,-0  
.0003409,-0.001184,-0.1180316,-0.0651214,0.0055977,0.0002563,0.0725473  
,0.1415465,-0.0025506,-0.000443,-0.0028463,-0.1352877,0.16187,-0.03053  
4,0.0007187,-0.0495198,-0.1375133,0.0018787,0.0008643,0.0019643,0.0656  
379,0.0509944,-0.0116148,0.0001624,0.0371323,-0.1855094,0.0025267,-0.0  
003025,0.0023138,0.0448661,-0.006763,0.0287065,0.0002526,-0.0802446,0.  
1572804,-0.003335,0.0013686,-0.0028762,-0.1313716,-0.1925848,0.0735252  
, -0.000909,-0.0353729,0.1267642,-0.0030544,0.0002322,-0.0025679,-0.156  
0223,0.2813633,-0.1991696,0.0033315,-0.1749862,0.0404254,-0.0013853,0.  
0031017,-0.0015021,-0.0212012,-0.0603158,0.1648198,-0.0013647,0.171581  
7,0.0163364,-0.0007585,-0.0014097,-0.0007879,-0.1309225,0.0040773,0.01  
18221,0.0004492,0.0708224,0.1508557,-0.0025301,-0.0001552,-0.0027839,-  
0.1275211,0.034835,0.0354612,-0.0007201,-0.0452617,0.1165645,-0.000170  
4,0.0000134,0.0002033,0.1191654,-0.0943029,0.0820878,-0.0017752,0.0880  
787,0.0123879,0.0014534,-0.0018371,0.0014284,0.1150285,-0.0959121,-0.0  
794245,-0.0000971,-0.088741,0.0131265,0.0006601,-0.0000051,0.000701,0.  
1142915,0.0520118,0.0337321,-0.0005932,-0.0262083,-0.1148503,0.0021926  
,0.0000376,0.002457,0.108161,0.0507481,-0.033591,0.0000928,0.0277422,-  
0.1182718,0.0024615,-0.0005539,0.0022049,0.1081831,0.0466584,-0.011619  
5,-0.0001212,0.0308564,-0.1207959,0.00242,-0.0005383,0.0022178,0.10250  
3,-0.097784,-0.0841115,-0.0000241,-0.0780478,0.0231436,0.0004884,-0.00  
00826,0.0004586,0.1044357,0.0451775,0.0342332,-0.0006218,-0.0172133,-0  
.1203554,0.0022474,-0.0001056,0.0024731,0.1072881,-0.0876016,0.0263804  
,0.0756672,0.0230585,0.0360811,0.0550516,0.1151883,0.024404,-0.0583861  
,0.0210945,-0.0603869,0.000395,0.0515524,-0.1347483,0.0022657,-0.00072  
1,0.0017799,0.0691882,-0.085962,0.0250884,-0.0764413,0.0212575,0.03446  
06,-0.0567271,-0.1158701,-0.0260589,-0.0584522\Polar=177.1339277,-6.05

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96083,119.6748578,0.6506541,-0.8211726,42.3617707\PG=C01 [X(C11H10)]\N  
Imag=0\

7<sup>+</sup>

1\1\MF (MLIB83-EXE) -MESON\Freq\RB3LYP\6-31G(d)\C11H9(1+)\THEIS\15-May-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2-methylnaf  
t\1,1\C,0.2113080953,0.8223460032,-2.7667361462\C,0.210274709,-0.5951  
837504,-2.7853681046\C,0.1194549571,-1.290238329,-1.6053341268\C,0.026  
1303144,-0.5857049257,-0.3600268233\C,0.0279393557,0.8650914055,-0.351  
601058\C,0.1222649769,1.5381573534,-1.5782218294\C,-0.0665110007,-1.26  
04343563,0.8467645356\C,-0.1597761288,-0.5511942689,2.0944595594\C,-0.  
1564817391,0.9006846987,2.0782505493\C,-0.0659370192,1.5688074611,0.89  
90770837\C,-0.2482148844,-1.2637593352,3.2586862829\H,0.283660889,1.36  
20982302,-3.7066832894\H,0.2812974865,-1.1202324051,-3.7320471328\H,0.  
1168245747,-2.3764433461,-1.5951427584\H,0.1254095533,2.6237422297,-1.  
5952336486\H,-0.0695759585,-2.347762753,0.8616247572\H,-0.2272691736,1  
.4326856068,3.0216759709\H,-0.0627777522,2.6545275643,0.8796431174\H,-  
0.3200254824,-0.7694843597,4.2241798373\H,-0.2502539551,-2.3505625049,  
3.2622836106\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-424.3229211\RMSD  
=2.306e-09\RMSF=3.518e-05\Dipole=-0.0637222,-0.5510101,0.8340757\Dipol  
eDeriv=0.0300022,0.0023798,-0.0471379,-0.0283655,0.4153123,0.3833529,-  
0.0477228,-0.0224098,0.6551435,-0.0778962,-0.030278,-0.0211766,-0.0096  
53,-0.481803,0.1184839,-0.0207056,0.3894405,0.2021255,-0.0406922,0.035  
4461,-0.0187505,-0.0115334,0.1714485,0.1574311,-0.0197334,-0.4622348,0  
.2085504,0.0260791,-0.036687,0.0580885,-0.0317771,-0.4079765,0.4099383  
,0.0581006,0.474465,-0.7269546,0.1402473,-0.0081744,-0.0709899,0.03751  
96,0.102792,-0.4958683,-0.069774,0.1070507,1.057899,-0.1235834,0.00748  
56,0.0920639,0.0085469,0.1867659,-0.1061241,0.0918531,-0.0917591,-1.33  
09263,0.031259,0.0368214,-0.0858552,0.0080303,0.2044491,-0.1002593,-0.  
0865272,-0.4822585,1.1591624,0.0531225,-0.022302,0.1008093,-0.0189401,  
-0.0520184,0.2478851,0.1014493,0.2945035,-1.2759788,-0.0751106,-0.0095  
193,-0.0389767,0.0282254,0.025227,-0.3718887,-0.0384798,0.1261803,0.43  
20336,-0.0991539,0.0099949,0.0449363,-0.0058816,0.1980675,0.0836497,0.  
0445737,-0.1256124,-0.687475,-0.0112284,0.0098489,-0.0543088,0.0188334  
,0.28995,-0.2433904,-0.0539087,-0.1229839,0.6974976,0.1188982,-0.00240  
14,0.0050783,-0.0024767,0.0724171,0.0315441,0.005075,0.0304878,0.05320  
98,0.1353496,0.0020848,0.0076385,0.0028559,0.0633418,-0.0392649,0.0076  
476,-0.0290707,0.0345345,0.1201627,-0.0034822,0.0035577,-0.0001574,0.0  
099132,-0.0004571,0.0036407,0.0435357,0.0734684,0.1314959,0.002824,0.0  
042469,-0.0001093,0.0008206,-0.0014748,0.0041644,-0.0399557,0.0761247,  
0.1159099,0.0002277,0.0050209,0.0001003,0.0241792,-0.0033601,0.0049599  
, -0.0050489,0.050485,0.1342726,0.0022096,0.0084258,-0.0019699,0.065154  
1,0.0248839,0.0083601,-0.0304443,0.0240293,0.1299409,-0.0025733,0.0043  
662,0.0001374,0.0079587,-0.0042686,0.0044136,0.031614,0.0727981,0.1324  
323,0.0015618,-0.0003577,0.0023681,0.0476463,-0.0333469,-0.0006189,-0.  
0232973,0.139765,0.1284927,0.0045329,0.003321,0.0042466,0.0563548,-0.0  
57466,0.0032324,-0.0622022,0.084508\Polar=36.03875,1.8522251,120.39028  
97,-13.8987326,-22.6820334,218.0062677\PG=C01 [X(C11H9)]\NImag=0\

8

1\1\MF (MLIB83-EXE) -BOSON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\03-Nov-20  
04\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\1methyl-2met  
hyoxy\0,1\C,-3.1912614911,0.3226845061,0.8317548792\C,-3.2189947676,-  
1.0922998169,0.8715890559\C,-2.0764737432,-1.8034975316,0.5875179187\C  
, -0.8649682774,-1.1410791068,0.2537161474\C,-0.8290134645,0.2932057055  
,0.2112690863\C,-2.0327520765,0.9946765143,0.5116722166\C,0.3191469412

, -1.8587144271, -0.0411338069\C, 1.4835012639, -1.2022598305, -0.362450001  
\C, 1.5164813695, 0.2158276664, -0.4037972331\C, 0.3821179932, 0.9722570782  
, -0.1228477905\C, 0.4350445427, 2.4809352187, -0.1713677498\O, 2.656625282  
9, 0.9108442892, -0.7197267271\C, 3.8425791814, 0.1944642674, -1.0149074801  
\H, -4.0949198098, 0.8835118497, 1.0564702325\H, -4.140033373, -1.609745562  
3, 1.1256722146\H, -2.0820321643, -2.8910654453, 0.6139884501\H, -2.0356994  
04, 2.0793376595, 0.4874833598\H, 0.3001800321, -2.9455283261, -0.011076866  
\H, 2.375963172, -1.77570749, -0.5838605164\H, 1.4328179458, 2.8266854048, -  
0.4415184765\H, 0.1750181005, 2.9215284165, 0.7995725129\H, -0.2734911529,  
2.8824262142, -0.9070619397\H, 4.599636824, 0.9509826667, -1.2313902528\H,  
3.7211368249, -0.4531604053, -1.8935197878\H, 4.1759759111, -0.4132207582,  
-0.1630365702\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7296709\RMS  
D=2.453e-09\RMSF=8.037e-06\Dipole=0.518772, -0.2686108, -0.1301089\Dipol  
eDeriv=0.0481095, -0.0904184, -0.0394646, -0.0943282, 0.1610612, 0.0185728,  
-0.0393776, 0.0175443, -0.0999413, -0.0619502, 0.1748358, -0.0222624, 0.1193  
105, -0.0719954, -0.0327381, -0.0209833, -0.0473346, -0.1247298, 0.1113805, -  
0.0943535, -0.0598673, 0.0907748, 0.1592325, -0.0303976, -0.0641273, 0.01828  
31, -0.1080923, -0.1070324, 0.0805974, 0.0353136, -0.0974372, -0.2383994, 0.0  
319001, 0.0394229, -0.0149073, 0.0242766, 0.3261842, 0.1063124, -0.0787687, 0  
.1237727, -0.1486812, -0.0283088, -0.0791778, -0.0237158, 0.05733, -0.147006  
, -0.0823499, 0.0031532, -0.049898, 0.0747395, 0.0081249, 0.0024006, 0.016641  
6, -0.1432289, 0.1508831, -0.1073432, -0.0710071, -0.0241642, 0.1315616, 0.00  
03529, -0.0729361, 0.0222173, -0.1098321, -0.2078423, -0.0319328, 0.0132486,  
-0.2964298, 0.0175378, 0.0738621, 0.019423, 0.0042891, -0.1655511, 1.4209853  
, 0.3387361, -0.3471109, 0.7703887, 0.095171, -0.2017859, -0.357195, -0.08829  
61, 0.2269258, -0.4526907, -0.1609796, 0.0965, 0.1065165, 0.2420693, -0.03586  
09, 0.090352, 0.0344753, -0.1243851, 0.0490493, 0.0219684, 0.0194102, -0.0204  
604, 0.0485138, 0.0071152, 0.0204074, -0.004013, 0.1195358, -2.0047962, -0.07  
05417, 0.4532109, -0.4359363, -0.4027502, 0.117312, 0.4616841, 0.0212613, -0.  
409501, 1.1068336, -0.0911671, -0.193235, -0.4558271, 0.3358267, 0.1205202, -  
0.1847796, 0.0246066, 0.4120023, -0.0855093, 0.0782567, 0.0499092, 0.0926573  
, 0.0073721, -0.0219776, 0.0495791, -0.0181919, 0.0985224, -0.0866044, -0.079  
6771, 0.0550312, -0.0854812, 0.0139262, 0.0248183, 0.0551629, 0.0232914, 0.10  
06705, 0.0548769, 0.0318004, 0.012779, -0.0319268, -0.1234777, 0.0136791, 0.0  
142443, -0.0030783, 0.1025853, 0.0731207, -0.0148752, 0.0087701, 0.0232146, -  
0.0960561, -0.0014749, 0.0078947, 0.0085518, 0.1028899, 0.0508219, -0.031259  
6, 0.0158673, 0.0100195, -0.1128531, 0.0024651, 0.0149087, 0.0133306, 0.10419  
93, -0.0516898, 0.0729641, 0.0436478, 0.0838623, 0.0362854, -0.0201107, 0.043  
3883, -0.017224, 0.1096863, -0.0376982, -0.1028775, 0.0324555, -0.0443771, 0.  
0534418, 0.0122049, 0.0311109, 0.0275731, 0.0680302, 0.062491, 0.0529746, 0.0  
491228, 0.0075239, -0.0568894, -0.0415816, 0.0311914, -0.0861209, -0.0884373  
, -0.0096377, 0.0848457, -0.0984162, 0.024193, -0.0521405, 0.0329578, -0.0780  
56, 0.0495909, -0.0210834, -0.1004323, -0.0630518, 0.0479704, -0.1215539, -0.  
0233357, 0.0342572, 0.0493189, 0.0188765, 0.0630903, -0.0438402, -0.033307, -  
0.0313417, 0.1302951, -0.029055, -0.131533, 0.0274466, -0.0812977, -0.100610  
5, -0.0580066, 0.0108426, 0.0050842, 0.1752913, -0.021105, 0.0476265, -0.0613  
033, 0.0836465, -0.0943521\Polar=190.3870053, 4.4972577, 139.2375604, -36.0  
500997, -3.1508836, 63.2421259\PG=C01 [X(C12H12O1)]\NImag=0\

8<sup>+</sup>

1\1\MF (MLIB83-EXE) -LEPTON\Freq\RB3LYP\6-31G(d)\C12H11O1 (1+)\THEIS\03-N  
ov-2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\1methyl  
-2methoxy\1,1\C, 0.5360176197, 0.3167336316, -3.2904288041\C, 0.56147095  
74, -1.0851880483, -3.3003031564\C, 0.377950886, -1.7732332789, -2.11357852  
34\C, 0.1673055671, -1.0681738967, -0.9060961421\C, 0.141254341, 0.35798464  
31, -0.8952496054\C, 0.3294290426, 1.0281416033, -2.1081840017\C, -0.020978

6584,-1.7757877697,0.3117553491\C,-0.2324425845,-1.1625654896,1.533426  
2881\C,-0.2673299386,0.2371358674,1.6002780832\C,-0.0819471329,1.05298  
1615,0.3893782717\C,-0.1257283892,2.4027545109,0.5161293923\O,-0.46171  
18307,0.9112367111,2.711107528\C,-0.6588259855,0.2376473133,3.97810468  
56\H,0.6791873483,0.8638683037,-4.2172648896\H,0.7233573953,-1.6223082  
149,-4.2288926755\H,0.3934393973,-2.8592727759,-2.0953396039\H,0.31850  
14452,2.1114449963,-2.1535550653\H,0.0031856886,-2.8626657423,0.277675  
1043\H,-0.3684891799,-1.7645400775,2.4226085963\H,-0.2922217842,2.8691  
416402,1.4799883088\H,0.0021442372,3.0678653602,-0.3299462201\H,-0.791  
7285445,1.0391101062,4.7022279561\H,0.2240197211,-0.3563492726,4.22756  
86354\H,-1.5547554281,-0.3867722209,3.9346786094\\Version=HP-PARisc-HP  
UX-G98RevA.11.3\HF=-538.8661671\RMSD=4.350e-09\RMSF=6.310e-06\Dipole=-  
0.1412029,-0.0568686,0.86402\DipoleDeriv=-0.0157746,-0.0163694,-0.0526  
051,-0.0120026,0.3470534,0.0345229,-0.0530605,0.0610345,0.291503,-0.07  
05831,-0.0513261,-0.0276497,-0.0444101,-0.3528513,0.2985386,-0.0283677  
,0.340657,0.0612469,-0.0525414,0.0531335,-0.0691263,-0.0347453,0.24104  
21,0.1797031,0.0600384,-0.3544818,0.3385083,-0.0009608,-0.0245502,0.1  
51525,-0.1019918,-0.252587,0.6484443,0.1595608,0.1779326,-0.9645422,0.  
0549775,-0.0393892,-0.0178206,0.0787872,0.0756901,-0.48136,-0.0300491,  
0.2369254,0.2095061,-0.1130085,0.0413803,0.0864245,0.0114782,0.118441,  
-0.0920943,0.0895435,-0.2738176,-0.6140123,0.0959415,-0.0446094,-0.277  
9753,0.0005253,0.4273001,-0.0423794,-0.2826646,0.2318343,1.7432606,-0.  
2231326,0.0647598,0.1317477,0.2438582,-0.6809197,-1.4321192,0.1132026,  
-0.3437931,-0.8526529,0.3248117,0.0048345,-0.2153876,-0.3025388,1.1220  
874,1.7520755,-0.1834925,-0.1157525,1.4159352,-0.0053513,-0.0164483,0.  
0027231,-0.0033026,-0.8236021,0.1045473,0.0013437,0.1845131,-0.0323126  
, -0.0589044,-0.0020164,-0.0099186,0.0060161,0.4299126,-0.087177,-0.010  
7499,-0.0385507,0.0087905,-0.2993441,0.0133353,0.3300871,0.1268514,-0.  
4164891,-0.7529242,0.3182717,-0.0632414,-2.1718175,0.2997576,0.0059051  
, -0.1472617,0.0583725,0.2249474,-0.3493854,-0.1526583,-0.0306036,1.206  
228,0.1201483,-0.00476,0.0153668,-0.0058321,0.0593045,0.0419886,0.0154  
763,0.0354706,0.0248586,0.127196,0.0072326,0.0195566,0.0080367,0.05966  
42,-0.0415285,0.0194736,-0.0366344,0.0159474,0.1194055,-0.0058727,0.00  
69112,0.0021084,-0.011633,0.00085,0.0060878,0.0493595,0.0783226,0.1148  
493,0.0106598,0.0054586,0.0012356,-0.0373421,0.0083176,0.0064305,-0.04  
8972,0.0818909,0.1100719,0.0068001,0.0033603,0.0005867,0.0235614,0.005  
4709,0.0040016,-0.0322975,0.089769,0.1450226,-0.0029919,0.0213154,-0.0  
006357,0.0849213,0.0104465,0.0210383,0.0248051,0.0180502,0.1267908,-0.  
0010686,0.0099967,-0.002996,0.1301167,0.0180415,0.0101869,0.0064357,0.  
0658185,0.1212434,-0.0069741,0.0174256,-0.0020882,0.1225381,0.0128339,  
0.0169258,0.0425448,0.0167229,0.1071476,0.0024816,0.0171486,0.0108379,  
0.0231872,-0.0568161,0.0162823,-0.0060789,0.0117591,-0.0251278,0.05204  
84,0.0057571,0.0371225,0.0446289,0.1193977,0.0506852,-0.0146847,-0.011  
9551,-0.0026355,-0.0461948,-0.0070595,-0.0752736,0.041028,0.1006058,-0  
.0474298,-0.0326045,-0.0308254\Polar=50.374842,-4.2878726,150.8763269,  
-26.6171279,15.2063667,206.1131274\PG=C01 [X(C12H11O1)]\NImag=0\

9

1\1\MF (MLIB83-EXE) -LEPTON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\02-Nov-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\l methyl-3-m  
ethoxy\0,1\C,-3.2031060419,0.8412683684,0.0888976621\C,-3.2101802595,  
-0.5717617741,0.1025063137\C,-2.0211328831,-1.2636728482,0.0730262896\  
C,-0.7731426364,-0.5853148817,0.028908055\C,-0.7595865722,0.851794133,  
0.0151655505\C,-2.0095208119,1.5288812928,0.0465258351\C,0.4441687805,  
-1.3170204306,-0.0013568458\C,1.6461237758,-0.6437589843,-0.0441385025  
\C,1.6648274472,0.7738009698,-0.0575131593\C,0.5100333845,1.5238237618

, -0.0293686793\C, 0.6441897312, 3.0338238441, -0.0477684901\O, 2.879497323  
, -1.2282250354, -0.075659632\C, 2.9425652646, -2.6447776489, -0.0642604874  
\H, -4.1422287429, 1.387437922, 0.1120208214\H, -4.1543476266, -1.10909369,  
0.1359402636\H, -2.0184438027, -2.3514131299, 0.0829857122\H, -2.032535758  
2, 2.6131794509, 0.0369161703\H, 0.3966328848, -2.4003805373, 0.0101948938\  
H, 2.637207369, 1.2584042374, -0.0912975982\H, 1.2298657649, 3.3804447997, 0  
.8120010049\H, -0.312260984, 3.5572263526, -0.0210444534\H, 1.1717468788, 3  
.3641704113, -0.9505284967\H, 4.0036622728, -2.8991324565, -0.0939900233\H  
, 2.439521308, -3.0771691893, -0.9396129345\H, 2.4937667791, -3.0603887003,  
0.8479504465\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.730221\RMSD=  
4.052e-09\RMSF=4.634e-05\Dipole=0.1032209, -0.3124663, -0.0004376\Dipole  
Deriv=-0.0560532, -0.1559912, -0.0007984, -0.1354045, -0.0398461, 0.0031796  
, -0.0011209, 0.0038207, -0.1326577, 0.0446331, 0.0867978, -0.0054662, 0.1077  
322, 0.110306, -0.0053168, -0.0055269, -0.0046702, -0.1095074, -0.1014569, 0.  
0772357, -0.002013, 0.0465414, 0.1321619, -0.0039676, -0.0016905, -0.0048897  
, -0.144019, 0.3175659, -0.17682, -0.0060326, -0.150434, -0.0351869, 0.005517  
7, -0.0063135, 0.0063509, 0.0664649, -0.0918755, -0.0463588, 0.0034389, 0.065  
161, -0.2997799, 0.0008858, 0.0024704, 0.0044418, 0.0066628, 0.0895499, 0.062  
6632, -0.0067956, -0.0871861, 0.1234101, 0.000367, -0.0054393, -0.0043267, -0  
.1158954, -0.5049688, 0.2582507, 0.0058567, -0.1066086, -0.0354113, 0.001417  
, 0.0092178, -0.0096441, -0.2302185, 1.4345475, -0.8217246, -0.0306243, -0.57  
98758, 0.5215027, 0.0141752, -0.032408, 0.0214797, 0.1666992, -0.1321329, 0.1  
951962, -0.0027419, 0.2803016, -0.2272247, -0.0077737, -0.0035207, -0.005259  
6, -0.1610097, 0.198047, 0.0829329, -0.0076746, 0.0898218, 0.3886473, -0.0067  
248, -0.007889, -0.0073518, -0.0302052, 0.0817089, -0.0819866, 0.001374, -0.0  
070117, 0.0045656, 0.0010671, 0.0007424, 0.0042724, 0.1018065, -1.460046, 0.7  
024529, 0.0287057, 0.8714162, -1.0832252, -0.0189309, 0.026729, -0.0137086, -  
0.2952879, 0.3258793, -0.0494096, 0.0014305, -0.5755042, 0.9298075, 0.011988  
5, 0.0063432, -0.0038698, 0.3584895, -0.0976398, 0.0802392, 0.005635, 0.09209  
13, 0.0070097, -0.0017567, 0.0055799, -0.0014172, 0.1143804, -0.0993595, -0.0  
811929, 0.007159, -0.0937127, 0.0132682, 0.0037671, 0.0071723, 0.0033838, 0.1  
12135, 0.0512085, 0.0341703, 0.0013326, -0.0259419, -0.1243779, 0.002931, 0.0  
019007, 0.0010615, 0.1056181, 0.0750575, -0.0055528, 0.0008108, 0.023262, -0.  
1210557, 0.001351, 0.00053, 0.0024076, 0.0994053, 0.0691222, -0.0324137, 0.00  
20963, 0.0367926, -0.0939752, 0.0009509, 0.0014628, 0.0030597, 0.1279073, -0.  
0531041, -0.0689003, 0.0055439, -0.0706148, 0.0423171, 0.0027243, 0.0055339,  
0.0026227, 0.1094036, 0.0052707, -0.0527122, -0.0838658, -0.0289336, -0.0445  
23, -0.0283507, -0.0781562, -0.0694686, -0.0437698, -0.0660566, 0.1199537, 0.  
0034482, 0.0451536, 0.0048015, -0.0008569, 0.004065, -0.0033837, 0.0698415, 0  
.0158731, -0.0463177, 0.080668, -0.0257988, -0.0432813, 0.0301578, 0.0747027  
, 0.0725495, -0.0561064, -0.143646, 0.0970179, 0.0058086, 0.0655166, 0.012724  
2, -0.0013703, 0.0060929, -0.0023164, 0.0778094, 0.0451383, -0.0917285, -0.09  
31308, 0.0802809, -0.072244, -0.0347782, -0.0413367, -0.0672886, -0.0941922,  
0.0527372, -0.0858015, 0.0858349, 0.0829556, -0.0703908, 0.0293465, 0.030858  
6, 0.0721446, -0.1037544\Polar=188.0337296, -10.3982735, 148.0877104, -3.96  
09951, -0.5672137, 53.9469991\PG=C01 [X(C12H12O1)]\NImag=1\

9<sup>+</sup>

1\1\MF (MLIB83-EXE) -MESON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\02-No  
v-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\1methyl-  
3methoxy\1,1\C, -0.2317900975, 0.8390417603, -3.2070297443\C, -0.1986405  
661, -0.5668723937, -3.2011773702\C, -0.1035579409, -1.2407678768, -2.00062  
49038\C, -0.0393775489, -0.5206434699, -0.7770748352\C, -0.073586689, 0.913  
3396349, -0.788344131\C, -0.1703070336, 1.567157501, -2.019869137\C, 0.0578  
51459, -1.2183881485, 0.4452721784\C, 0.1256531944, -0.5686270545, 1.696542  
7377\C, 0.0940216842, 0.8195636851, 1.7133334802\C, -0.003624664, 1.5968856

166,0.511913038\C,-0.0261431069,2.9575615428,0.6507178543\O,0.21894275  
25,-1.1856524877,2.8831262713\C,0.2562244944,-2.6191182786,2.942784774  
\H,-0.3065949831,1.3701984869,-4.1509325467\H,-0.2477090943,-1.1149627  
882,-4.1362468438\H,-0.0766542361,-2.326227938,-1.9759905392\H,-0.1991  
870253,2.6500486404,-2.0733848723\H,0.0804561832,-2.3031520171,0.40618  
16851\H,0.1456091834,1.3248359604,2.6729780264\H,0.0281769977,3.415448  
3294,1.6338968059\H,-0.0976238381,3.6374352776,-0.1913983548\H,0.33245  
82696,-2.8590934706,4.002371577\H,1.1326180301,-3.0112075429,2.4145714  
045\H,-0.6634306175,-3.0528981485,2.5342798406\\Version=HP-PARisc-HPUX  
-G98RevA.11.3\HF=-538.8478277\RMSD=3.660e-09\RMSF=1.080e-05\Dipole=-0.  
0188334,0.4035234,-0.1390495\DipoleDeriv=-0.018428,-0.0046893,0.019030  
3,-0.0078751,0.4200869,0.0358512,0.0179202,0.0843342,0.280999,-0.06789  
18,0.0295917,0.0010347,0.0291061,-0.3044049,0.3565569,0.0008635,0.3639  
808,0.074054,-0.0687877,-0.024263,0.0212215,0.0030683,0.2553802,0.1611  
521,0.0307812,-0.2517317,0.3060133,0.0469205,0.0056047,-0.0633542,0.04  
23755,-0.1524905,0.5687839,-0.0503665,0.0138475,-0.7057086,0.0445783,0  
.0226376,0.0201564,-0.0336711,-0.0155563,-0.5300773,0.0003473,0.321272  
7,0.162617,-0.0910688,-0.0310318,-0.0327745,-0.0125352,0.1256085,-0.11  
32156,-0.0262702,-0.3931473,-0.6253378,-0.0232458,0.03487,0.0637602,-0  
.017225,0.3567876,-0.1252929,0.0454901,0.6596551,0.8951572,0.1960134,-  
0.0965135,0.0877235,-0.1038954,-0.1679089,-1.6935012,0.0846519,-1.5770  
097,0.9054684,-0.0454863,-0.0195492,-0.0258407,0.0446935,0.5171963,0.8  
736261,-0.0030754,-0.1003451,-0.125351,0.0497315,0.0185708,0.0107843,0  
.0036077,-0.8986181,-0.2799758,0.0054586,-0.0519201,0.1132654,-0.04241  
91,-0.0059572,0.014454,-0.0108179,0.5213247,0.0355036,0.0127051,0.1093  
412,0.1877368,-0.2915003,0.0854162,-0.0866116,0.0812762,-1.1062097,0.9  
360707,-0.0878104,0.9971778,-1.2556796,0.3236725,-0.0212602,0.00975,-0  
.049956,1.0253839,-0.5063427,-0.0004293,-0.0739936,0.2906937,0.1228051  
3,0.0037901,-0.0066789,0.0038054,0.064397,0.0367603,-0.0066572,0.036531  
3,0.035502,0.1305007,-0.0007707,-0.0063839,-0.0009838,0.0600354,-0.039  
8564,-0.0064542,-0.0366331,0.0203989,0.1198401,0.0065924,-0.0028421,0.  
0031291,-0.0039279,0.0036299,-0.0040564,0.0558437,0.0785575,0.1168175,  
-0.0007865,-0.0033791,0.0043884,-0.0274049,0.0153168,-0.0015639,-0.063  
2106,0.0709891,0.1151434,0.0001545,-0.0004996,0.0032933,0.0386064,0.02  
28067,0.0006648,-0.0257097,0.1160339,0.1282633,0.0022511,-0.0020601,-0  
.0000406,0.0736242,-0.0200376,-0.0027402,0.0145695,0.092019,0.1313307,  
0.0009499,-0.0067124,0.0028997,0.1313274,0.0437188,-0.0060167,0.014426  
1,0.0458202,0.1274025,0.0015811,-0.0083241,0.0005851,0.1222987,0.00685  
16,-0.0086745,0.0212642,0.0041837,0.1040866,0.0050116,-0.0094155,0.002  
9435,0.051728,0.0259132,-0.0101325,0.0569118,-0.0273744,-0.04537,0.028  
8029,0.0607863,0.0087446,-0.0427466,0.094012,0.0946091,-0.088024,0.020  
3155,-0.0629084,-0.0410033,-0.0538247,0.0030835,-0.0445172,0.0917456,-  
0.0792444,-0.0874309,0.0396268\Polar=46.9785564,-2.7176364,175.1015712  
,9.9886353,4.4602335,198.7679616\PG=C01 [X(C12H11O1)]\NImag=0\

## 10

1\1\MF (MLIB83-EXE) -PROTON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\03-Nov-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\1-me-4meo\  
0,1\C,-1.480215641,0.9956345676,-2.4613789829\C,-1.328944611,-0.405422  
8727,-2.5483373692\C,-0.6843710804,-1.0930324983,-1.542705276\C,-0.166  
7677974,-0.4100661251,-0.41333952\C,-0.3148242803,1.0116609905,-0.3150  
488029\C,-0.985696554,1.6827147435,-1.3732573816\C,0.5055770016,-1.113  
8557974,0.6391205279\C,0.9997139788,-0.4266053864,1.7263586935\C,0.842  
2226996,0.9790034655,1.8029186309\C,0.2064329526,1.7105849513,0.825025  
7904\C,0.0641582137,3.2082315881,0.9538325162\O,0.6015325014,-2.465186  
722,0.4634267316\C,1.254594911,-3.2250851614,1.4658097739\H,-1.9891514

937,1.5346427691,-3.2563501969\H,-1.7212284928,-0.9406767141,-3.408906  
4813\H,-0.5624557901,-2.1688163496,-1.5989225306\H,-1.1097733885,2.759  
651903,-1.3206211724\H,1.5107814622,-0.9416105625,2.5314103343\H,1.243  
2212656,1.4925884584,2.6738136447\H,-0.9878324344,3.5220043162,0.96198  
01597\H,0.5499357761,3.7400394984,0.1253866631\H,0.5204306273,3.560007  
3612,1.8842658077\H,1.2177265672,-4.2626064375,1.1283983802\H,0.742687  
2906,-3.1384219543,2.4334132571\H,2.3021198392,-2.917883303,1.58472667  
9\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7323953\RMSD=3.224e-09\  
RMSF=1.266e-05\Dipole=0.2476711,-0.2080333,0.401064\DipoleDeriv=-0.054  
5664,-0.0782642,0.0812044,-0.0482772,0.1025449,-0.033397,0.0889513,-0.  
0884958,0.0306035,-0.0999705,0.0813487,0.0679949,0.0174474,-0.0291276,  
0.0571631,0.051384,0.1746368,0.0145395,-0.0882987,-0.072025,0.0213779,  
0.0125346,0.0591303,0.0671322,0.0433996,-0.0882854,-0.0533725,0.006444  
,0.111554,0.0229316,0.0039427,-0.2679829,-0.0651183,-0.0050878,0.13266  
36,0.0350045,0.080197,0.02859,0.0832702,0.0710611,-0.1616794,0.0783201  
,0.094311,0.0002614,0.212346,-0.1341993,-0.0356096,-0.0001901,-0.04486  
08,0.0815961,-0.0249164,-0.0025891,-0.0079476,-0.1459584,0.1446195,-0.  
0755536,0.0135607,-0.350882,1.5521108,-0.2735048,-0.0581471,0.2325856,  
0.0802589,-0.1445547,-0.1630818,0.0404082,0.0771218,-0.2956778,0.11414  
13,0.1028968,-0.3273455,-0.0858588,-0.0685411,0.0354773,0.1238413,-0.1  
009353,0.1573804,-0.1104553,0.0884115,0.1402463,0.0681509,-0.108069,-0.  
.0277203,-0.0855657,0.0186113,0.1760956,0.0971769,-0.073504,0.0120446,  
-0.1974346,0.1125337,0.0212232,-0.0166192,0.0094646,0.1089254,0.013321  
9,-0.0196769,0.034946,0.0975146,-0.4152394,0.3199403,-0.1563812,0.4411  
812,-1.8321592,0.4077421,-0.124853,0.1850045,-0.4660653,0.4833805,-0.3  
455793,0.1373594,-0.1680922,0.7176489,-0.2156384,0.1836362,-0.5419603,  
0.5558917,0.0530135,0.0499214,-0.0934708,0.0554367,0.0123066,0.0761991  
, -0.0919911,0.0660321,-0.0409466,0.0726433,-0.0263746,-0.0811793,-0.03  
20777,0.0130782,-0.0850155,-0.0826866,-0.0745378,-0.0583404,0.1038189,  
0.015609,-0.0049961,0.0053313,-0.0504266,-0.0316743,-0.0076789,-0.0127  
84,0.0913054,0.0935294,0.0162262,-0.0154983,0.0325017,-0.0997693,0.006  
5617,-0.0112594,-0.0233288,0.077484,0.077816,0.0593074,-0.0814844,0.05  
02005,0.0166348,0.0625831,-0.0838134,0.079312,-0.0028185,0.0685736,-0.  
0309711,-0.072426,-0.033947,-0.0036247,-0.0903186,-0.0732562,-0.084860  
4,-0.0531512,-0.1191015,0.0982336,0.0193584,0.0398596,-0.0608689,-0.01  
55809,-0.0086244,0.0131955,0.0744533,0.0271844,-0.029705,0.0651825,-0.  
0246739,-0.0910995,0.0372987,0.0792652,0.106543,-0.0415782,0.0331552,-  
0.0524211,-0.0843863,-0.0020969,0.0143933,-0.0187674,-0.0712697,-0.111  
2719,-0.0883714,0.0674248,0.0029848,-0.0179074,0.0322832,-0.1557141,-0.  
.0013469,-0.0102848,-0.0551839,0.0443822,-0.0354124,0.045644,0.0691482  
,0.0275345,0.0247889,-0.0455402,0.0342602,0.1307995,-0.1410922,-0.1563  
809,0.0512457,-0.0355331,-0.0886695,0.0114959,-0.0063663,-0.0417935,0.  
1077303,-0.0069463\Polar=82.8791529,-14.6123865,158.4123725,49.6843345  
,0.4056426,145.2027851\PG=C01 [X(C12H12O1)]\NImag=0\

10<sup>+</sup>

1\1\MF (MLIB83-EXE) -PROTON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\03-N  
ov-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\lme-4me  
o\1,1\C,-1.3938743633,0.9774825905,-2.5469225134\C,-1.1805235444,-0.4  
067547023,-2.6291952905\C,-0.5610222475,-1.0677177136,-1.5839662729\C,  
-0.1451103769,-0.3517718279,-0.4385347505\C,-0.3599621278,1.0551201303  
, -0.3503684888\C,-0.9899332327,1.6950411707,-1.4259680547\C,0.50087811  
56,-1.0367691718,0.6526060598\C,0.9289426307,-0.3387221543,1.818308499  
\C,0.7243920805,1.0073478636,1.9052385025\C,0.0856888917,1.7711310687,  
0.8580880447\C,-0.0615508085,3.1076898972,1.060752639\O,0.664212513,-2  
.328361319,0.4989383064\C,1.297014637,-3.1535847118,1.5090203015\H,-1.

8798333314,1.4988747237,-3.3659107801\H,-1.4998537071,-0.9564931,-3.50  
84573035\H,-0.3891146882,-2.1363677034,-1.6325937048\H,-1.1715930732,2  
.763634593,-1.3980454167\H,1.412109908,-0.870575932,2.6280261706\H,1.0  
509857047,1.5391662065,2.7943839536\H,0.2908738394,3.5711254198,1.9773  
091281\H,-0.5265209145,3.7709486531,0.3397065006\H,1.2824795189,-4.159  
1372107,1.0931896004\H,0.7203412756,-3.1195008443,2.436457928\H,2.3267  
874365,-2.8257388899,1.6700754172\\Version=HP-PARisc-HPUX-G98RevA.11.3  
\HF=-538.8698279\RMSE=4.798e-09\RMSF=1.060e-05\Dipole=0.4554337,0.1916  
233,1.0281692\DipoleDeriv=0.0375825,-0.0417631,0.117849,-0.0454625,0.2  
91714,0.0264005,0.1164734,0.0341106,0.230883,-0.0837819,0.176499,0.045  
3687,0.1292833,-0.2982025,0.184777,0.0272595,0.2837615,0.0924383,0.007  
0377,-0.1840048,0.0556866,0.0293393,0.1043835,0.1217253,0.1374814,-0.3  
254187,0.1103762,-0.2362358,0.2479804,-0.34848,0.2766227,-0.3761778,0.  
4450304,-0.3376059,0.384821,-0.5847883,0.0988567,0.0666713,0.1283044,-  
0.2037597,0.2001488,-0.3693623,0.0247225,0.197496,0.1772145,-0.1589623  
, -0.1185374,-0.1731273,-0.06333,0.1167755,-0.0506017,-0.1519353,-0.166  
3979,-0.4800724,0.5399109,-0.0316794,0.4751585,-0.5397371,2.1547383,-0  
.4223814,0.2801902,0.6432592,1.1412249,-0.1506469,-0.1760046,-0.004706  
8,-0.0875531,-0.981971,-0.4907662,0.0293474,-0.6766017,-0.3782921,0.04  
35392,-0.289902,-0.0608155,-0.0359917,0.989153,0.2960189,0.0364904,-0.  
236386,0.0058089,0.0238722,0.2452957,0.0570253,0.1372036,-0.9113087,-0  
.0772355,0.0155779,0.1498254,0.1313422,-0.0507239,-0.0733704,0.0543577  
, -0.0978914,0.4862529,0.0153482,0.0449203,0.0671347,0.0299774,-0.40596  
14,0.3523019,-0.2075683,0.6359093,-2.1177646,0.6134587,-0.0986176,0.01  
8715,-0.4420038,0.4078793,-0.3610044,0.1448551,-0.2445893,0.8493891,-0  
.2914637,0.1894901,-0.5354942,0.4645298,0.0963071,0.0242786,-0.044297,  
0.0268723,0.0637744,0.0340957,-0.0433159,0.028672,0.0420671,0.1104611,  
-0.0050127,-0.0392398,-0.0080509,0.0578561,-0.0437967,-0.0404158,-0.03  
73947,0.0292906,0.1100536,0.0267658,-0.0053254,0.0124105,0.032013,-0.0  
066752,-0.0108217,0.0233705,0.1037425,0.1104932,-0.0020145,-0.0140048,  
0.0241607,-0.0302225,-0.0055985,-0.003997,-0.0604786,0.0852985,0.11902  
4,0.0274119,-0.0415773,0.0271509,0.0561285,0.0233233,-0.0416939,0.0236  
232,0.0654776,0.1052978,0.0063866,-0.0234256,-0.0073943,0.0509973,-0.0  
410488,-0.0287306,-0.0122197,0.052685,0.1096911,-0.0000022,-0.0493319,  
0.01263,0.117343,0.0204254,-0.0445057,-0.0062043,0.0375149,0.1041951,0  
.0145873,-0.0484554,0.0082724,0.1195243,0.0133637,-0.0508399,0.0264051  
,0.0334405,0.0971441,0.0017356,-0.0273612,0.0232179,-0.0060077,0.00397  
81,-0.0191417,-0.0410106,0.0547101,-0.0056525,0.0758305,0.0375784,0.05  
91062,0.0323056,-0.0228561,0.0058409,0.0991633,-0.0299264,-0.029381,0.  
0175508,-0.0284673,-0.0684192,-0.0008426,0.0238409,-0.0361728,0.117248  
7,0.0270608\Polar=71.8377899,-21.8392495,186.2097372,46.0932862,7.9751  
587,145.517195\PG=C01 [X(C12H11O1)]\NImag=0\

## 11

1\1\MF (MLIB83-EXE) -BOSON\Freq\RB3LYP/6-31G(d)\C12H12O1\THEIS\03-Nov-20  
04\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\lme=5methoxy  
\0,1\C,-2.3009606272,0.7776508647,-0.0112238692\C,-2.1742418767,-0.62  
4902992,-0.1433609349\C,-0.9180668339,-1.1990595377,-0.1518224618\C,0.  
2595100136,-0.3909350763,-0.0283152562\C,0.1130957281,1.0280004881,0.1  
04726033\C,-1.1964457127,1.5867277564,0.1096359967\C,1.5545359788,-0.9  
69829836,-0.0358309861\C,2.667458972,-0.1705196097,0.0843570673\C,2.52  
88459162,1.229362968,0.2158562589\C,1.2890832486,1.8382781559,0.228417  
3616\C,1.1791044645,3.3380203448,0.3707117876\O,-0.6852835233,-2.53923  
41468,-0.2738248172\C,-1.7994685256,-3.4062107112,-0.4010424385\H,-3.2  
965033744,1.2138175474,-0.0063936625\H,-3.0675919235,-1.2312139172,-0.  
2364109723\H,-1.3224537796,2.6592536287,0.2095274888\H,1.6481036555,-2



.044838016,-0.1372779321\H,3.6603375834,-0.6124222558,0.0787760205\H,3  
.4215101554,1.843778416,0.3096894771\H,2.17061524,3.7930783467,0.45352  
71515\H,0.6067827848,3.6221850237,1.2630238485\H,0.6746303457,3.793553  
5183,-0.4910006055\H,-1.3877042865,-4.4137872569,-0.483560704\H,-2.386  
0224737,-3.1777045096,-1.3007062189\H,-2.4541402148,-3.3513242398,0.47  
8753297\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7325578\RMSD=4.27  
9e-09\RMSF=2.899e-06\Dipole=-0.4565223,-0.2412205,-0.041039\DipoleDeri  
v=0.1431319,-0.1176517,-0.0020085,0.1259481,0.2790957,0.0424522,0.0217  
98,0.0332173,-0.1027386,-0.0667247,0.3825895,0.0424898,-0.109843,-0.30  
43071,-0.0141705,-0.0056166,0.0045293,-0.2015927,0.0811512,-0.3073222,  
-0.0321433,0.3062154,1.5647355,0.1510902,0.0277655,0.1277193,0.1500079  
,0.0444873,-0.1416638,-0.012456,0.0127104,-0.2804428,-0.0276743,0.0026  
106,-0.0335451,0.0046058,0.2584093,0.0080129,0.0091877,-0.0364781,-0.1  
7469,-0.0220267,0.0048781,-0.0202998,0.0349082,-0.2607988,-0.0649469,-  
0.0098889,-0.1175398,-0.0561112,0.0063499,-0.0150424,0.008322,-0.16682  
01,-0.0633528,0.0805824,0.0099808,-0.0855949,0.0125212,0.0096234,-0.00  
62455,0.015922,-0.1178539,0.0744886,-0.1876006,-0.0111898,-0.0276634,0  
.0061447,0.0106696,0.0044251,0.00463,-0.1131724,0.0554675,0.1640864,0.  
0230759,0.0309423,-0.0096798,0.0130102,0.0100859,0.0180496,-0.128745,-  
0.1296448,-0.053038,-0.0084509,0.0279997,0.3089954,0.0354522,-0.000555  
9,0.0322011,-0.0402186,0.0870558,0.0426406,0.0032952,0.0321644,0.06338  
21,-0.0034135,0.0022673,-0.0027921,0.1103817,-0.4971512,-0.195517,-0.0  
271645,-0.4928484,-1.8618615,-0.1726808,-0.0561832,-0.1612683,-0.30361  
59,0.6035079,0.6129138,0.0692087,0.2698209,0.7926476,0.052654,0.035709  
8,0.0656989,0.3667816,-0.1083243,0.0734923,-0.0011066,0.0677451,0.0224  
314,-0.0060015,-0.0016851,-0.0057903,0.1095686,-0.03599,-0.1012399,-0.  
0162065,-0.0893715,0.0060193,-0.0155704,-0.0150418,-0.0160193,0.128642  
2,0.0635444,0.002449,-0.0015991,0.0378359,-0.0967927,-0.0189679,0.0018  
525,-0.0202766,0.1103217,0.0846911,0.0148241,0.0004856,0.037979,-0.046  
6071,-0.0138722,0.0027528,-0.0147531,0.1088135,-0.1125411,0.0709282,-0  
.0015699,0.0738095,0.0197318,-0.0062145,-0.0012928,-0.0063254,0.111275  
8,-0.0704829,-0.094153,-0.0158074,-0.1174346,-0.0199726,-0.0165725,-0.  
0180988,-0.0157042,0.1018624,-0.1115983,-0.1346371,-0.0202653,-0.03266  
56,0.000113,-0.0083259,-0.0102745,-0.012249,0.0708233,0.0250323,0.0673  
389,0.0979001,0.0081006,-0.0373469,-0.0300834,0.0716177,-0.06014,-0.06  
12548,0.036946,0.0794245,-0.0766785,0.0186728,-0.0563415,0.0334378,-0.  
0621155,0.0680251,-0.0543744,0.0327941,0.0657759,0.0046844,0.002103,-0  
.1498949,-0.022133,-0.0015296,-0.0197047,0.0758366,-0.0608836,-0.12573  
11,-0.0878535,0.0349323,0.0051317,0.0657334,-0.0812239,-0.0080725,-0.0  
989226,-0.0732148,-0.1415573,0.0640806,0.0224599,0.0130984,-0.0427657,  
0.0891421,0.018626,-0.0945205\Polar=170.2651806,14.1258745,160.7598038  
,5.7934972,10.984816,55.0538322\PG=C01 [X(C12H12O1)]\NImag=0\

## 11<sup>+</sup>

1\1\MF (MLIB83-EXE) -BARYON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\03-N  
ov-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\1me-5me  
o\1,1\C,0.3225522427,0.7957524794,-2.291814\C,0.4944420419,-0.5800231  
136,-2.1467194518\C,0.3372222731,-1.1573101133,-0.885747516\C,0.000420  
7397,-0.321875304,0.2424554226\C,-0.1698918429,1.0973322159,0.05654781  
52\C,-0.0042141452,1.6310866599,-1.2160045226\C,-0.1605587478,-0.88603  
17781,1.5121436721\C,-0.4892306298,-0.1182616144,2.6496158741\C,-0.660  
4227504,1.2351475223,2.5189705751\C,-0.5134754323,1.9007598126,1.24481  
02024\C,-0.7042162845,3.250821038,1.2180917969\O,0.4750123149,-2.45564  
91777,-0.6204927313\C,0.8095993074,-3.3754730582,-1.6769529049\H,0.447  
0156393,1.2355098361,-3.2770016857\H,0.7469050099,-1.1837072877,-3.009  
2782728\H,-0.1228118128,2.6922667468,-1.4011462257\H,-0.0255596357,-1.

9578576269,1.6182001837\H,-0.6027687969,-0.6042264814,3.6124425476\H,-  
0.9135643806,1.8419389668,3.3837005815\H,-0.9559467954,3.7915933472,2.  
1254586434\H,-0.6183200996,3.8465121769,0.3157966\H,0.859044259,-4.352  
8572151,-1.1995055837\H,1.7812901767,-3.1216816334,-2.1111689413\H,0.0  
312572863,-3.373845886,-2.4459377745\Version=HP-PARisc-HPUX-G98RevA.1  
1.3\HF=-538.8574403\RMSD=3.282e-09\RMSF=6.967e-06\Dipole=-0.1385221,0.  
5902778,0.2748934\DipoleDeriv=0.0594268,-0.174518,-0.1704286,-0.228216  
4,0.9158476,0.5002994,-0.1296027,0.2189504,0.5136086,-0.1517984,-0.065  
1987,-0.0395664,0.1166311,-0.837219,-0.1031855,-0.177843,0.8494222,0.1  
169724,0.2555632,-0.0978521,-0.1154179,-0.3988596,2.0281884,0.7139651,  
0.1132547,-0.8625078,0.2809984,-0.0538739,0.1029221,0.1343463,-0.08873  
69,-0.159921,0.5755187,0.2798674,-0.427788,-1.1529466,0.0756247,-0.052  
9735,0.0169176,0.13198,-0.0362768,-0.6090589,-0.1233799,0.3586197,0.44  
46616,-0.177312,0.1145674,0.1808998,0.008476,-0.0069732,-0.1348958,0.2  
61374,-0.6899028,-0.9702474,0.1434197,-0.1882995,-0.2297392,-0.0555561  
,0.395426,0.0456494,-0.3305162,0.7405275,1.2397444,-0.1729836,0.208565  
6,0.1453664,0.288729,-0.941058,-0.8840192,0.0846193,-0.4650082,-0.2049  
879,0.0337603,-0.0505603,-0.0616797,-0.2287256,0.8884675,0.5339112,0.0  
734569,-0.3983459,-0.0673682,0.0200081,0.1006144,0.0296593,0.1856461,-  
0.9542106,-0.2168199,-0.0349152,0.2285409,0.0494923,-0.0538584,-0.0814  
307,-0.0325604,-0.0807231,0.4999479,-0.0115909,-0.0330875,-0.0079212,0  
.1074166,-0.3281146,0.2731389,0.1302378,0.4415348,-2.2213235,-0.825018  
3,0.0025091,0.0562446,-0.3198674,0.3486593,-0.2123187,-0.1078652,-0.16  
53165,0.9301819,0.3849809,-0.1439966,0.6330195,0.5707973,0.1185217,-0.  
0006932,0.0130006,-0.0006715,0.0789218,0.0353887,0.0130522,0.0353146,0  
.0257998,0.133853,0.0228362,0.0232287,0.0242031,0.0425413,-0.0513852,0  
.0221747,-0.0441167,0.0590642,0.1184,0.0307464,0.0069185,0.0183771,-0.  
0274943,0.0189974,0.0162936,-0.0457038,0.0736091,0.1042097,0.00723,-0.  
0020386,0.0054043,0.0671994,0.0002507,-0.0006784,-0.0091078,0.1153149,  
0.1364306,0.006375,0.0176124,0.005865,0.0721685,0.0212883,0.0180531,0.  
018505,0.0322224,0.1116732,0.0105243,0.0166039,0.0199305,0.0426522,-0.  
0483886,0.0094593,0.0008627,0.0661991,0.1308962,0.0016393,0.0137261,-0  
.0045561,0.1255513,0.0300818,0.0183984,-0.0022113,0.0391088,0.1230782,  
-0.0018708,0.024911,0.0009869,0.1171935,0.0027006,0.0227782,0.0174727,  
-0.0049578,0.0994541,0.0107176,0.0132613,0.0218564,-0.039679,-0.006112  
3,0.004913,0.0518524,0.0389933,-0.0449778,0.0040537,0.0505786,-0.07385  
12,-0.0012648,0.0093417,0.0587744,-0.1248297,-0.0081727,-0.0300601,0.0  
317847,-0.0579725,0.0555927,0.021133,0.0181008,-0.0249588,-0.131889,-0  
.0454552\Polar=55.6054767,-27.3794415,192.7557884,-29.2992921,31.93340  
79,175.1209638\PG=C01 [X(C12H11O1)]\NImag=0\

## 12

1\1\MF(MLIB83-EXE)-BARYON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\11-Nov-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\6-meo\0,1\  
C,-1.5298625019,1.118607681,0.1260650459\C,-1.9494108,-0.2275774303,-0  
.0141345822\C,-1.0046743154,-1.2315680467,-0.1250620004\C,0.3782881069  
, -0.9408016331,-0.1013217972\C,0.8139494088,0.4203690668,0.0403890852\  
C,-0.1837295943,1.4214369185,0.1512655845\C,1.3544284591,-1.971054721,  
-0.2152196483\C,2.6922272756,-1.6647922922,-0.1896391266\C,3.119538121  
8,-0.3208672024,-0.0496959265\C,2.2173102606,0.716520171,0.0645876617\  
C,2.7034971822,2.1388017097,0.2124600094\O,-3.2593698106,-0.6183571747  
, -0.0487751763\C,-4.267322434,0.3727262513,0.0606236911\H,-2.257225847  
2,1.9177054892,0.2142423612\H,-1.343065022,-2.2582231972,-0.2318999079  
\H,0.1130347531,2.459888589,0.2595368717\H,1.0207005535,-3.0002691449,  
-0.3223503009\H,3.4351436118,-2.4534205108,-0.2768040481\H,4.184965223  
5,-0.1040937342,-0.0321700641\H,3.7968927367,2.1769719692,0.211588141\

H, 2.3555592029, 2.5935327619, 1.1488963552\H, 2.3477006957, 2.7785820759, -0.6053780653\H, -5.2176525263, -0.1621330455, 0.0086566122\H, -4.2174717644, 1.0976998155, -0.7628701537\H, -4.2090581482, 0.9098134932, 1.0168456288  
\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.731119\RMSD=3.709e-09\RM  
SF=3.227e-06\Dipole=-0.329619, 0.5908562, 0.0638787\DipoleDeriv=-0.3215342, 0.0335587, 0.0043056, -0.2683712, 0.0640419, 0.0261734, -0.0275771, 0.0246387, -0.1679232, 1.8328479, 0.0380542, -0.0044102, 0.4844705, 0.0068416, -0.018701, 0.0426238, -0.0164741, 0.1590677, -0.4845821, -0.0134119, 0.0000371, 0.2631523, 0.0794385, 0.0274828, 0.0292643, 0.0288967, -0.1902828, 0.3595185, 0.0035356, -0.0011288, -0.0596745, -0.0965562, -0.0165908, -0.0078181, -0.0169205, 0.0615551, -0.1256226, 0.0017984, 0.000845, -0.0982919, -0.2797633, -0.02948, -0.0097175, -0.0299613, 0.0006147, 0.1480739, -0.1098294, -0.0129637, -0.0250073, 0.1379185, 0.027181, -0.0040037, 0.0276002, -0.1151403, -0.1530942, 0.0075525, 0.0008023, 0.0158051, 0.1157347, 0.0281545, 0.0016851, 0.0282006, -0.1482975, 0.0285309, -0.0602975, -0.007017, -0.0333405, 0.1990959, 0.0316664, -0.0041637, 0.0318187, -0.0954168, 0.0156728, 0.157197, 0.015774, 0.0295925, -0.2230631, -0.0079153, 0.0022956, -0.0085717, -0.1505002, 0.14238, -0.0363606, -0.004722, 0.1850319, 0.2746555, 0.0311707, 0.0186148, 0.0321672, -0.0259331, 0.1007294, 0.0223906, 0.0024237, 0.0028845, 0.0392954, -0.0076044, 0.00043, -0.0075355, 0.110134, -2.209976, 0.2519517, 0.0362018, -0.0831518, -0.3871179, -0.0091689, 0.0008577, -0.0108021, -0.2972177, 0.9689897, -0.204796, -0.0246336, -0.6303332, 0.4811886, 0.0155441, -0.0694904, 0.0133878, 0.3655886, -0.019078, 0.0818077, 0.0093637, 0.1046344, -0.0027455, -0.0136672, 0.0117859, -0.0135539, 0.1200298, 0.0477174, -0.0225408, -0.0020005, -0.0641965, -0.0560874, -0.0186228, -0.0064099, -0.0188394, 0.121158, 0.0549081, -0.0536988, -0.0054312, -0.0346162, -0.0812852, -0.019264, -0.0034145, -0.0191463, 0.1005729, 0.0322674, -0.0822784, -0.0083037, -0.0200262, -0.0955174, -0.0216457, -0.0017194, -0.0213339, 0.1079215, -0.0402811, 0.1022316, 0.011581, 0.1002701, -0.0518185, -0.0178046, 0.0113692, -0.0178157, 0.109798, -0.1398995, -0.0400449, -0.0029838, -0.0654852, 0.0444017, -0.0063147, -0.0056873, -0.0064481, 0.106557, -0.1545584, -0.0658007, -0.0059151, 0.0296293, 0.0447849, -0.0031163, 0.0041756, -0.0026843, 0.0727623, 0.0461579, 0.0256342, 0.0720742, -0.0312678, -0.0492328, -0.0629275, 0.0341761, -0.0855984, -0.0751556, 0.0451795, 0.0409343, -0.0659842, -0.0228413, -0.0807811, 0.0619328, -0.0408453, 0.0839748, -0.0427723, -0.1562225, -0.0409891, -0.0031921, -0.0883154, 0.0194739, -0.0057483, -0.0082022, -0.0059806, 0.0772512, -0.0089539, -0.0220738, 0.0374639, 0.1574219, -0.0700911, 0.0895494, -0.0058629, 0.0952596, -0.0836133, -0.0091709, -0.0145245, -0.0421863, 0.1520262, -0.0328119, -0.0802836, 0.0376341, -0.0842785, -0.1207581\Polar=200.4089493, -8.8957218, 139.0006642, -1.6805146, 9.0423422, 54.8580329\PG=C01 [X(C12H12O1)]\NImag=0\

## 12<sup>+</sup>

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\03-Nov-2004\0\#\N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\lme-6meo\1,1\C, -1.2374648088, 0.6730120805, -1.291242974\C, -1.2211169941, -0.7406323807, -1.3373426962\C, -0.3762519972, -1.4263154843, -0.4656950135\C, 0.4432328111, -0.721685972, 0.4411026822\C, 0.4249788792, 0.7146979611, 0.4859106319\C, -0.4312856235, 1.3749576861, -0.3986924776\C, 1.2948291872, -1.4290499329, 1.319076675\C, 2.1350634921, -0.7906054327, 2.2449135837\C, 2.1389384274, 0.584826147, 2.3105712716\C, 1.3010723197, 1.3867571207, 1.451727676\C, 1.3842290953, 2.7419965639, 1.6012809276\O, -1.9637790678, -1.4895105983, -2.1641792256\C, -2.856721314, -0.85530039, -3.0899244934\H, -1.8847425078, 1.231480272, -1.9573429533\H, -0.3592673323, -2.511087932, -0.4959906444\H, -0.4883614691, 2.4583071967, -0.4108522762\H, 1.2952365981, -2.5156845731, 1.2708977315\H, 2.7704495152, -1.3797916761, 2.8971149443\H, 2.7827661985,

1.0960355351,3.0204877066\H,2.053855184,3.1791777805,2.3359249985\H,0.8016488926,3.4407058404,1.0100448338\H,-3.3319921137,-1.6699650101,-3.6347969739\H,-2.3068759769,-0.2167320945,-3.7901151618\H,-3.6195052908,-0.2723083525,-2.5620531612\\Version=SGI64-G98RevA.7\HF=-538.8501966\RMSD=8.644e-09\RMSF=5.705e-05\Dipole=0.8348772,1.0021605,0.9363161\DipoleDeriv=-0.0216778,0.0812798,0.0849131,-0.2286167,0.2233813,-0.229766,0.0708057,0.1008419,-0.0171417,0.8660804,0.6578526,0.7209773,0.868851,-0.0365889,0.9170137,0.7311053,0.6915387,1.0299688,-0.1375752,-0.3314275,-0.0254696,0.1471605,0.3189241,0.1771787,-0.0045618,-0.334821,-0.1474461,-0.3076093,0.0896488,-0.3760795,0.5162039,-0.2079042,0.5394565,-0.3573183,0.0844443,-0.3290242,0.0010215,0.134915,-0.0131786,-0.3936172,-0.0555196,-0.4239952,-0.0365028,0.1407127,-0.0141705,-0.1997399,-0.2670217,-0.142035,-0.0135728,0.2089784,-0.001415,-0.129677,-0.2717508,-0.2295448,0.6419196,0.3460319,0.6296511,-0.0453935,0.4729012,-0.0302395,0.6124314,0.3880877,0.7385385,-0.2411265,-0.3808017,-0.1581013,-0.6687658,-0.6879409,-0.7404294,-0.1708585,-0.4327541,-0.311338,-0.0554977,-0.1839389,-0.0948959,0.4426808,0.8456433,0.5092279,-0.067728,-0.1601699,-0.0537876,0.1559866,0.2171697,0.1147869,-0.0810829,-0.920127,-0.130323,0.1017426,0.1888046,0.1750554,0.0226221,-0.0260047,0.0803514,-0.0044882,0.5029037,0.0201313,0.0821376,-0.0015329,0.0336444,-1.1267599,-0.306446,-0.9130364,-0.4589204,-0.4718263,-0.4983738,-0.9200329,-0.3358636,-1.2829706,0.7261824,0.0413032,0.4329289,-0.2578704,0.2313608,-0.2796101,0.4196445,0.0402537,0.7730457,0.079361,0.0204821,-0.0514892,0.0287009,0.0958721,0.0291081,-0.0515629,0.0206322,0.0745504,0.1085527,0.0249428,-0.0271853,0.0008144,0.0456844,-0.0032174,-0.0279081,0.0231318,0.1063132,0.0941719,-0.032708,-0.0242809,0.0046575,-0.0296823,-0.0015595,-0.0229863,-0.041916,0.0889771,0.1012828,-0.0279377,-0.0086663,-0.0015304,0.0441022,-0.004413,-0.0077541,-0.0330634,0.0985424,0.0955186,0.018129,-0.0497886,0.0136169,0.0736689,0.0115683,-0.0499391,0.015873,0.0902261,0.0925898,-0.0062403,-0.0256503,-0.0303418,0.0516459,-0.0351717,-0.0264283,-0.0091999,0.0880511,0.0888685,0.0082589,-0.0458281,0.0289519,0.1207608,0.030552,-0.0452565,0.007269,0.084251,0.069108,0.0190059,-0.0609092,0.0123713,0.1232743,0.0131639,-0.0619112,0.0197213,0.0618558,0.0456738,-0.0278369,-0.0603258,-0.052053,0.01287,-0.0596301,-0.0613121,-0.0334365,0.0341929,-0.0602303,-0.08482,0.0267506,0.0295192,0.0145388,0.1490785,-0.01452,0.0119512,-0.0308195,-0.0387222,0.0161652,-0.0134374,0.1427252,0.0230817,0.0416656,0.0383922,-0.0787524,-0.0609682\Polar=121.9287059,14.698911,165.9612977,81.4237601,21.0781255,134.239921\PG=C01 [X(C12H11O1)]\NImag=0\

### 13

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\29-Jul-2004\0\#\N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\En methoxy gr\0,1\C,-0.4107453811,-1.1041283277,1.7898592066\C,-0.6115279746,0.2944752492,1.6782299387\C,-0.3248869236,0.945415798,0.490353031\C,0.1707499845,0.2423731128,-0.633137587\C,0.3747851991,-1.1745870823,-0.5220703884\C,0.0712528124,-1.8083733856,0.7075830999\C,0.4752837489,0.8957145392,-1.8755681297\C,0.9551296331,0.1398267053,-2.9253075351\C,1.1563058258,-1.2585393236,-2.8152526831\C,0.8716671579,-1.902933092,-1.6366340397\C,-1.0848217729,1.0774617123,2.694980331\C,-1.3974944574,0.4656499527,3.9351739041\C,0.2742222931,2.3836221416,-2.0313640047\H,-0.631485884,-1.6247045731,2.7147187814\H,-0.492700746,2.0156960676,0.4471299435\H,0.2255535421,-2.8816344835,0.792590618\H,1.1864791452,0.6323294952,-3.867212991\H,1.5363010747,-1.8133185733,-3.6688121595\H,1.0212442966,-2.9756933577,-1.5378418459\H,-1.751703867,1.2698560956,4.5830143182\H,-0.5155316934,-0.0023758489,4.3925812377\H,-2.1904054115,-0.2868961488,

3.8299058766\H,-0.7718730834,2.6724519994,-1.8665298323\H,0.8787646762  
,2.9531840405,-1.3136886413\H,0.5554806253,2.7103138625,-3.0368868288\  
\Version=SGI64-G98RevA.7\HF=-539.7313614\RMSD=2.058e-09\RMSF=2.095e-05  
\Dipole=-0.1272602,-0.2375711,0.498797\DipoleDeriv=-0.1959122,0.002696  
6,0.068543,0.1046792,-0.0771885,-0.3619583,0.0170084,-0.056872,-0.1939  
23,0.3681051,-0.1666083,-0.5378195,-0.3396551,0.3456193,0.9184127,-0.4  
51111,0.4044199,1.302161,-0.2240535,0.0140045,0.093856,-0.0591801,0.02  
32258,0.0690232,0.1312471,-0.1492996,-0.5072996,0.0735932,-0.0227491,-  
0.1066292,-0.0113164,-0.1349551,0.1179753,-0.1127013,0.1540821,0.29300  
74,0.0136774,0.0104097,0.0547789,0.0440134,-0.2170721,-0.0035327,0.038  
0519,0.0971189,-0.1297946,-0.08009,-0.0198666,-0.1059619,-0.0418317,0.  
1676513,-0.0202484,-0.094588,-0.0857471,0.2076239,-0.0528357,-0.028506  
,0.0354942,-0.0197749,0.2798757,-0.1058013,0.0317693,-0.0807168,-0.098  
0099,-0.118247,0.0167049,-0.0470114,-0.00032,0.0198921,-0.076321,-0.03  
88657,-0.127242,0.0484008,-0.0973569,-0.0731,-0.0284332,-0.0478961,-0.  
014286,0.090561,-0.0413101,0.1650915,-0.0794065,-0.1031833,-0.0083781,  
-0.0883167,-0.0706015,0.1056948,0.0895505,-0.0562035,-0.0958143,0.0853  
316,-0.5233665,0.0972221,0.6341601,0.2369775,-0.4798862,-0.6132652,0.5  
633428,-0.197015,-1.8763757,0.4254983,0.01263,-0.1919317,0.1370452,0.2  
965293,-0.37504,-0.2540555,-0.003802,1.1237703,0.103117,0.0241633,0.00  
77407,0.0205476,0.0469788,-0.0283791,0.0105359,-0.0391141,0.0981247,0.  
1090543,-0.0099158,0.047609,-0.0147864,0.0546587,0.0796514,0.0499153,0.  
.0642035,-0.0595926,0.1095692,0.0254581,0.0125068,0.0333846,-0.0533001  
, -0.0125414,0.0083087,0.0097211,0.0881912,0.095412,0.040093,0.0132259,  
0.0273827,-0.1094962,0.0281838,0.0195858,-0.0109452,0.0537694,0.090498  
6,-0.0101719,0.0471816,-0.0191787,0.0090273,0.1060805,0.0516224,0.0788  
514,-0.0902774,0.0827807,0.0459173,0.0729682,0.0449726,0.0003232,-0.07  
69414,0.073139,-0.0791177,-0.0650171,0.0977869,0.0203602,0.0200316,0.0  
420582,-0.1169999,-0.011653,0.0089434,0.0531475,0.0539745,0.0470916,0.  
0410024,0.0699602,0.0574017,-0.034599,-0.1140064,0.0613572,-0.0652249,  
-0.0723726,-0.1012544,0.06362,-0.0903813,0.0253707,0.0150554,0.1622916  
, -0.0025014,0.0059079,-0.0825529,-0.0763044,-0.0807192,0.0188915,-0.15  
05364,-0.0402691,0.1197819,-0.0142776,-0.0459324,-0.052199,-0.1079308,  
0.0782697,0.005837,0.0339417,-0.0356478,0.0199687,0.039999,-0.0196799,  
0.0766768,0.0074011,-0.0437597,-0.0682852,-0.0350144,-0.0714056,-0.021  
5768,-0.0850516,-0.0886058,-0.0023118,0.05695,-0.0287778,0.0619836,0.0  
023157,0.0205759,0.0197845,0.0458377,0.112585,-0.1218962\Polar=70.9598  
88,-13.8701566,137.5519755,-44.0901555,-1.1001524,186.1458438\PG=C01 [ X(C12H12O1) ]\NImag=0\

### 13<sup>+</sup>

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\19-Jul-2004\  
0\#\N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Monomethoxy\1,  
1\C,1.6037184106,0.315776822,-1.3763905029\C,1.8195677563,0.0099290769  
, -0.0067037855\C,0.7268520574,-0.1908010666,0.8668934903\C,-0.57558327  
23,-0.0954705915,0.4135222151\C,-0.8019829516,0.2155779019,-0.97859371  
4\C,0.3155592507,0.4137191479,-1.8399813474\C,-1.7614780188,-0.2936477  
992,1.2719734704\C,-3.0741144586,-0.1644768755,0.6770914858\C,-3.24359  
84199,0.1324963669,-0.6494462223\C,-2.1061424253,0.3197384901,-1.46742  
18714\O,3.0158644599,-0.1106284969,0.5555228658\C,4.2154942694,0.06953  
34742,-0.2219255332\C,-1.6933653124,-0.5935602764,2.5984184494\H,2.439  
0513753,0.4700132539,-2.0480900647\H,0.9687808445,-0.4203748406,1.8983  
424541\H,0.133496396,0.6471961108,-2.8850825747\H,-3.9374454294,-0.311  
785532,1.3195710869\H,-4.2362550561,0.2249075323,-1.0762439037\H,-2.24  
89669237,0.5552997039,-2.5195656458\H,5.0335950304,-0.0833931461,0.480  
02303\H,4.2591351827,1.0835134259,-0.6305100558\H,4.2681076722,-0.6730

874876,-1.0236482801\H,-2.598677367,-0.7289198404,3.182533714\H,-0.757  
298718,-0.7112292291,3.1338705082\\Version=SGI64-G98RevA.7\HF=-538.860  
1713\RMSD=9.824e-09\RMSF=2.468e-05\Dipole=-0.5590033,0.0106885,-0.0602  
992\DipoleDeriv=-0.4820188,0.0468143,-0.2156375,0.1866331,-0.1578923,0  
.0192527,-0.8402504,0.0163579,-0.2459731,2.2821371,0.0261743,-0.073342  
5,-0.1903134,0.2862995,-0.0780791,0.8869993,-0.0738577,0.6180469,-1.12  
87286,-0.0928309,0.3894879,-0.0833224,-0.1456946,-0.0175465,0.3502058,  
-0.0177221,-0.064393,0.6073811,0.0594328,-0.252357,-0.1207182,0.068418  
4,-0.0077955,0.5508637,-0.0036662,0.0961761,-1.3284068,-0.0375708,0.13  
95474,0.1056006,0.0153134,0.0417779,-0.4962277,0.0386472,-0.159071,0.9  
015127,-0.0081529,0.0548215,0.0315412,-0.028032,-0.0597674,-0.1226356,  
-0.0605814,0.2256618,0.0120316,0.0501811,-0.2232089,-0.0736616,-0.0044  
111,0.1974611,0.3218422,0.1990062,-0.8360062,-0.1732366,-0.094017,0.41  
39196,0.1360472,0.0435693,-0.1696714,-0.6067774,-0.17346,0.7650831,-0.  
1997172,-0.089252,0.3935879,-0.2306724,-0.1548069,0.1739383,1.0240439,  
0.1775944,-0.8833965,1.4305552,0.141112,-0.5978891,0.0426852,0.0680183  
, -0.1040981,-0.1633962,-0.1028459,0.4993723,-2.6061768,-0.0494173,0.17  
07482,0.1284573,-0.26844,0.0146556,-0.6175519,0.0113113,-0.3295496,1.2  
779613,0.0434915,-0.1719952,0.1110004,0.2975166,-0.0050225,-0.4709254,  
-0.0062715,0.3152007,0.1474442,0.0029339,-0.0098554,0.0125027,-0.04843  
08,-0.1251022,-0.0552414,-0.1263314,0.4802173,0.0199444,-0.0091963,0.0  
386429,-0.0087832,0.1357386,0.0142744,0.03687,0.014006,0.0771101,0.072  
0016,-0.006002,0.0262508,0.0040462,0.1221592,0.0278659,-0.0156524,0.02  
79558,0.0057114,0.067449,0.0108815,-0.0492008,0.0012677,0.1155676,0.02  
30178,-0.0060874,0.023299,0.0174934,0.0705181,-0.0004666,0.0023153,-0.  
011456,0.1142864,0.0169269,0.050142,0.0175468,0.0410515,0.0234402,0.00  
3309,-0.0166206,0.0035799,0.1384072,0.0149818,-0.0160739,0.0146078,0.0  
760256,0.1040917,-0.0060357,0.0266485,-0.0000829,0.1057866,0.0209497,-  
0.0003355,0.0209619,0.0170343,-0.0310891,0.0022133,-0.0141123,0.011900  
8,0.1016603,0.0169275,-0.0576504,0.0165233,0.0293779,-0.04418,0.052550  
3,-0.0028162,-0.0295997,-0.0579054,0.0457663,0.1351212,0.0464634,0.037  
0104,-0.0438998,-0.0462791,-0.0244174,-0.0318116,-0.0059319,-0.0658879  
,0.1357162,-0.0652765,-0.0156755,0.0347072,-0.0036755,0.0153704,0.0066  
065,0.1324846,0.0023979,-0.0279828,0.0026831,0.1204542,-0.0137186,0.00  
38026,-0.0198879,-0.0014478,0.1263187,0.0027777,0.0049837,0.0030481,0.  
1130407\Polar=230.2639429,5.0829456,51.6138862,-18.9348056,-24.1051173  
,152.9616652\PG=C01 [X(C12H11O1)]\NImag=0\

#### 14

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\04-Nov-2004\0\#\#  
N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\\lme-8-me0\\0,1\C,2.  
0446990127,-0.199992831,-0.8774817885\C,1.9922601047,-1.610981645,-0.8  
573754\C,0.8802208057,-2.254947499,-0.3811308214\C,-0.2343797502,-1.51  
33332883,0.0987057981\C,-0.2150187487,-0.0739194976,0.0926900588\C,0.9  
781403181,0.5521302851,-0.4184339321\C,-1.375603955,-2.2010385111,0.58  
76261185\C,-2.4629976888,-1.5072327167,1.0555707076\C,-2.4459577999,-0  
.0974992833,1.0503186205\C,-1.3656024837,0.6359953117,0.5875901779\C,-  
1.4781393723,2.1458161112,0.6376721085\O,0.9920792036,1.9189500861,-0.  
4217488499\C,2.1375479027,2.5902419069,-0.9173318592\H,2.9348416346,0.  
2852799466,-1.2584440427\H,2.8445265344,-2.1767138606,-1.2241822813\H,  
0.8298967783,-3.3403345914,-0.3614196116\H,-1.3671163297,-3.2881948097  
,0.5821997995\H,-3.3366962888,-2.0343022289,1.429870537\H,-3.314900178  
,0.4385046436,1.4239673821\H,-2.4503058269,2.4273809975,1.055169603\H,  
-1.3880419607,2.5974969922,-0.3545219017\H,-0.6964173194,2.595673439,1  
.2566231281\H,1.9204554488,3.6561821169,-0.8248614597\H,2.323315202,2.  
3468862415,-1.9717166718\H,3.0327986054,2.3491103663,-0.3292124149\Ve

rsion=SGI64-G98RevA.7\HF=-539.7270489\RMSD=5.827e-09\RMSF=1.326e-05\Di  
pole=0.4799356,0.3635851,-0.2077493\DipoleDeriv=-0.0759027,0.3249696,-  
0.0536772,-0.1582455,-0.292011,0.0680499,-0.0542905,-0.1398801,-0.1792  
298,0.1194838,-0.1068571,-0.0968385,0.1404758,0.2281908,-0.0597832,-0.  
0964256,0.0465481,-0.06407,-0.2561587,0.0135934,0.0378649,-0.058117,0.  
0396488,0.0254318,0.0376776,-0.0058235,-0.1841326,0.2251022,-0.0365787  
, -0.0681328,-0.0538675,-0.1077475,0.0227959,-0.0686155,0.0151758,0.095  
7591,0.0581136,-0.1479588,-0.0310211,-0.0044784,-0.3114961,0.0017553,-  
0.0307265,0.0634349,-0.0003944,0.116384,-0.0594654,0.0040721,0.4486277  
,1.4566138,-0.1908701,0.0050943,0.0283576,0.1227302,-0.176111,0.025308  
,0.0115911,0.0398514,0.1068363,-0.0167494,0.0118087,-0.0106605,-0.1540  
098,0.0894464,0.1039938,-0.0794081,0.000362,0.1300381,0.0001506,-0.079  
4822,-0.0449566,-0.0617695,-0.0028427,-0.222418,-0.0609135,0.013014,-0  
.1404906,-0.0055429,-0.0606576,0.0955423,-0.1177157,-0.0405076,0.12070  
88,0.0077188,-0.1002924,0.3139214,0.0435399,0.0074164,-0.0517275,-0.02  
61896,0.1368195,-0.0904549,-0.0244963,-0.0141489,-0.0025044,0.0057658,  
-0.0243188,0.0378575,0.0906988,-0.6257407,-0.3590053,0.1564692,-0.5835  
744,-1.6427332,0.2493865,0.1563545,0.1520174,-0.3290483,0.6943426,0.54  
73141,-0.1455099,0.257032,0.6078178,-0.1104976,-0.1465655,-0.2359099,0  
.418024,-0.0303791,-0.0804877,0.0684763,-0.0709721,0.0302538,0.0302289  
,0.068511,0.0341606,0.100356,-0.0537317,0.0883407,0.0710357,0.0751326,  
0.0021764,-0.0324239,0.0709673,-0.0376476,0.0808769,0.0568818,-0.04010  
31,0.0250309,0.0153393,-0.1194272,-0.0070174,0.0251785,0.0168434,0.104  
553,0.0598742,0.0349098,0.0211347,-0.0211222,-0.1206337,0.0087209,0.02  
08485,-0.0145712,0.0999255,-0.0644405,-0.083933,0.0752202,-0.0796035,0  
.0086024,0.0340289,0.0753154,0.0363044,0.0786878,-0.057692,0.0706317,0  
.0696425,0.0992343,-0.0007751,-0.0427607,0.0698707,-0.0305603,0.074196  
, -0.1327536,0.1049104,0.0855172,0.009597,0.0130047,-0.0041575,0.085492  
8,-0.0452686,0.0293024,0.0902671,0.005984,0.0109888,0.0130992,-0.05186  
84,0.042079,0.0046577,0.0715425,-0.0787043,-0.0062218,-0.0468708,-0.08  
71747,-0.0214688,-0.0510511,-0.0384236,-0.0810556,-0.0527804,0.0179271  
,0.0475405,0.0364966,0.0113572,-0.0273015,-0.1494681,0.0118375,0.01148  
27,-0.0153928,0.0693088,-0.0309298,-0.1013976,0.0348447,0.0151888,0.02  
65529,-0.0774715,0.059596,0.0427353,-0.1481783,-0.1408413,-0.1016291,-  
0.0437929,0.0662383,0.0265527,0.0419258,-0.0681352,0.0446587,-0.038903  
4\Polar=156.7099265,5.4296656,156.228897,-44.4489704,-2.1992764,72.266  
935\PG=C01 [X(C12H12O1)]\NImag=0\

#### 14<sup>+</sup>

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\03-Nov-2004\  
0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\1-me-8meo\1,1\  
C,-0.4976273511,-0.2033479582,-2.1563235504\C,-0.4459272848,-1.6014792  
688,-2.1015229989\C,-0.1501335709,-2.2328349759,-0.9110755391\C,0.0993  
370492,-1.4572057584,0.249631305\C,0.0515558356,-0.0229016801,0.217040  
8716\C,-0.2552248726,0.590820951,-1.0242294797\C,0.4003432526,-2.12392  
33257,1.4582531465\C,0.6607304906,-1.4481039849,2.6546618018\C,0.62149  
15246,-0.0711071505,2.6529592645\C,0.3232854181,0.6932881682,1.4678290  
15\C,0.323600141,2.0567811611,1.6351595939\O,-0.3003051149,1.938263561  
8,-1.0587982409\C,-0.6089182314,2.6194984471,-2.2869044815\H,-0.731557  
8975,0.2715563692,-3.1013368175\H,-0.6399194553,-2.1772683602,-3.00039  
4524\H,-0.1049074004,-3.3152755071,-0.8476432022\H,0.4283014371,-3.210  
9044151,1.4468176624\H,0.8878126574,-1.9994128141,3.5604870476\H,0.820  
0166822,0.4769038411,3.5696054299\H,0.5401698823,2.4753939566,2.614116  
6087\H,0.1161777207,2.7453095597,0.8301073417\H,-0.5823239485,3.680450  
1633,-2.0406630398\H,-1.6086064336,2.3492539764,-2.6411693049\H,0.1422  
032698,2.4009769866,-3.0524149669\Version=SGI64-G98RevA.7\HF=-538.852

0944\RMSD=3.784e-09\RMSF=2.113e-05\Dipole=0.1285224,0.0225114,0.559658  
5\DipoleDeriv=-0.0722078,-0.0253618,0.0778037,0.062247,0.1833014,0.301  
0749,0.0878862,-0.0747933,0.2761943,-0.0499833,0.1003394,0.0626377,0.0  
281248,-0.2405405,0.0982607,0.0539939,0.4096153,0.2184841,-0.0753283,-  
0.0916163,0.0423955,0.0320101,0.1462301,0.1659704,0.0575649,-0.3612309  
,0.1134823,-0.000708,0.0345956,-0.2098488,0.1111644,-0.130657,0.456374  
4,-0.2004685,0.1253889,-0.7929993,-0.0023068,0.0928456,0.0220045,-0.07  
3993,-0.1373515,-0.3339603,0.0014584,0.3821317,0.049304,0.1398763,-0.1  
246669,-0.1568499,-0.2260141,1.2332487,-0.8459181,-0.1675504,-0.412230  
2,-0.5955349,0.1137138,0.0837931,0.2581189,-0.000978,0.4663702,0.04571  
65,0.2475712,0.4070415,1.1654524,-0.1123273,-0.0988952,-0.0254537,-0.1  
851252,-0.6954858,-0.8647906,-0.0355959,-0.4926238,-0.3223406,0.029902  
7,-0.0884236,-0.0233396,0.109309,0.8480303,0.5689991,0.0011716,-0.2772  
267,0.0023055,0.0495508,0.0669784,0.0275989,0.0057903,-0.9809993,-0.10  
44643,0.0204584,0.1597798,0.1525579,-0.0269943,0.0078851,0.0477549,-0.  
0279494,0.563014,-0.0450992,0.0429462,0.1064508,0.1587191,-0.3099692,0.  
.1251107,-0.1046406,0.2484654,-1.3549806,0.9367836,-0.0909087,0.410828  
4,-0.6193796,0.3375214,-0.1282256,0.1210746,-0.0929426,0.5678759,-0.36  
39535,0.1253231,-0.5219932,0.7771152,0.1242882,0.0145663,-0.0189077,0.  
012691,0.0744216,0.0470897,-0.0192003,0.0562728,0.0553659,0.1247732,-0.  
.0065244,-0.0230263,-0.005945,0.0567651,-0.0337289,-0.0230551,-0.03847  
33,0.0273382,0.1251838,0.0169338,-0.0119212,0.0057678,0.011211,0.00992  
56,-0.0133082,0.0565043,0.0784181,0.1084349,-0.0072319,-0.0045365,0.00  
20461,0.0329398,-0.0005141,-0.0034322,-0.040085,0.0897931,0.1366574,0.  
0078051,-0.0227103,0.0067869,0.0749049,0.0207226,-0.0230017,0.023774,0.  
.0472758,0.1114851,0.0005069,-0.0098223,-0.0101309,0.0450759,-0.051657  
3,-0.01134,-0.0069986,0.0643366,0.1131247,-0.001457,-0.023923,0.008758  
3,0.1166861,0.037669,-0.0230178,-0.0074929,0.0207363,0.1254998,-0.0085  
859,-0.0133202,0.0049358,0.1160522,0.0205637,-0.0110963,-0.035685,0.07  
52796,0.0974478,-0.0081199,-0.0120353,0.0108349,-0.0483341,0.0271305,-  
0.0100029,-0.0528492,0.0505827,-0.0596901,-0.006649,-0.0461573,-0.0835  
138,0.0231455,-0.0313792,-0.0318376,0.0965426,-0.0276592,-0.027945,0.0  
443965,0.0471042,0.0576604,0.0290793,-0.0608155,0.0254418,0.0873523,-0.  
.0648241\Polar=53.4397502,-1.3319515,173.941572,31.6343563,9.8340669,1  
82.7108135\PG=C01 [X(C12H11O1)]\Nimag=0\

## 15

1\1\MF (MLIB83-EXE) -PROTON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\11-Nov-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me1meo\0,  
1\C,-2.9971473756,0.1224362225,-0.0722051994\C,-3.0496372401,-1.291012  
9061,-0.0072590364\C,-1.8859207075,-2.0267834057,-0.005803752\C,-0.618  
3462961,-1.3880989122,-0.0610418158\C,-0.5684913697,0.041976864,-0.110  
9530568\C,-1.785216314,0.7749087462,-0.1247048682\C,0.6011624639,-2.11  
53675405,-0.0766510331\C,1.8060787533,-1.4587071809,-0.1491101486\C,1.  
8873651617,-0.0399606766,-0.1900330806\C,0.7065825998,0.6826794916,-0.  
1580912476\O,0.7350610528,2.0665343384,-0.2191979217\C,3.2307282923,0.  
6431665282,-0.2711805929\C,0.84593179,2.709100102,1.0507115713\H,-3.92  
13722373,0.6941196242,-0.0863509916\H,-4.012585074,-1.7929990205,0.034  
4661768\H,-1.9204912506,-3.1131699699,0.0336439914\H,-1.7396079785,1.8  
563658716,-0.1954753893\H,0.5676423632,-3.2016463873,-0.0431250471\H,2  
.731493745,-2.0297819764,-0.1770956985\H,3.1377320412,1.6395120144,-0.  
71034476\H,3.9281949523,0.0577100172,-0.8802640153\H,3.6891751339,0.75  
67144044,0.7209629423\H,0.8283620777,3.7842773065,0.8557525567\H,1.786  
1454837,2.4476963195,1.5535024838\H,0.0062837732,2.4429030941,1.705844  
6839\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7280478\RMSD=2.919e-  
09\RMSF=8.969e-06\Dipole=0.16916,0.0262742,0.4917841\DipoleDeriv=0.043



3014, -0.1458947, 0.0051173, -0.0777822, 0.0625392, -0.0057252, 0.0037991, -0.0022962, -0.1190029, 0.0304204, 0.1392821, -0.0107129, 0.0769158, 0.0145811, -0.0105204, -0.0065714, -0.0087768, -0.116739, -0.0371431, -0.0209377, -0.021064, 0.079306, 0.1561442, -0.0129687, -0.0081484, -0.0038433, -0.1323163, 0.1109928, -0.001742, -0.0091528, -0.0765816, -0.1645175, 0.0068522, -0.0136994, 0.0011486, 0.0466867, 0.0973634, -0.0510467, 0.0124667, 0.0587032, -0.2165637, -0.0359578, 0.0080831, -0.0003744, 0.0291829, -0.0760188, 0.0299228, -0.0028769, -0.0653761, 0.0676324, -0.0163009, -0.0070138, -0.0361214, -0.1207079, -0.090087, -0.0223854, -0.0052221, -0.0642411, 0.1046626, -0.0167726, -0.0003901, -0.0003951, -0.1393209, -0.0110591, -0.1349099, 0.0049618, -0.082549, 0.1092856, 0.0047814, -0.0072934, -0.0059288, -0.1287606, 0.194839, 0.2478042, -0.0141162, 0.0930006, -0.1285451, -0.0470251, 0.0428994, -0.0061004, -0.0518794, 0.0882767, -0.0202266, -0.0005657, 0.188783, 1.1266827, 0.2177946, -0.002108, -0.0472109, -0.0071011, -0.412738, -0.0968529, -0.0297106, -0.2038366, -1.3655765, -0.3707919, -0.0652604, -0.2993504, -0.5902045, 0.0565362, -0.0321592, 0.004541, -0.0020416, 0.0551463, 0.0174366, -0.0860248, 0.0087293, 0.1192187, 0.3259856, 0.0736516, 0.0281642, 0.0646163, 0.6083912, 0.2257767, 0.1165396, 0.5043252, 0.6733766, -0.0909596, 0.0780394, -0.0027775, 0.0929723, 0.006652, 0.0038105, -0.0006148, 0.0037705, 0.1117955, -0.1005241, -0.0816905, 0.0068285, -0.0861023, 0.0184481, 0.0052549, 0.0088848, 0.0047141, 0.1138659, 0.0512468, 0.0263065, -0.0007698, -0.0331482, -0.1192863, 0.0072932, 0.0041302, 0.0065578, 0.1080978, 0.0868986, -0.0087504, 0.0098913, 0.0203084, -0.0660466, 0.0054477, 0.0005201, 0.0095511, 0.1048552, 0.0445738, -0.040199, 0.0035444, 0.0106503, -0.1169765, 0.0060716, 0.0059062, 0.0056264, 0.112354, -0.0903251, 0.0920611, 0.008865, 0.0736032, 0.0119866, -0.0058793, 0.0101435, -0.0010946, 0.1039363, 0.0437677, 0.0142058, -0.0288308, -0.0555779, -0.0652331, 0.0581498, 0.0121056, 0.0527341, 0.0481857, -0.0699001, 0.0197548, 0.0622516, 0.0717967, -0.0036116, -0.0782869, 0.1022258, -0.0471046, 0.0146047, -0.0830204, -0.046878, -0.044454, -0.079646, 0.0562833, -0.0102031, -0.0899124, -0.0297043, -0.0999766, 0.0694965, 0.0030541, -0.002495, -0.0178837, -0.1869593, -0.0106617, -0.0087244, 0.0103611, 0.0288901, -0.1104839, -0.0127855, -0.103338, 0.0631489, 0.0144848, 0.0251461, -0.0703529, -0.0653646, -0.0429006, -0.0714397, -0.0078029, 0.1104968, -0.0490387, 0.0203963, 0.0372781, 0.0508768, -0.0538524, -0.0650215, Polar=185.6305107, 7.1569535, 142.5017193, -2.3233459, 3.3460325, 55.333366, PG=C01 [X(C12H12O1)] \NImag=0\

### 15<sup>+</sup>

1\1\MF(MLIB83-EXE)-LEPTON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\11-Nov-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\lmeo2me+\1,1\C, -3.0329090618, -0.0102419613, 0.268015605\C, -3.0153571486, -1.4056362372, 0.0797992054\C, -1.8176365031, -2.0838864876, -0.1207441685\C, -0.5998206111, -1.3907145206, -0.1505670543\C, -0.6144553356, 0.0299200188, 0.0381232719\C, -1.8495618788, 0.6998027758, 0.2559629618\C, 0.652625889, -2.0859261772, -0.3397986096\C, 1.8174652267, -1.4105841649, -0.4046559778\C, 1.8666216199, 0.046230717, -0.3048421658\C, 0.6194631662, 0.7454818077, 0.0428938955\O, 0.5180690025, 2.01280217, 0.36424207\C, 3.0108413925, 0.6859569692, -0.6679199874\C, 1.57226538, 2.9269735812, 0.7426668021\H, -3.9752658276, 0.5044430525, 0.4232683905\H, -3.9485980142, -1.960800901, 0.0949231033\H, -1.8178792405, -3.1612218676, -0.2554361476\H, -1.8522321307, 1.7735988729, 0.3997049175\H, 0.6323865328, -3.1660278988, -0.4465823113\H, 2.7561943648, -1.9252222674, -0.5828403388\H, 3.8734973324, 0.1013868183, -0.9755797411\H, 3.1235326424, 1.758398229, -0.7305909397\H, 1.957202269, 3.4310345354, -0.1467803334\H, 2.3649841675, 2.4037526187, 1.2813865305\H, 1.0843730725, 3.6539835227, 1.3909876392\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-538.8532788\RMSD=2.808e-09\RMSF=4.349e-05\Dipole=1.0830294, 0.6821388, 0.0074796\DipoleDeriv=0.1794331, -0.3484714, -0.089098, -0.0623915, -0.44

96994,-0.0686607,-0.043473,-0.0210198,-0.0845478,0.559647,0.0513211,-0.0695032,-0.2611847,0.2975549,0.0970664,-0.0793837,0.0334575,0.0196037,-1.0666065,-0.0234697,0.1339976,0.0751446,0.2019747,0.0298621,0.0905792,0.0406801,-0.1217573,0.8114399,-0.0930481,-0.133175,0.4287769,0.2065495,-0.0077991,0.0288661,0.0513205,0.1243176,-0.8016233,-0.7867336,-0.06328,-0.3751157,-0.5432465,-0.0656596,0.0346918,-0.0177718,-0.0641627,0.1405599,0.5202523,0.077927,-0.1372114,0.0679518,0.0260519,-0.0491883,-0.0604758,-0.0395394,-0.3013535,0.1077243,0.0781123,-0.1170419,0.167794,0.046433,0.0176591,0.0135531,-0.1029386,0.146057,-0.1125733,-0.0509076,0.1603878,-0.0036866,-0.0389996,-0.1361247,0.00006,-0.0827173,-0.8803679,0.0555027,0.245557,-0.0211092,0.0611817,-0.0145349,0.3633581,0.003852,-0.0787266,1.2965095,0.4347775,-0.1502926,0.5084781,1.6879405,0.3995715,-0.1141426,0.2448357,0.3861988,-0.4461157,-0.1706346,-0.0442556,-0.5721939,-1.8345373,-0.4530086,-0.1257789,-0.3525147,-0.3342343,0.3806198,-0.0117618,-0.1358935,0.0468697,0.1066955,-0.022581,-0.170418,-0.0079645,-0.0273028,0.4045755,0.4673993,0.1700768,0.2711794,0.7750939,0.163365,0.0640027,0.1848226,0.337692,0.0165123,0.0286913,0.0143587,0.0438799,0.0576371,-0.0143881,0.0174313,-0.0096938,0.1276863,0.0304355,-0.0368002,0.0028701,-0.0430734,0.0670357,-0.002164,0.007006,-0.0021033,0.1176502,0.0759194,0.0394848,0.008855,0.0041686,-0.0125824,-0.0185456,-0.0071,-0.0209084,0.127225,0.0917073,-0.0212567,0.0004515,0.0025481,0.0238947,-0.012361,0.010897,-0.0060951,0.11013,0.0636691,-0.032399,0.0052462,0.0095941,-0.0010546,-0.0138089,0.0187448,-0.0076664,0.1246238,0.0072461,0.0345818,0.022126,-0.0285328,0.0583622,0.0022596,0.029447,-0.0038293,0.1303209,0.1272385,0.0186954,0.0049684,0.0417315,0.0375324,-0.0200978,0.0175794,-0.002451,0.1267123,0.0879463,0.0273823,0.0007461,0.0257895,0.017615,-0.0027218,-0.0163168,-0.0003739,0.1274361,0.0179388,-0.1157058,-0.0102493,-0.0115826,0.0426595,-0.01763,0.0260346,0.010106,-0.0420331,0.0077227,-0.0464891,-0.0553861,0.0256344,-0.0605264,0.0498,0.0064258,0.0074724,0.0559151,0.050889,0.0135305,0.036748,-0.0147454,0.02786,-0.0414488,0.008827,-0.077292,0.0624479\Polar=212.4121001,30.5330517,148.4610071,-19.9502197,11.6173503,52.7938765\PG=C01 [X(C12H11O1)]\NImag=0\

## 16

1\1\MF (MLIB83-EXE) -BOSON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\12-Nov-2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me3meo\0,1\C,-2.9144836074,1.0103532496,1.7770876629\C,-2.8957018399,-0.4024927415,1.8527390711\C,-1.8805785444,-1.1193519234,1.2564826736\C,-0.8365579114,-0.4589928688,0.5566973391\C,-0.8561473434,0.9687239262,0.4806206091\C,-1.9140505957,1.6785289453,1.1043656891\C,0.2247283901,-1.1694657424,-0.0690428633\C,1.2214630371,-0.492972026,-0.7400462059\C,1.219104031,0.937533448,-0.8275038082\C,0.1928923664,1.6238541418,-0.2222440966\C,2.3276809242,1.6368367003,-1.5709438947\O,2.2773174082,-1.0908340732,-1.3697908862\C,2.3625697588,-2.505719628,-1.3369069271\H,-3.7195749119,1.5655410749,2.2507844276\H,-3.6877211728,-0.9230732791,2.384770081\H,-1.8672424904,-2.2055210173,1.3153234538\H,-1.9223431152,2.7645956426,1.0423353876\H,0.2277275799,-2.2520850334,-0.0039375066\H,0.1773477433,2.7105845801,-0.2798553622\H,2.1853725549,2.7214065272,-1.5489926272\H,2.3707345651,1.3140767577,-2.6179455362\H,3.3071090416,1.4068268337,-1.1350074857\H,3.2658293477,-2.7657823109,-1.8919635961\H,1.492076238,-2.9718173973,-1.8173504453\H,2.4466551293,-2.8790926787,-0.3076651958\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7351855\RMSD=2.968e-09\RMSF=2.200e-05\Dipole=0.2247744,-0.4574844,-0.114096\DipoleDeriv=-0.0772559,-0.1133701,-0.0274127,-0.128381,-0.0261305,0.0744787,-0.0265251,0.0650148,-0.1191474,-0.0298281,0.0675183,-0.0577929,0.0994521,

0.0808726,-0.0748827,-0.0597371,-0.0547172,-0.0737344,-0.0823007,0.048  
9236,-0.0407622,0.0555921,0.1363057,-0.0523445,-0.0411913,-0.0481025,-  
0.1131061,0.1994689,-0.1256707,-0.0858475,-0.1173492,-0.0660168,0.0813  
339,-0.0863154,0.086533,0.1001937,-0.0320584,0.000861,0.0480036,0.0849  
658,-0.2081117,-0.0380103,0.0427278,0.0151007,0.0161753,0.0387958,0.02  
17481,-0.1057079,-0.0934464,0.1582583,0.0413579,-0.0985725,-0.0313965,  
-0.0623956,-0.3533583,0.1759874,0.075686,-0.114415,0.0062934,0.0584322  
,0.0936482,-0.1248311,-0.2676518,0.9803571,-0.6590805,-0.4951332,-0.55  
85259,0.4547512,0.3325453,-0.5014802,0.396076,0.4235179,0.0573256,0.15  
16318,-0.0741072,0.3265373,-0.0496371,-0.2058813,-0.0849138,-0.0954569  
,0.0143768,0.0046122,-0.0197363,-0.094426,0.0174577,0.1349627,-0.02851  
25,-0.0966727,-0.0049935,-0.08558,0.037297,-0.0117563,0.0405414,0.0428  
562,0.1454246,-0.0298773,0.0370988,0.0046021,0.0764912,-1.1180685,0.56  
76034,0.4943257,0.74316,-1.0911257,-0.4190165,0.4837033,-0.3085075,-0.  
5656121,0.3404346,-0.0606985,0.0127256,-0.4852432,0.9343057,0.270523,0  
.0388333,0.0026958,0.3299539,-0.0418539,0.074071,0.0946717,0.0809904,0  
.0073198,-0.0444185,0.0942546,-0.0400581,0.0584179,-0.0394391,-0.06292  
06,0.1000635,-0.0733017,0.0153995,0.052301,0.1006793,0.045734,0.046567  
1,0.0661978,0.0325047,0.0229908,-0.0211729,-0.123321,0.0275582,0.02630  
61,-0.0063228,0.0896058,0.0686897,-0.0250096,0.0255906,0.0288057,-0.12  
08419,-0.0040916,0.0222563,0.0299027,0.0908825,0.0806539,-0.0192151,0.  
029366,0.0340183,-0.0965472,-0.0077187,0.0260328,0.0258626,0.1072789,0  
.0631011,0.0139741,0.0231529,-0.020025,-0.1189777,0.0262914,0.0252387,  
0.0048274,0.0848971,0.0358442,0.0553663,0.017986,-0.0370131,-0.1453813  
,0.0368104,0.0237624,-0.0215029,0.0561963,0.012709,-0.0335477,0.031947  
7,-0.0467144,0.0476975,-0.0385154,0.068251,-0.0157292,-0.1320985,-0.14  
43461,-0.0120249,-0.009179,-0.0003916,0.0559229,0.0555193,-0.0453741,0  
.0317643,0.0167018,-0.0809977,0.0836318,0.0946425,0.0526358,0.013473,-  
0.0293207,0.0965654,-0.0489397,0.0188573,-0.0474494,-0.1165557,-0.1110  
337,0.0478945,-0.0775079,-0.0654018,-0.067383,-0.0103136,0.0042303,0.0  
614692,-0.0342357,-0.0102917,0.0816134,-0.0673878,-0.0191598,-0.071192  
8,0.1027579,-0.1150176\Polar=160.1470985,-9.649405,138.6092658,-66.644  
36,0.8267574,95.6371096\PG=C01 [X(C12H12O1)]\NImag=0\

## 16<sup>+</sup>

1\1\MF(MLIB83-EXE)-MESON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\11-No  
v-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me3meo+  
\1,1\C,0.7345488624,1.0969920681,-3.2799041174\C,0.712652742,-0.32776  
53538,-3.2990605411\C,0.4515629634,-1.0704251042,-2.1628698813\C,0.195  
0729312,-0.4298812912,-0.9316366864\C,0.215708191,1.0260138105,-0.9041  
155384\C,0.4918233771,1.7602887906,-2.110003223\C,-0.0761940283,-1.171  
3420785,0.2512114199\C,-0.3247846283,-0.5355385656,1.4456360748\C,-0.3  
097664634,0.9348797882,1.5008937922\C,-0.0328902775,1.6650224935,0.290  
7136546\C,-0.5491319715,1.6097281025,2.6587154075\O,-0.5889943428,-1.1  
258701624,2.6081808896\C,-0.6320964649,-2.5633354587,2.6852659524\H,0.  
9436755442,1.6421636834,-4.1940578119\H,0.9071955899,-0.8429171624,-4.  
2354516007\H,0.4421885791,-2.1549343587,-2.2109377361\H,0.5023637143,2  
.8455771918,-2.0672700265\H,-0.0819230889,-2.2528829751,0.1864709059\H  
, -0.0241526443,2.7507816525,0.3415498103\H,-0.5350869335,2.6955971577,  
2.6861084242\H,-0.7603400171,1.0866637678,3.5855602494\H,-0.8629015649  
, -2.7882497037,3.725250735\H,0.3399632221,-2.9874111074,2.4157197586\H  
, -1.4180590585,-2.9552500551,2.0325322925\Version=HP-PARisc-HPUX-G98R  
evA.11.3\HF=-538.8565146\RMSD=3.443e-09\RMSF=1.066e-05\Dipole=-0.07686  
25,0.3069389,0.3798168\DipoleDeriv=-0.0780049,0.0977591,-0.0516474,0.0  
18321,-0.5811266,-0.1254267,-0.0583222,-0.4898822,0.1354653,0.0508647,  
0.0366426,-0.1358172,0.1007168,0.6866106,-0.4063606,-0.1304524,-0.1122

712, 0.6100355, -0.1972031, -0.097855, 0.2727098, -0.0202423, 0.1388527, 0.1160512, 0.2792141, 0.4723526, -1.3781649, 0.206497, 0.1281095, -0.2679555, -0.0617917, 0.3353266, 0.2998391, -0.2838612, -0.5720936, 1.4007636, -0.0031614, 0.1146656, 0.1286834, 0.0547114, -0.5403924, -0.2986726, 0.123605, -0.5737857, -0.5933008, -0.0427771, -0.1101828, -0.0598133, 0.0384489, 0.1601143, -0.1586267, -0.0472817, 0.5237473, 0.2074828, -0.2729326, -0.1599376, 0.2513115, 0.0407933, 0.0951777, -0.1611381, 0.268141, 0.7600532, -1.3821757, 0.2983396, 0.261717, -0.3935532, -0.0161133, 0.4494977, 0.0950064, -0.4169941, -1.1803463, 2.0220289, -0.0243614, 0.0766124, 0.2325432, 0.0130249, -0.3226, -0.0893803, 0.2273757, -0.3818012, -1.0520005, 0.046054, -0.1125688, -0.208552, -0.0053476, 0.1831853, 0.039447, -0.1995384, 0.5323582, 0.9641406, 0.0075024, -0.0333412, -0.1175649, -0.0488043, 0.3288271, 0.2534974, -0.1188605, 0.1823037, 0.5442743, -0.3257375, -0.2314043, 0.2846017, -0.1926534, -1.1441911, 0.8095428, 0.2878845, 0.9875689, -1.4973545, 0.3030844, 0.0417505, -0.0184978, 0.1531141, 1.0012233, -0.6435997, -0.0091308, -0.1326089, 0.3290394, 0.1302754, -0.0088677, 0.0240309, -0.0109489, 0.052155, 0.043246, 0.0238528, 0.0336862, 0.0290015, 0.1143234, 0.0076053, 0.0158389, 0.0071589, 0.068374, -0.0369988, 0.0158028, -0.03906, 0.0418129, 0.1254406, -0.0114752, 0.0122691, -0.0008553, -0.0194848, -0.008495, 0.0131618, 0.0402464, 0.0712855, 0.1177739, 0.0084632, 0.0106516, -0.0030434, 0.0036945, 0.004218, 0.0096875, -0.0486402, 0.0713868, 0.1406152, 0.0001213, 0.0143991, -0.0063173, -0.0027582, 0.0166626, 0.0138448, -0.0129838, 0.0790928, 0.1135651, -0.0018036, 0.0136004, -0.001774, 0.027591, 0.0006913, 0.0135772, 0.0007736, 0.0542407, 0.1234694, -0.0154006, 0.0068771, -0.0098782, 0.0519764, 0.039186, 0.0073538, 0.0646327, 0.0969129, 0.1294463, -0.0057352, -0.0046301, -0.0050427, 0.0664151, 0.0179788, -0.0046655, 0.0212238, 0.1517269, 0.0984068, -0.0125642, 0.0287924, -0.0040525, 0.0421702, 0.0133207, 0.0295128, 0.0523991, -0.0260875, -0.0554805, 0.0453385, 0.0154363, -0.0252536, -0.0407881, 0.0880682, 0.0537116, -0.0585524, 0.0853963, -0.0059996, -0.0176486, -0.0537142, -0.0141709, -0.0398503, 0.0919429, -0.0976186, -0.0693204, 0.034997, Polar=54.9965816, 2.0669981, 146.6297005, -40.1815298, -1.0183405, 230.6224076, PG=C01 [X(C12H11O1)] \NImag=0\

## 17

1\1\MF(MLIB83-EXE)-MESON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\13-Nov-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me4meo\0,1\C,-2.9936313002,1.19365222,-0.7359881397\C,-2.9726206736,-0.2070323414,-0.9284239879\C,-1.8214381846,-0.9249597573,-0.6821365616\C,-0.6470822775,-0.2700953746,-0.2339954643\C,-0.6604526273,1.1453998392,-0.0371345309\C,-1.8638659219,1.8515381254,-0.3009028124\C,0.5707051494,-0.9778411024,0.0337966296\C,1.6939500756,-0.3066464744,0.4688091433\C,1.6749218847,1.1043448093,0.663364233\C,0.517520144,1.8047966306,0.4127187517\C,2.9304723016,1.7937963812,1.1410587551\O,0.5082357739,-2.3256226736,-0.1764525243\C,1.6708598104,-3.0998318702,0.0651372676\H,-3.9056701022,1.7512776482,-0.9327214853\H,-3.8681989967,-0.7178571911,-1.2717975691\H,-1.7970038191,-1.9992166596,-0.827235536\H,-1.8775714622,2.928826734,-0.1521509469\H,2.614507497,-0.8437092567,0.6710563806\H,0.4895227385,2.8824244482,0.5571933406\H,3.2559776786,1.4020486671,2.1134882612\H,2.7774984681,2.8719247635,1.2483670441\H,3.7616545383,1.6402964058,0.440632902\H,1.3974122184,-4.1314021492,-0.16432256\H,1.9883340212,-3.0318479239,1.1140267381\H,2.5016207444,-2.7905106107,-0.5827360764\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7342419\RMSD=3.249e-09\RMSF=8.726e-06\Dipole=0.5928449,-0.2761657,0.1400292\DipoleDeriv=0.0686299,-0.1104142,0.0389859,-0.0571471,0.0892579,0.011286,0.0465556,-0.0048301,-0.0986649,-0.0057328,0.1679074,0.0612278,0.0426193,-0.0323707,0.0266576,0.0434354,0.064548,-0.1070716,-0.0206386,-0.1022578,0.0121437,0.0797102,0.06574,0.0488805,0.0379733,-0.0061588,-0.098161,-0.005618

8, 0.1699356, 0.0227276, -0.0534882, -0.2875065, -0.0568476, -0.0089819, 0.010717, -0.0022233, 0.2840576, 0.0541417, 0.0710027, 0.1343024, -0.0799066, 0.0186793, 0.0824041, -0.0055608, 0.0988238, -0.1436009, -0.0302231, -0.0049744, -0.060912, 0.144981, 0.0222118, -0.0093287, 0.0315019, -0.1396845, 0.1539873, 0.0856728, 0.016586, -0.3930626, 1.5214071, 0.0773424, -0.0514081, 0.2221262, 0.1553936, -0.1463495, -0.3592445, -0.0308229, 0.0407391, -0.3140071, -0.002033, 0.0260088, -0.1229902, -0.2226589, 0.3341016, 0.1475821, 0.1274256, -0.0627849, 0.2448532, 0.0183256, 0.09748, 0.0819114, 0.0231902, -0.3759621, -0.0505655, -0.0638293, 0.0569806, 0.0086116, 0.0452158, -0.0485968, 0.0126856, -0.2015582, 0.0561511, -0.025692, -0.0233095, 0.047966, 0.1058081, 0.0123349, -0.0126869, -0.0099018, 0.1158586, -0.566077, 0.338998, -0.0366801, 0.5300617, -1.7630114, -0.0494618, -0.009501, -0.1072734, -0.3037436, 0.6411273, -0.5928424, 0.002259, -0.2529732, 0.7090036, -0.0263045, 0.0504912, -0.1290359, 0.3523361, -0.086012, 0.0877738, -0.0475466, 0.0958427, 0.0096, 0.0144033, -0.0464047, 0.0119642, 0.100033, -0.0799597, -0.0665579, -0.0680225, -0.078646, 0.0165767, -0.0375731, -0.0697377, -0.0339133, 0.0878058, 0.0882642, 0.0018957, -0.0058831, -0.0230839, -0.051587, -0.0297178, -0.0094308, -0.0221651, 0.1026023, 0.0564558, -0.0267936, -0.0193693, 0.0293664, -0.114445, -0.0226788, -0.0114028, -0.039665, 0.098844, -0.0502589, 0.0972402, -0.038068, 0.0750622, 0.0319415, 0.0100326, -0.0412436, 0.0167438, 0.1111251, 0.048243, 0.0187294, -0.015998, -0.0224719, -0.1179053, -0.0391337, -0.0218483, -0.0266734, 0.09952, -0.0347832, -0.0236961, -0.073012, -0.0152983, 0.0222028, 0.0702659, -0.1132306, 0.0335575, -0.1047613, 0.029548, 0.0583312, -0.0040436, -0.0419955, -0.1349601, -0.0419416, -0.0183415, -0.0116025, 0.0632015, -0.1417043, -0.0278607, 0.0491269, -0.0115116, 0.0457664, -0.0513453, 0.0928321, -0.0221384, -0.0214801, 0.0429829, -0.0398625, -0.0163707, 0.017455, -0.1510734, -0.0273329, -0.0082236, -0.044679, 0.0694762, -0.031406, 0.1215837, -0.0330095, -0.0103225, 0.0229837, -0.0494055, -0.0661379, 0.0585533, -0.1386297, -0.1154449, 0.1062188, 0.0794543, -0.066408, 0.0080394, 0.05814, 0.0693246, 0.0422787, -0.0395729, Polar=177.2386888, -7.205992, 146.6994114, 36.2844134, 10.9955857, 66.4228606\PG=C01 [X(C12H12O1)]\NImag=0\

### 17<sup>+</sup>

1\1\MF(MLIB83-EXE)-BOSON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\11-No v-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Naftyl\1,1\C,-3.014144301,1.2588076633,0.2993675419\C,-3.0389220371,-0.1391915668,0.0835148395\C,-1.8696044421,-0.8791562328,-0.0716684866\C,-0.6247669968,-0.242875882,-0.0160284077\C,-0.5836600755,1.1850363598,0.2039043607\C,-1.8075859306,1.9124912027,0.3589673372\C,0.6190654798,-0.9833256816,-0.1738400697\C,1.8240196541,-0.3357131896,-0.1148017096\C,1.8680784636,1.0909174052,0.1048710258\C,0.6449044443,1.8267232705,0.2611227797\C,3.0456720866,1.7884891531,0.1726752421\O,0.4439714857,-2.296800739,-0.3716438175\C,1.594672025,-3.1364406684,-0.5425037394\H,-3.9447188917,1.8041012766,0.4160571086\H,-3.9964676814,-0.650077827,0.0374849982\H,-1.9146619354,-1.9488020329,-0.2359537181\H,-1.760379418,2.9850695368,0.5235480271\H,2.7603710718,-0.8671411975,-0.2292306347\H,0.6929675289,2.8998082637,0.4259184655\H,3.0589795714,2.8617029866,0.3395933176\H,4.0086179196,1.2967458117,0.062844441\H,1.2020215118,-4.1421756556,-0.6860104942\H,2.2282395679,-3.1083445992,0.3506024826\H,2.1668886488,-2.831051652,-1.4251877372\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-538.8521904\RMSD=5.678e-09\RMSF=2.204e-05\Dipole=0.8272815,0.9626911,0.1207372\DipoleDeriv=0.1952457,-0.3964519,-0.0709246,-0.1445293,-0.442695,-0.0514159,-0.0318648,-0.0426903,-0.0843337,0.6247117,0.0278468,-0.0166499,-0.3859863,0.4035965,0.073137,-0.0808996,0.0588572,0.029524,-1.2980387,0.1076736,0.0581631,0.129239,0.0985064,0.0256522,0.0616467,0.0263776,-0.0936952,1.019525,-0.0086157,-0.033444,0.5601888,-0.022

3114, -0.0365535, 0.0546717, -0.0170158, 0.0839035, -0.7432458, -0.4320669, -0.0402546, -0.4159238, -0.3200104, -0.0401994, -0.0377862, -0.039629, 0.0269027, 0.2180298, 0.4502197, 0.0607646, -0.1563136, 0.1641576, 0.0376122, -0.0332582, 0.0166743, -0.0401136, -0.5837284, 0.4413191, 0.0949973, -0.198127, 1.6450403, 0.2338838, -0.0042104, 0.211626, 0.216118, 0.3540654, -0.4214832, -0.0850244, 0.3155144, -0.4587326, -0.0485713, 0.029509, -0.0230789, -0.2211014, -1.2827917, -0.2327661, 0.0106399, -0.1173935, 0.3703919, 0.0498569, 0.0281735, 0.0537013, 0.0826517, 1.1885399, 0.4718855, 0.0326348, 0.1780085, 0.0885422, 0.0057841, -0.0130528, -0.0043617, 0.0112153, 0.63199, 0.0472857, -0.0159725, 0.1516532, 0.1640455, 0.0271375, 0.0007909, 0.0309846, -0.0391745, -0.3967862, 0.2497711, 0.0430192, 0.3147653, -1.7774126, -0.2440204, 0.0532145, -0.241615, -0.3161989, 0.5052939, -0.5888568, -0.098081, -0.2346985, 0.7341477, 0.0731153, -0.0430856, 0.0855905, 0.3306262, 0.0299799, 0.0322337, 0.008607, 0.0435285, 0.0628566, -0.0125956, 0.0103483, -0.0122046, 0.1321508, 0.0430643, -0.0289963, -0.0019173, -0.0330979, 0.0704601, -0.0061517, -0.0025579, -0.0062915, 0.116636, 0.1014762, 0.0051161, 0.0017165, 0.0022125, 0.0508461, -0.0121065, 0.0012706, -0.0122063, 0.1264882, 0.0722953, -0.0454252, -0.0054168, -0.0017593, 0.0099801, -0.0168901, 0.0013675, -0.0153727, 0.1169039, 0.0309231, 0.05308, 0.0123313, -0.0115164, 0.0537911, -0.0145385, 0.0022837, -0.0168, 0.1475149, 0.0517758, 0.0067287, 0.0033317, -0.0049443, 0.0259294, -0.0141677, 0.0015239, -0.0145426, 0.11602, 0.0791215, 0.0585507, 0.0108927, 0.0563552, 0.0504994, -0.0144317, 0.0105629, -0.0146066, 0.1282928, 0.1298102, 0.0276141, 0.0043544, 0.0359382, 0.0447108, -0.0147356, 0.0053437, -0.0144963, 0.1289672, 0.0566729, -0.0449905, -0.0055136, 0.0023944, -0.0429798, -0.0225825, 0.0018668, -0.0209823, 0.0980357, -0.0172399, 0.1169216, -0.0309711, -0.0376912, 0.0267639, -0.0579264, -0.0558174, -0.0093627, -0.0588606, -0.01069, 0.1034063, 0.0627175, -0.0478169, -0.0001239, 0.0807079, 0.0399591, 0.0214446, -0.0384732, Polar=233.9983175, 14.7213919, 148.074112, -4.1901806, 15.2884794, 48.8013819, PG=C01 [X(C12H11O1)]\NImag=0\

## 18

1\1\MF(MLIB83-EXE)-LEPTON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\11-Nov-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me5meo\0, 1\C, -2.4126512867, 1.1913775238, 0.1370514923\C, -2.4625180194, -0.2235468284, 0.0844928354\C, -1.2897145506, -0.9506768826, 0.0121564743\C, -0.0211872698, -0.2865310642, -0.0102749662\C, 0.0083445393, 1.1411879655, 0.0435767866\C, -1.214674787, 1.8635487353, 0.1176299884\C, 1.2054261467, -0.9959260241, -0.0839820209\C, 2.4049440105, -0.3223836182, -0.1033892209\C, 2.4569633234, 1.0972829452, -0.0506417522\C, 1.2690756178, 1.7958350325, 0.0211412918\C, 3.7914759829, 1.8031041837, -0.0738441421\O, -1.2263444948, -2.3137583007, -0.0427105472\C, -2.4413893983, -3.0440533568, -0.0247814247\H, -3.3469793007, 1.743780596, 0.1936323878\H, -3.4263135027, -0.7186869893, 0.1018892138\H, -1.1854470923, 2.9492622445, 0.1583079152\H, 1.1811595868, -2.0792449755, -0.1247840909\H, 3.3356099999, -0.8830606972, -0.1601658616\H, 1.2841948142, 2.8833768494, 0.0624585804\H, 3.6715037554, 2.889940927, -0.0268179599\H, 4.3521004358, 1.5662962314, -0.9872455527\H, 4.4190031721, 1.4975517245, 0.7732334916\H, -2.1592074111, -4.0973278237, -0.0759088859\H, -3.0735200411, -2.7942600941, -0.8871202331\H, -3.0059143107, -2.8628732584, 0.8993933218\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7341724\RMSE=2.883e-09\RMSEF=5.538e-06\Dipole=-0.329635, -0.2601166, 0.0025003\Dipole Deriv=0.1431155, -0.0947744, -0.0131728, 0.1409671, 0.2557255, 0.0087004, -0.0041031, 0.0176163, -0.1080408, -0.0689408, 0.3385448, 0.0078457, -0.1485505, -0.3288723, 0.0008885, -0.0109005, -0.0175407, -0.2062579, 0.1406349, -0.1183535, -0.0046158, 0.5292343, 1.541056, 0.0339437, 0.0203012, 0.0584658, 0.1403473, -0.0273292, -0.1672279, -0.0055653, -0.0217997, -0.2945916, -0.0103524, 0.0000328, -0.0048484, -0.0043849, 0.3064638, 0.0004868, -0.0087381, -0.0

588338,-0.0742345,-0.0035104,-0.0109869,-0.0057531,0.0750815,-0.278694  
1,-0.0279128,0.0030292,-0.095249,0.028159,0.0112333,0.0004376,0.008677  
8,-0.169783,0.0073801,0.0687931,-0.0015707,-0.0837043,0.0614133,0.0095  
383,-0.0074331,0.0037821,-0.1038321,-0.068035,-0.2118535,-0.0108541,-0  
.1286486,-0.0162511,0.0095917,-0.0076403,0.0127383,-0.1381629,0.330236  
5,0.1882261,-0.0058508,0.1250482,0.0756098,-0.0011829,-0.0084008,-0.00  
36026,-0.0163357,-0.2721555,-0.0505902,0.0022335,0.0330223,0.1342105,0  
.0101309,0.00544,0.0132942,-0.1611565,0.0377174,-0.0382209,0.001569,0.  
0441019,0.1231073,-0.0014961,0.0049513,0.0016764,0.1185426,-0.6167722,  
-0.3482759,-0.0008958,-0.6744132,-1.7508815,-0.0308431,-0.0134269,-0.0  
431906,-0.287434,0.7253533,0.6153617,0.0098341,0.2895896,0.6801545,0.0  
013878,-0.0027171,-0.01096,0.3590084,-0.0920493,0.0900614,0.0111665,0.  
0808484,0.0040214,-0.0071981,0.0108162,-0.0075458,0.1109526,-0.0618635  
, -0.0925793,0.0037502,-0.0814751,0.0265324,-0.0009589,0.0041775,-0.000  
5381,0.1313394,0.0470086,-0.0400007,0.0010638,0.0212961,-0.1157569,-0.  
0097204,0.0034207,-0.0073998,0.1154607,0.0826868,-0.0033881,0.000807,0  
.0171732,-0.0570064,-0.0069887,0.0015999,-0.0062099,0.107245,-0.100290  
2,0.081173,0.0108182,0.0820459,0.0178412,-0.0063908,0.0108326,-0.00635  
6,0.1025067,0.0458567,0.0066952,0.0023785,-0.034906,-0.1241678,-0.0073  
958,0.0007654,-0.0089785,0.1017014,0.0213651,0.0564995,0.0039973,-0.05  
65556,-0.1385639,-0.0059414,-0.0004298,-0.0102269,0.0681378,-0.0819605  
, -0.0306594,0.0748482,-0.0242358,0.0364261,-0.0525346,0.116343,-0.0212  
688,-0.0692936,-0.0963786,-0.0228079,-0.0746198,-0.0107745,0.0299334,0  
.0610781,-0.1154351,0.0304858,-0.0483029,0.0379246,0.0422365,0.0031175  
, -0.0242902,-0.156668,-0.0080812,0.0005603,-0.0105951,0.077106,-0.0865  
315,-0.118145,-0.0744635,0.0457409,0.0190721,0.065676,-0.0852477,0.006  
6902,-0.0890115,-0.074743,-0.1232886,0.063888,0.0343684,0.0237316,-0.0  
595738,0.0870424,0.0115876,-0.1054336\Polar=189.9966742,15.5759886,147  
.5638912,-4.5408421,3.0109189,54.3344271\PG=C01 [X(C12H12O1)]\NImag=0\  
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### 18<sup>+</sup>

1\1\MF(MLIB83-EXE)-PROTON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\11-N  
ov-2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me5meo  
\1,1\C,-0.1331938724,1.2615210297,-2.3498824425\C,-0.135651894,-0.152  
3683672,-2.3875106432\C,-0.0695642169,-0.9205598763,-1.2203853631\C,0.  
0020568824,-0.268350969,0.0384778419\C,0.0038727941,1.1776893014,0.064  
3650707\C,-0.0650775153,1.9291507819,-1.1533220909\C,0.0715004672,-1.0  
112031941,1.2632366892\C,0.1399446238,-0.377904984,2.4653163762\C,0.14  
36183282,1.0702570834,2.5232761391\C,0.0739809909,1.8139151952,1.29455  
60138\C,0.2105056205,1.7541308698,3.706696204\O,-0.0678883275,-2.26332  
00397,-1.1855132011\C,-0.1371355039,-3.0066717365,-2.4110395286\H,-0.1  
861443886,1.8094565164,-3.284851327\H,-0.1905518409,-0.6434134977,-3.3  
522909778\H,-0.0624125955,3.0135763563,-1.1103254631\H,0.0679520745,-2  
.0930646863,1.2049177192\H,0.1925421685,-0.9390784024,3.3926825222\H,0  
.076935645,2.9001444582,1.3400714218\H,0.2122156813,2.840482753,3.7374  
892995\H,0.26419723,1.235837578,4.6606765163\H,-0.1200387349,-4.054346  
494,-2.1134125562\H,0.7274678952,-2.7901447275,-3.0476434029\H,-1.0681  
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3\HF=-538.849943\RMSD=5.877e-09\RMSF=1.779e-05\Dipole=0.050905,0.97509  
28,0.8925425\DipoleDeriv=-0.0681002,-0.0215561,0.0262724,0.0046819,-0.  
2610328,0.0834032,0.026197,-0.3790545,0.3935251,-0.0759232,0.0156276,0  
.0373089,-0.0372612,0.0480325,-0.6576033,0.037493,0.2754256,0.5815583,  
0.1594428,0.002262,-0.0892387,0.0546935,1.749632,0.9584822,-0.0893259,  
0.0323989,-1.4104832,0.0688396,-0.0195219,0.0483862,0.0183934,-0.05565  
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114,-0.0129665,-0.3136347,-0.226655,-0.0436755,-0.5182255,-0.7272198,-  
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6,0.4476635,0.0033216,-0.0727307,0.0121641,-0.0293547,-0.0083348,0.113  
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06781,0.0207958,0.0628393,0.5089132,1.1249904,-0.0195483,0.0064066,0.0  
368059,0.0073421,0.2882137,0.1288644,0.0371311,0.1140607,0.6340767,-0.  
2783892,-0.0207868,-0.0092088,-0.0586621,-1.8148712,-1.029662,-0.00919  
64,-0.3612032,-0.4397544,0.3186306,0.0353771,0.028253,0.0227591,0.6772  
453,0.4005186,0.028375,0.6247831,0.8161811,0.1318714,0.0020194,-0.0061  
068,0.002146,0.0555022,0.0380685,-0.0061206,0.0359293,0.0243003,0.1283  
568,-0.003207,-0.0034829,-0.0028525,0.0733577,-0.0499493,-0.0034939,-0  
.0561417,0.0672409,0.1274573,-0.0028281,-0.0028656,-0.0004198,0.010816  
3,-0.0068732,-0.0028882,-0.0497052,0.0769812,0.1260682,-0.0003475,-0.0  
01389,0.0004269,0.0492944,0.007799,-0.0014228,-0.0059662,0.1011137,0.1  
331781,0.0017718,-0.0067353,-0.0016582,0.0579471,-0.0290106,-0.006706,  
0.0313159,0.015274,0.1151302,0.0001568,-0.0040424,-0.0002286,0.021171,  
-0.0036519,-0.0040123,0.0034095,0.0444829,0.1278059,0.0035383,-0.00256  
69,0.0032875,0.0500025,0.058389,-0.0025926,0.0621251,0.0819335,0.13175  
18,0.0012294,0.0006984,0.0016624,0.0439279,0.029582,0.0006611,0.021853  
1,0.1432747,0.1007253,0.0021915,-0.002642,-0.0013782,-0.0540907,-0.024  
5529,-0.0026398,0.038103,0.0547107,-0.0461323,-0.0314765,0.0541187,-0.  
069255,0.0204527,0.0625179,0.040956,-0.1100438,-0.0577327,-0.0569686,0  
.0188286,-0.0542246,0.0758099,0.0204857,0.0542377,-0.0410905,-0.112937  
4,-0.0469505\Polar=46.960702,1.7977188,150.0937047,11.4547709,31.34692  
,248.0914882\PG=C01 [X(C12H11O1)]\NImag=0\

## 19

1\1\MF(MLIB83-EXE)-BARYON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\11-Nov-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me6meo\0,  
1\C,-2.0053546646,0.8020351187,0.0735387785\C,-2.039388622,-0.61493796  
53,0.0044580335\C,-0.857591485,-1.3326234239,-0.0509332035\C,0.3924785  
531,-0.6737169508,-0.0397835863\C,0.434412186,0.7569564219,0.029847468  
\C,-0.7935751625,1.460471155,0.0852868673\C,1.6288346507,-1.3782756491  
, -0.0954380507\C,2.8259395584,-0.7054954711,-0.0827533973\C,2.88133698  
12,0.7173942014,-0.0137036657\C,1.6944941512,1.4157290975,0.0408337693  
\C,4.2187844084,1.4177929937,-0.0019374214\O,-3.1948840338,-1.34731164  
42,-0.0119120055\C,-4.4348256745,-0.6625614576,0.0426777517\H,-2.92517  
54289,1.3740285235,0.1173016018\H,-0.9052557783,-2.4165650043,-0.10342  
83394\H,-0.7745150039,2.5466543395,0.1383945899\H,1.6104580084,-2.4643  
816508,-0.1485187017\H,3.757883798,-1.2654955402,-0.1262424305\H,1.708  
2468022,2.5030114834,0.0940079783\H,4.1007277281,2.5045529406,0.053812  
1384\H,4.7984218883,1.1898563915,-0.9058840749\H,4.8285299418,1.102867  
4588,0.8548628217\H,-5.203995041,-1.4369999838,0.0175683199\H,-4.56983  
88138,0.0061275416,-0.8181289012\H,-4.5396851125,-0.0817717692,0.96899  
09814\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-539.7323924\RMSD=3.166e  
-09\RMSF=1.309e-05\Dipole=-0.3389556,0.397583,0.0252193\DipoleDeriv=-0  
.2424481,-0.0367871,-0.0006211,-0.368894,-0.0350698,0.0130062,-0.01692  
71,0.0073504,-0.1714942,1.5800099,0.45275,-0.0018965,0.9484668,0.26829  
38,-0.0107089,0.0224629,-0.0022996,0.1580658,-0.5051084,-0.1732542,-0.  
0031987,0.1211949,0.1049888,0.0125318,0.01127,0.0175366,-0.1911049,0.3  
108585,0.1413173,0.0025511,0.0799265,-0.0982965,-0.0087368,-0.0004779,  
-0.0097857,0.0513381,-0.0745998,0.0958105,0.0066871,-0.0175788,-0.2178  
033,-0.0124563,0.0011121,-0.014387,0.0409485,0.1984015,-0.1054968,-0.0



106096,-0.0244304,0.168408,0.014627,-0.0066336,0.016044,-0.1197408,-0.0791358,-0.0887114,-0.0053363,-0.0673885,0.1456531,0.0150021,-0.0042608,0.0153837,-0.1356417,-0.0453638,-0.1188379,-0.0072167,-0.1714058,0.132659,0.0145931,-0.0098565,0.0137153,-0.1231712,0.1966442,0.2174431,0.0068145,0.1925875,-0.0526698,-0.0042723,0.0056061,-0.0046939,-0.0326324,-0.0232543,-0.1223844,-0.0081293,0.0829044,0.1319017,0.0123055,0.0019479,0.0157583,-0.1465355,0.0637318,-0.0226837,-0.0000804,0.0629708,0.1195852,-0.0013307,0.0042125,0.000137,0.1248679,-2.1808548,-0.2155813,0.0213958,-0.5917257,-0.4749905,0.001284,0.0028819,-0.0050876,-0.2968142,1.1776389,-0.0253916,-0.0150307,-0.4593013,0.3050217,0.0048279,-0.0363226,-0.00254,0.3659517,-0.0690893,0.0674346,0.0065801,0.0869778,0.0459353,-0.0052573,0.00754,-0.0049197,0.1224351,0.0617865,0.0115644,0.0016156,-0.0336473,-0.071767,-0.0090226,-0.0006072,-0.0097923,0.1228611,0.0480732,-0.0315192,-0.0005589,0.0116444,-0.1103431,-0.0108562,0.0015663,-0.0101421,0.1059219,0.0438599,-0.037476,-0.0007584,0.0170417,-0.1175229,-0.0113572,0.0019281,-0.0104384,0.1070716,-0.1020226,0.0879067,0.0078208,0.0841414,0.0191558,-0.0055575,0.0076435,-0.0056327,0.1025946,0.04474,0.0084997,0.0013654,-0.0427756,-0.1238797,-0.010311,-0.0011628,-0.0111672,0.1000731,0.019434,0.0569046,0.0036431,-0.0610513,-0.1380035,-0.0091458,-0.0021891,-0.0111537,0.0676135,-0.1019087,-0.0297464,0.0756139,-0.029433,0.041,-0.051794,0.1214371,-0.020722,-0.0691638,-0.1086331,-0.0213117,-0.0766564,-0.0154159,0.0327478,0.0623243,-0.1221868,0.0313541,-0.0541498,-0.1130754,-0.07651,-0.0005359,-0.1259092,-0.0277572,-0.0030534,-0.0029691,-0.003891,0.0774017,-0.0503934,-0.0162961,0.0129981,0.1644972,-0.0226354,0.095968,-0.040837,0.0870651,-0.0940706,-0.0492909,-0.017643,-0.0164566,0.1566033,-0.0052182,-0.09261,0.054822,-0.0776915,-0.1126255\Polar=218.7765191,10.2833571,129.2976185,-2.2916152,3.5175492,54.425006\PG=C01 [X(C12H12O1)]\NImag=0\

## 19<sup>+</sup>

1\1\MF (MLIB83-EXE)-BARYON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\11-Nov-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me6meo+\1,1\C,-0.532779778,0.8847655937,-1.8704941222\C,-0.5607061465,-0.5462420081,-1.9007438966\C,-0.2364639772,-1.2989177287,-0.7515507643\C,0.115847406,-0.6696865527,0.4301583093\C,0.1479692883,0.7841983995,0.4732526691\C,-0.1872864897,1.5214853136,-0.7126005758\C,0.452798168,-1.4106699295,1.6227106376\C,0.7956414212,-0.7769559152,2.7703028671\C,0.8337619106,0.6758276833,2.8328974245\C,0.4978306239,1.4195499232,1.6452633948\C,1.1753915424,1.3452072901,3.9717682232\O,-0.8813191892,-1.2537786437,-2.9701161822\C,-1.2345828802,-0.615408134,-4.2152959781\H,-0.782767339,1.4566596188,-2.7554535187\H,-0.2724575771,-2.3808915841,-0.8252151402\H,-0.1622005006,2.606933427,-0.6758661769\H,0.4247095847,-2.4951471165,1.5775567554\H,1.0480120644,-1.3396272339,3.6636800617\H,0.5246391474,2.505804687,1.6867152999\H,1.2006493522,2.4306636285,4.0078602574\H,1.434618861,0.8173119822,4.8853076438\H,-1.4440914854,-1.4345421127,-4.9010116218\H,-0.3976405508,-0.0189754073,-4.5894015791\H,-2.1274445764,0.0031156482,-4.0872516547\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-538.8624668\RMSD=6.077e-09\RMSF=2.764e-05\Dipole=0.1608956,0.9270783,0.5079935\DipoleDeriv=-0.1634839,-0.0795591,-0.0235298,-0.1917984,-0.5427119,-0.6410488,-0.0182889,-0.2555545,-0.2067903,0.476476,0.1349233,0.6285092,0.2277744,0.8285819,0.7582827,0.624503,0.4390885,2.4170684,-0.3023441,-0.0274706,-0.4220994,0.0884776,0.1090085,0.2904833,-0.4278279,-0.1078884,-1.6435806,0.216487,0.0171218,0.3127307,0.1429263,0.1670683,0.4890962,0.3070628,0.056944,1.1773298,-0.0670639,-0.1076213,-0.2835263,-0.1144976,-0.3166568,-0.3778194,-0.2831778,-0.3540496,-0.9391131,0.0320656,0.1010358,0.2017923,0.0020233,0.1775074,-0.002292

6, 0.206415, 0.3378955, 0.6653484, -0.1517561, 0.0159168, -0.1520978, -0.0050094, 0.1570576, -0.0297661, -0.1510901, 0.0421817, -0.6284244, -0.0385803, -0.0140346, 0.1489175, 0.0871465, 0.0627061, 0.2922823, 0.1439997, -0.0553663, 0.4154136, -0.0398143, -0.0579093, -0.3570612, -0.0811225, -0.0241865, -0.2744887, -0.3552831, -0.1940455, -1.1452792, 0.1040279, 0.1021974, 0.3394757, 0.0537651, 0.1821761, 0.1767907, 0.3414878, 0.3423719, 1.1600655, -0.0216128, 0.019552, 0.1787932, 0.0731937, 0.2016393, 0.2382778, 0.1766224, 0.0546985, 0.5290748, -0.4557823, -0.1204039, -0.6685871, -0.2718353, -0.5642413, -0.9198608, -0.6619659, -0.3997041, -2.515869, 0.3775456, 0.0240394, 0.2977906, -0.099466, 0.214543, -0.3384701, 0.3040441, 0.086407, 1.3313885, 0.1297658, 0.0067084, -0.0329442, 0.0085591, 0.0779978, 0.032253, -0.033026, 0.0258662, 0.0246444, 0.1378568, 0.0033982, -0.0184072, 0.000506, 0.0310475, 0.0069139, -0.0183021, 0.0168771, 0.0794911, 0.1146576, -0.010519, -0.0134366, 0.000018, 0.0060285, 0.0052379, -0.0139474, -0.0310607, 0.0722065, 0.1236697, -0.0107745, -0.0167453, 0.0010102, -0.00369, 0.0097144, -0.017327, -0.0307347, 0.0706273, 0.1220393, 0.0099462, -0.032246, -0.0043734, 0.052428, -0.0112596, -0.0316244, 0.0379102, 0.0209284, 0.1099467, 0.0001415, -0.0182287, 0.0032498, 0.0034703, 0.0163172, -0.0184012, 0.0057618, 0.0518645, 0.127519, 0.015007, -0.0113662, 0.0141347, 0.0329205, 0.0531607, -0.0114997, 0.0557142, 0.0886166, 0.1341009, 0.0064361, -0.0032037, 0.0078683, 0.0366591, 0.0315264, -0.0035937, 0.0264715, 0.1215065, 0.0969969, -0.0083638, -0.0339471, -0.016977, 0.0214799, -0.0547753, -0.0336537, -0.0251279, -0.0076216, -0.0438684, -0.0676412, -0.0045354, -0.0258508, 0.0461071, 0.1429509, -0.0523523, -0.0200012, -0.0584777, -0.0188487, 0.0478732, -0.0160472, 0.1002776, 0.0430599, 0.1064941, 0.0272265, -0.0546551, -0.0804183, Polar=65.9529711, 12.2444609, 128.472505, 66.9830171, 38.218543, 274.5395186, PG=C01 [X(C12H11O1)] \NImag=0\

## 20

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\13-Nov-2004\0\#\N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me7meo\0,1\C, -2.0311956992, 0.3353677319, 0.0482716939\C, -2.0007416969, -1.0823199371, -0.0095818085\C, -0.7891791001, -1.7394347399, -0.0568881716\C, 0.4378364058, -1.0334707338, -0.0493662018\C, 0.4019760077, 0.3980318816, 0.0090985585\C, -0.8488922951, 1.0546370889, 0.0570857037\C, 1.7014563176, -1.6830867813, -0.0972538486\C, 2.8684848246, -0.9592104721, -0.0879069339\C, 2.8503731225, 0.4652592819, -0.0300059965\C, 1.6342279626, 1.1118795145, 0.0168421903\C, 4.1525298334, 1.2291921122, -0.0210389559\O, -3.1851333607, 1.0680933728, 0.0976743589\C, -4.4267047473, 0.384017977, 0.0914923495\H, -2.9212805464, -1.6547029232, -0.0169506213\H, -0.76967119, -2.826042901, -0.1011737513\H, -0.897019126, 2.1388684971, 0.1017706556\H, 1.72982327, -2.7697585803, -0.1417057702\H, 3.8262472667, -1.473591729, -0.1251090408\H, 1.6011921464, 2.1987533238, 0.0612544065\H, 3.9833269713, 2.309452536, 0.0250118468\H, 4.744126105, 1.0197958115, -0.9216204069\H, 4.7733940434, 0.9493610653, 0.8398656328\H, -5.1940697901, 1.1593632698, 0.1359858219\H, -4.532595244, -0.2767612821, 0.9623279075\H, -4.5634326343, -0.2046616135, -0.8255430258\Version=SGI64-G98RevA.7\HF=-539.732586\RMSD=3.599e-09\RMSF=1.520e-05\Dipole=-0.3377087, -0.3424552, -0.0078907\DipoleDeriv=1.5980442, -0.4018674, -0.0410033, -0.9355963, 0.2887711, 0.0211236, -0.062298, 0.0115385, 0.1626557, -0.2741735, 0.0412114, 0.0033831, 0.3659484, -0.0656801, -0.0019334, 0.0164355, 0.0036476, -0.1759983, 0.2594634, 0.0785622, -0.0032958, 0.0329175, 0.1835325, 0.011588, -0.0053348, 0.0110934, -0.1164612, -0.1886029, -0.0652081, 0.0010842, 0.0256654, -0.2551367, -0.0118398, 0.0045189, -0.0101626, 0.0212576, 0.4210642, -0.0890088, -0.0096818, -0.0560283, -0.0560142, -0.0044176, -0.0082369, -0.0030269, 0.0717489, -0.5593608, 0.1249405, 0.0113495, -0.1179783, 0.0895971, 0.0135792, 0.0015783, 0.0098824, -0.1951384, 0.1808149, 0.0534562, -0.0030884, -0.1153968, 0.1526844, 0.0128974, -0.0096763, 0.0103435, -0.1175

685,-0.1568581,-0.1981743,-0.0079348,-0.2042299,-0.0712893,0.0065859,-  
0.0079692,0.0061141,-0.1440063,0.3034711,0.1554458,0.001034,0.1899923,  
0.1376479,0.0028422,0.0025157,0.0034104,-0.0164376,-0.2799557,-0.00044  
82,0.0020714,0.0214507,0.1191606,0.0109991,0.0027718,0.0116946,-0.1640  
327,0.0375588,-0.0416313,-0.000332,0.0440127,0.112323,-0.0011342,0.003  
7065,0.0013289,0.1203745,-2.1667456,0.1711785,0.0390261,0.5850675,-0.4  
597744,-0.0165886,0.0554339,-0.0088301,-0.2977283,1.1747337,0.0412456,  
-0.0121842,0.4541855,0.3121677,-0.0099248,0.0045819,-0.0015442,0.36478  
81,-0.068316,-0.0687632,0.0005741,-0.0871911,0.0452783,-0.0016197,-0.0  
002898,-0.0020772,0.1235091,0.0464092,0.0314959,0.0022841,-0.0129826,-  
0.1159043,-0.0086565,0.0007253,-0.0096773,0.106107,0.0632686,-0.012011  
2,0.0005352,0.0323675,-0.0715834,-0.0083194,0.0022972,-0.0080404,0.122  
9062,0.0446899,-0.0320596,-0.0002752,0.028554,-0.1247445,-0.0096127,0.  
0021959,-0.0093968,0.104879,-0.1084838,0.0816562,0.0070335,0.0764247,0  
.0241245,-0.0046159,0.0067204,-0.0045639,0.1055614,0.0454904,0.0145105  
,0.0015578,-0.0316843,-0.1194161,-0.0082193,-0.00035,-0.0094175,0.1024  
672,0.0211735,0.0634237,0.0033368,-0.0522734,-0.1340137,-0.0070802,-0.  
0013158,-0.0092845,0.0682048,-0.0872691,-0.0291697,0.077151,-0.0307359  
,0.0365039,-0.0498779,0.1178839,-0.019594,-0.065697,-0.0943557,-0.0228  
457,-0.0781944,-0.0193401,0.0306814,0.0581123,-0.1194858,0.0270529,-0.  
0529973,-0.1131795,0.0740177,0.0061954,0.1263737,-0.0272035,-0.0063655  
,0.0084744,-0.0056866,0.0771819,-0.0488018,0.0170266,-0.0148108,-0.159  
8582,-0.0226186,0.1005215,0.039801,0.0857081,-0.0961804,-0.0500768,0.0  
130166,0.0141846,-0.1596645,-0.0090918,-0.0880435,-0.0546844,-0.080513  
3,-0.1093956\Polar=218.2069977,2.4493458,129.6349411,-2.7054809,3.0214  
017,54.3702074\PG=C01 [X(C12H12O1)]\NImag=0\

## 20<sup>+</sup>

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\12-Nov-2004\  
0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me7meo\1,1\C,  
-0.1157362173,0.3896343226,-1.9798193644\C,-0.1342674257,-1.0340415649  
, -1.9211236883\C,-0.0704494368,-1.7144933298,-0.7123410706\C,0.0152006  
517,-1.0245284244,0.504477793\C,0.0346590038,0.4257307139,0.4546117482  
\C,-0.0316704479,1.1041212378,-0.7945560345\C,0.0826520859,-1.70154014  
18,1.7688897717\C,0.1653232755,-1.0107725793,2.9363358457\C,0.18636920  
98,0.4402230818,2.9150604706\C,0.119261315,1.1247897099,1.6523368318\C  
,0.2677248111,1.1819861004,4.061370894\O,-0.17461463,1.1011992429,-3.1  
147429348\C,-0.2630665548,0.4301488435,-4.3795240714\H,-0.1996743888,-  
1.6080415719,-2.8386770461\H,-0.0873994173,-2.800183194,-0.712858834\H  
, -0.0170945177,2.188727235,-0.8309797309\H,0.0660617715,-2.7874215795,  
1.771873825\H,0.2165108314,-1.5212167388,3.8924355551\H,0.135778467,2.  
2118106174,1.6455530349\H,0.2830009899,2.2684778984,4.036897201\H,0.32  
02427845,0.7123226904,5.040297669\H,-0.2966876904,1.2252745095,-5.1232  
775919\H,-1.1776417019,-0.1695718563,-4.4434090208\H,0.6178182904,-0.1  
973197718,-4.5542263366\Version=SGI64-G98RevA.7\HF=-538.8485245\RMSD=  
4.451e-09\RMSF=2.137e-05\Dipole=0.0871514,0.0187236,1.4163349\DipoleDe  
riv=0.2147641,-0.0538686,0.0941424,-0.0710948,-0.2995647,-1.0336026,0.  
0990383,-0.7495707,1.9975838,-0.0553465,0.0006362,0.0259181,0.0044046,  
0.2720639,-0.010889,0.0248632,-0.0657158,0.3706517,-0.1062273,0.016907  
3,-0.056657,0.0052102,0.2642366,-0.0048264,-0.0538566,0.1830219,-1.025  
4169,0.1064908,-0.0112641,0.051476,0.0366152,-0.0233235,0.6203537,0.03  
95847,-0.1504255,0.7817848,0.034409,-0.0387789,-0.041381,-0.0412924,-0  
.4388654,-0.5598673,-0.0397343,-0.5035562,-0.4972338,-0.1244793,0.0382  
847,-0.018299,-0.0112338,0.2114143,-0.2625491,-0.0059687,0.5445569,-0.  
3511532,-0.0870231,0.0124118,-0.0280107,-0.0044387,0.2469292,-0.160332  
3,-0.0224849,0.1232868,-0.4960356,-0.0973085,-0.0068454,0.0308337,0.02

22312,-0.0148801,0.3379582,0.0232783,-0.1364668,0.3132365,0.0603984,-0.0217939,-0.0875433,-0.0170378,-0.0941759,-0.2229942,-0.0904054,-0.3057724,-1.3118642,0.0224639,0.0350445,0.0692892,0.0098282,0.2418394,0.1056617,0.0768779,0.4972061,1.1454249,-0.0142026,0.0131739,0.0483316,0.0210251,0.3466249,0.2470093,0.0468052,0.1148692,0.713163,-0.2913846,0.0112258,-0.1128383,0.040087,-0.3561016,0.6660119,-0.1196633,0.203183,-2.2795523,0.3264154,0.0028293,0.0604148,0.025696,0.2786732,0.4264671,0.0559817,0.0643128,1.2143377,0.1226353,-0.0018487,-0.0054782,-0.0030834,0.1024407,-0.0418612,-0.005574,-0.030574,0.0412967,0.1285282,0.0003707,-0.0038892,-0.001906,-0.0044536,0.0058654,-0.0033094,0.0359798,0.0658422,0.134188,-0.0026811,-0.0032652,-0.001092,0.0416994,0.0031655,-0.0040736,-0.0274238,0.0752263,0.1270917,-0.0036249,-0.0027559,-0.0017184,-0.0023105,0.0085491,-0.0037502,-0.0325185,0.0743382,0.1360274,0.0005376,-0.0079062,-0.0025863,0.068691,-0.0287993,-0.0075267,0.0305764,0.0163664,0.1155176,-0.0015721,-0.0032543,-0.001691,0.028279,0.0013151,-0.00417,0.0062176,0.0476792,0.1277099,0.0025868,-0.0017041,0.0026918,0.0550162,0.0586008,-0.0019419,0.0646884,0.0798641,0.1314389,0.0003094,0.0004411,0.0007932,0.0474502,0.0365802,0.0008439,0.0216855,0.1355844,0.1010835,0.0007102,-0.0065789,0.0035761,0.0179942,0.0790028,-0.0075196,0.0342806,-0.0273738,-0.0569386,-0.0652909,-0.0047679,-0.0838002,0.0076498,-0.1302976,0.0399392,0.0427899,-0.0440023,-0.0562516,0.0725402,0.0034828,0.0688157,0.0026748,-0.140523,-0.0372338,0.0353687,-0.0397464  
\Polar=47.3358622,2.3907265,135.3561174,13.5439771,16.6189334,263.2082313\nPG=C01 [X(C12H11O1)]\NImag=0\

## 21

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H12O1\THEIS\12-Nov-2004\0\#\#  
N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me8meo\0,1\C,-2.454777147,-0.0494212602,0.0255771595\C,-2.4134108967,-1.4668037672,0.032435986\C,-1.2180437413,-2.1418010939,0.0236164524\C,0.0086112139,-1.4211294767,0.0071673267\C,-0.0095122932,0.0093371131,0.0001119809\C,-1.2798788213,0.6759241474,0.0099394314\C,1.2694480309,-2.0701422269,-0.002546386\C,2.4422564872,-1.3481915762,-0.0185196271\C,2.4337727107,0.0700076806,-0.0252012151\C,1.2136278763,0.7226850561,-0.0159830803\C,3.7313492484,0.8472749329,-0.0431272823\O,-1.2133674188,2.0401031024,0.0019669928\C,-2.4279093776,2.7710331626,0.0109303995\H,-3.4171527933,0.4489352209,0.0327090502\H,-3.3513133786,-2.0157229395,0.0447681724\H,-1.1919479091,-3.2283777598,0.0288839593\H,1.2967366182,-3.157452645,0.0029116756\H,3.3964368088,-1.8704235123,-0.0257116491\H,1.1775256371,1.8075361926,-0.020940105\H,3.8166513799,1.5068078646,0.8293255857\H,3.8070007222,1.4824852981,-0.9344191419\H,4.5978040834,0.1780940421,-0.0388505782\H,-2.144088484,3.8250312308,0.0026670227\H,-3.0176396326,2.5593260734,0.9126771711\H,-3.0362734433,2.5502999653,-0.8761639788\Version=SGI64-G98RevA.7\HF=-539.7331812\RMSE=2.533e-09\RMSF=3.267e-05\Dipole=-0.3417646,0.3592487,0.0013514\DipoleDeriv=-0.0461663,-0.3323494,0.0002589,0.1347661,-0.2844878,-0.0007616,-0.0022033,0.0036462,-0.202415,0.101517,0.1133133,-0.0029035,-0.131233,0.216922,-0.000272,-0.0014977,-0.00317,-0.1127659,-0.2054229,-0.0115526,0.0005553,0.1063221,0.0453813,-0.0019532,-0.000223,-0.0009498,-0.1665408,0.1786784,0.0414671,-0.0013703,0.0809705,-0.1173656,0.0002799,-0.0014476,0.0004718,0.0552193,0.0608389,0.1888965,-0.0016757,0.0232349,-0.2496046,0.0011755,-0.0004772,-0.0007387,0.0076888,0.1000237,0.099699,-0.0000199,-0.5185221,1.4880093,-0.0017524,0.0027927,-0.0093057,0.1333545,-0.0632311,-0.0310994,-0.0006623,-0.055633,0.1636827,-0.0014213,-0.0004791,-0.0005414,-0.129697,-0.0086122,-0.1395526,-0.0009459,-0.1399539,0.0469536,0.0010194,-0.0001473,0.0004354,-0.1249228,0.2280213,0.2477442,-0.0042241,0.2258563

, 0.0373663, -0.0029016, -0.006904, -0.003478, -0.0274033, -0.1869681, -0.1471342, 0.001425, 0.0482402, 0.047773, -0.00185, 0.0004376, 0.0004986, -0.1257018, 0.1377614, -0.0251315, -0.0004453, -0.1172664, 0.0650494, 0.0013874, 0.005214, -0.0007651, 0.1107551, -0.6152037, 0.3405866, 0.0017177, 0.6710664, -1.7123602, 0.0002269, 0.0002249, 0.0048857, -0.284342, 0.7259581, -0.5994337, -0.0007206, -0.2914431, 0.6696235, 0.001487, -0.002177, 0.0047909, 0.3588224, -0.0639369, 0.0884716, 0.0015147, 0.0822608, 0.0278949, -0.0002949, 0.0014513, -0.0002366, 0.1309257, -0.0912796, -0.0936379, 0.0025333, -0.0795464, 0.0022326, 0.0013566, 0.0025313, 0.0017303, 0.1123061, 0.0451122, 0.03929, 0.0006071, -0.0241843, -0.1205047, 0.0009935, 0.0009069, 0.0011061, 0.11613, 0.0459914, -0.0291717, 0.0007588, 0.0201281, -0.1235451, 0.0013532, 0.0006457, 0.0008622, 0.1069831, -0.1144194, 0.0889781, 0.0021914, 0.0766479, 0.0263537, -0.0006455, 0.0015811, -0.0002237, 0.1048934, 0.0929913, -0.0118832, 0.0000607, -0.030943, -0.0585732, 0.0014556, -0.0000003, 0.0008028, 0.0997528, -0.0454201, -0.0273451, 0.0076023, -0.0785163, -0.0178372, -0.092419, -0.0439999, -0.0990221, -0.0539132, -0.0468133, -0.0277421, -0.0058232, -0.0770293, -0.0138583, 0.0924538, 0.0449332, 0.1000954, -0.0595856, -0.1048822, 0.0359413, 0.0005218, 0.130649, -0.0267294, 0.0005468, -0.001223, 0.001224, 0.0681189, 0.0377027, -0.0443448, 0.0005828, 0.0248928, -0.1557155, 0.0008503, 0.000117, 0.0016282, 0.0772382, -0.0794873, 0.1182464, 0.068448, -0.0392525, 0.0218875, 0.0627891, 0.0868481, -0.0045674, -0.0994204, -0.0827524, 0.1177435, -0.0699874, -0.0415132, 0.0214562, -0.0631033, -0.0869047, 0.0008211, -0.0954833\ Polar=188.2428167, -2.3835417, 148.342449, -1.3960762, -0.4714072, 53.9814347\ PG=C01 [X(C12H12O1)]\ NImag=1\ \

## 21<sup>+</sup>

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C12H11O1(1+)\THEIS\12-Nov-2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\2me8meo+\1,1\C, -0.9231174471, -0.0218191789, -2.2353091807\C, -0.8992153973, -1.4202573666, -2.1679051041\C, -0.4380367784, -2.1183298462, -1.0456014245\C, 0.0226733953, -1.4195150846, 0.0657524284\C, 0.0153916224, 0.0335774095, 0.0377084925\C, -0.4724244461, 0.7210815725, -1.148307332\C, 0.5074761104, -2.0893909793, 1.2452976446\C, 0.9543141085, -1.3955605779, 2.3216874638\C, 0.9538876602, 0.0561135538, 2.3081199215\C, 0.4703693078, 0.7346120734, 1.1334832885\C, 1.3954000959, 0.7968259502, 3.3675574694\O, -0.4429087744, 2.0476550114, -1.0851943426\C, -0.9023385735, 2.8339756976, -2.2032727826\H, -1.2910517319, 0.4641807087, -3.1299327111\H, -1.2550513381, -1.9832002863, -3.0262205755\H, -0.4402222466, -3.2033569225, -1.0432115966\H, 0.5060851819, -3.1751820151, 1.2508742052\H, 1.3179409011, -1.9078737389, 3.2068385222\H, 0.4671734767, 1.819971522, 1.1178175708\H, 1.3894344821, 1.8829492311, 3.3436670792\H, 1.768896064, 0.3271931247, 4.2735331364\H, -0.7728969565, 3.870367374, -1.8959216067\H, -1.9584381854, 2.6300146106, -2.4023153422\H, -0.2948774017, 2.6258169591, -3.0888392599\Version=SGI64-G98RevA.7\HF=-538.8595185\RMSD=3.495e-09\RMSF=3.120e-05\Dipole=0.1669652, 0.3847936, 0.3993676\DipoleDeriv=-0.1015214, -0.2426074, 0.2029273, 0.2242523, -0.8953318, 0.5476587, 0.2002101, -0.5833188, 0.3032683, 0.1666381, -0.0349615, 0.3416974, -0.3649095, 0.6491349, -0.8870118, 0.3442741, -0.0853916, 0.860246, -0.3705516, 0.0685404, -0.5444861, 0.0018577, 0.123336, 0.0023442, -0.5444409, 0.1641936, -1.4647401, 0.2759865, -0.0466457, 0.3487972, 0.2419343, 0.0677318, 0.5862804, 0.347003, -0.1134799, 0.9724251, -0.1609527, -0.0679614, -0.341794, -0.1541808, -0.3838016, -0.3697848, -0.3414916, -0.1625563, -0.8436258, 0.209559, 0.2834949, -0.0609476, -0.4480831, 1.6520182, -1.093687, -0.0565682, 0.6767333, 0.0924253, -0.1814423, 0.0428219, -0.1875602, -0.0415478, 0.1875259, -0.1031549, -0.1873136, 0.1015649, -0.5575331, -0.0061352, -0.0503003, 0.1886228, 0.1238324, 0.0174679, 0.2987346, 0.1865498, -0.1226845, 0.3695757, -0.122231, -0.071288, -0.4422641, -0.0974216, 0.0400916, -0.2362063, -0.4409289, -0.

1706133,-1.0043467,0.1949536,0.1212024,0.3889608,0.083728,0.073196,0.2  
02963,0.3894799,0.2940636,0.9727053,0.0328959,0.0332522,0.224914,0.075  
0512,0.2088951,0.179114,0.224291,0.076396,0.4810245,-0.2883413,0.07391  
97,-0.071963,0.5071471,-1.7813401,1.2374441,-0.0744716,0.1906221,-0.44  
03353,0.3626816,-0.221396,0.1763756,-0.1876926,0.7140186,-0.4568302,0.  
1761405,-0.5379775,0.7205136,0.1309223,0.0171361,-0.0349814,0.0241057,  
0.053476,0.0587369,-0.035182,0.041955,0.0603083,0.1074135,-0.0134117,-  
0.0266733,-0.0159937,0.071608,-0.0387457,-0.0267166,-0.035027,0.053422  
5,0.1274481,0.015572,-0.0237057,0.0029209,-0.0027164,0.0082524,-0.0233  
937,0.0394092,0.0801997,0.1202573,-0.0117651,-0.0201003,0.0032209,-0.0  
047576,0.0089818,-0.0200825,-0.0284891,0.0801618,0.1153304,0.0138622,-  
0.0421976,-0.0083982,0.0599853,-0.0194447,-0.0416554,0.0341384,0.03075  
07,0.1025182,-0.0031658,-0.0171133,0.0016815,0.0464647,0.0039058,-0.01  
74869,-0.007572,0.0674216,0.121583,0.0229547,-0.0191299,0.0213279,0.03  
62769,0.0527555,-0.019177,0.0558684,0.0825815,0.1325702,0.0081814,-0.0  
036228,0.0139305,0.0469623,0.0341533,-0.0037926,0.0215843,0.1250896,0.  
094572,-0.0174186,-0.0234735,0.0100813,-0.0365763,0.0252278,-0.0236524  
,-0.0409576,0.0471414,-0.0608255,0.0190592,-0.0432862,-0.0742775,0.028  
5851,0.006341,-0.0259991,0.1045597,-0.0157603,-0.0033282,0.060924,0.03  
10044,0.0574326,0.0277534,-0.0480278,0.0144051,0.0869786,-0.0729183\Pol  
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=C01 [X(C12H11O1)]\NImag=0\

## 22

1\1\MF(FIRST)-NEUTRON\Freq\RB3LYP\6-31G(d)\C13H14O2\THEIS\29-Jul-2004\  
0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3LYP/6-31G(D) FREQ\  
\smgl.med orto subst.\0,1\C,-2.183069001,-0.3499148869,0.433434005\C  
, -2.1336867636,0.7398365727,-0.4678338606\C,-0.9129415719,1.2027899448  
, -0.9305998541\C,0.3047405117,0.6103269664,-0.5235026173\C,0.250239215  
2,-0.4937675793,0.3899334213\C,-1.008870847,-0.9456854354,0.8461782076  
\C,1.5776188028,1.0813979991,-0.9964314025\C,2.7135811728,0.4468793382  
, -0.5491170763\C,2.6813967318,-0.6460592705,0.3536140932\C,1.470772486  
7,-1.1111800875,0.8174348021\O,-3.2407528203,1.3943789758,-0.933540421  
6\C,-4.5180386413,0.9650965356,-0.4925758441\C,1.6660859551,2.24097454  
27,-1.9578575288\O,1.3182997348,-2.1542426137,1.6872792906\C,2.4847702  
596,-2.8114758752,2.1517063632\H,-3.1307399157,-0.7233121455,0.8041407  
246\H,-0.917252999,2.0396508655,-1.6198455764\H,-1.0426965861,-1.78091  
63655,1.536644255\H,3.6841810627,0.7923276484,-0.8983561062\H,3.615692  
3175,-1.0985553241,0.6643749968\H,-5.2390430722,1.6212057677,-0.984230  
3756\H,-4.6270016999,1.062079947,0.5959125395\H,-4.7210769742,-0.07441  
9334,-0.7828936687\H,2.7094443081,2.4585199084,-2.2066205627\H,1.22696  
55846,3.1557877207,-1.5384655003\H,1.1364250465,2.0358869158,-2.897536  
5018\H,2.1389530462,-3.5989910226,2.8240779242\H,3.1409159213,-2.12454  
43682,2.7024671919\H,3.0492687793,-3.2611236993,1.3241234557\Version=  
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06\Dipole=-0.0501491,-0.4321984,0.3606939\DipoleDeriv=-0.2163531,0.084  
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.1479336,1.5408847,-0.4105979,0.2464994,-0.7788419,0.3611599,-0.110747  
3,0.5504697,-0.1355716,0.2383773,-0.6152155,0.1307197,-0.0795953,-0.03  
89918,-0.0629347,-0.1057062,0.0603349,-0.1170071,-0.1019086,0.4847257,  
-0.1233164,0.0723018,-0.0330169,-0.0215498,0.0569819,-0.0020624,0.0629  
568,-0.0068503,-0.2067046,0.076988,-0.0505135,0.0043819,-0.2123369,0.1  
64076,0.0092908,0.159271,-0.1447391,0.2376817,-0.0250147,-0.0016208,-0  
.0023102,0.011452,-0.0885238,-0.0203541,-0.087025,-0.0231048,-0.304993  
5,0.0865292,-0.055783,0.091067,0.062231,-0.1168434,-0.059564,-0.116474  
7,0.0277724,0.1426753,0.0645903,-0.0710887,-0.1191139,0.1064088,-0.183

4309, 0.0802427, -0.1956477, 0.0300554, -0.1391237, -0.3129326, 0.2537355, 0.0871142, -0.2980481, 0.0734114, -0.0759144, 0.1000295, -0.2793255, 0.2499804, 0.2119471, -0.1824482, -0.3591062, 1.0010447, -0.6908353, 0.2881792, -0.7289109, 0.7153144, -2.0932878, 0.284355, -0.1138947, 0.5763808, -0.4541101, 0.092978, -0.3547361, 0.1126972, -0.363857, 1.1877742, -0.0477503, -0.0160928, 0.2772396, 0.304409, 0.0289725, -0.2844386, 0.0507806, 0.3392736, 0.084026, 0.0348122, -0.0260026, 0.0259597, 0.1116394, 0.008786, -0.018717, 0.0081846, 0.1189106, -0.5721447, 0.2200446, -0.1622678, 0.4675028, -1.2615484, 0.7738419, -0.3663174, 0.7904423, -0.9119004, 0.6659559, -0.5092613, 0.3992825, -0.2315964, 0.6186371, -0.198803, 0.1705137, -0.1804277, 0.4960932, -0.0786634, -0.039236, 0.0456902, -0.0572383, 0.0833437, 0.0358734, 0.0604746, 0.0346841, 0.0896405, 0.0847211, -0.000775, 0.0027906, 0.0179437, 0.0108426, 0.0864433, -0.012612, 0.0876764, 0.0458112, 0.0857218, -0.0094644, 0.0092122, -0.0164259, 0.0151432, 0.0766047, 0.0149841, 0.0761412, 0.0430499, -0.1001514, -0.0612393, 0.0639489, -0.0679539, 0.0463817, 0.0506922, 0.0695037, 0.0502289, 0.0563866, -0.0536789, 0.0840487, -0.0569008, 0.0691708, 0.05268, 0.0608733, -0.0446644, 0.059882, 0.0857654, -0.1007665, 0.0673591, -0.0435178, 0.1067904, 0.0010521, 0.0553342, -0.0759687, 0.0579805, 0.0343692, -0.0557733, 0.0097588, -0.0233852, -0.0843428, 0.043268, -0.0193823, 0.1334251, -0.043631, -0.1525387, -0.0603863, 0.0153366, -0.0035562, -0.1576804, -0.1249334, -0.0654958, 0.060735, -0.0592663, 0.0200057, -0.1371174, -0.0862495, 0.0849634, -0.0057423, 0.0415088, 0.0249709, 0.0186132, 0.0303302, 0.0451093, 0.0501875, 0.0961271, 0.0207618, 0.0379889, -0.139287, 0.0106849, 0.0376247, -0.0293985, -0.0101129, 0.0356172, -0.0025365, -0.1121985, -0.0331372, -0.0090886, 0.0049156, -0.0559214, 0.0390742, -0.1257055, 0.0356182, -0.0407066, 0.0363097, 0.0115874, -0.0645241, 0.1156627, -0.0068048, 0.1191534, -0.0210778, -0.083737, 0.0551626, -0.1413606, -0.0835819, -0.051237, -0.088871, -0.0434361, -0.0283463, -0.0200739, -0.0674726, 0.1470244, -0.0282921, 0.0298775, -0.0108428, -0.0187172, 0.0847049, -0.096233, -0.0768065, Polar=211.4158298, -15.8584023, 129.0238371, 3.340325, -51.3015094, 107.537329, PG=C01 [X(C13H14O2)] \NImag=0\

## 22<sup>+</sup>

1\1\MF (FIRST) -LEPTON\Freq\RB3LYP\6-31G(d)\C13H13O2(1+)\THEIS\29-Jul-2004\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3LYP/6-31G(D) FREQ\smgl. med orto subst.\1,1\C, -2.1886241573, -0.3068417523, 0.44414061\C, -2.1447036048, 0.744961454, -0.5002734573\C, -0.9074576905, 1.1945170444, -0.9985565241\C, 0.2870234256, 0.6255530052, -0.5825537502\C, 0.2418621256, -0.440280848, 0.3747513702\C, -1.0101360153, -0.8815026776, 0.8668358789\C, 1.6026565963, 1.0730152461, -1.0855276219\C, 2.7822547781, 0.4051077237, -0.5778253676\C, 2.7253490946, -0.6060198257, 0.3318671289\C, 1.4551464012, -1.0437048249, 0.8211516359\O, -3.2160988668, 1.3771706044, -0.9825723314\C, -4.5323394641, 1.0027903689, -0.5449623905\C, 1.7816139697, 2.0674782195, -1.9921760501\O, 1.3321679644, -2.0161243109, 1.700857835\C, 2.4799283503, -2.7135377661, 2.2386305107\H, -3.1330060704, -0.6632625576, 0.8364006837\H, -0.938129186, 2.003246028, -1.7193318881\H, -1.0352938906, -1.6878586435, 1.5904007019\H, 3.7485023353, 0.7355862959, -0.9481681616\H, 3.6355753829, -1.075628096, 0.6821990158\H, -5.2112223241, 1.6631508502, -1.082789014\H, -4.6412818836, 1.15782583, 0.5332583603\H, -4.7456555909, -0.0390964027, -0.8046355787\H, 2.7789706799, 2.3456511947, -2.3188674368\H, 0.9622893073, 2.6261241386, -2.4311171878\H, 2.0622614454, -3.4447936041, 2.928295245\H, 3.1285203504, -2.0177939031, 2.7768595352\H, 3.0244738062, -3.2207336819, 1.4381998586\Version=PA64H-G03RevC.02\State=1-A\HF=-653.4022187\RMSD=7.201e-09\RMSF=1.458e-05\Dipole=1.099869, -0.3382873, 0.2180147\DipoleDeriv=-0.2541477, 0.1735645, -0.1479684, 0.5795362, -0.3668076, 0.1416434, -0.5112054, 0.1730823, -0.2735729, 1.9711612, -0.3726012, 0.1994805, -0.9242768, 0.6038877, -0.2431458, 0.6934426, -0.2857913, 0.4539794, -1.1230467, 0.

0666685,0.0159999,-0.0530815,-0.0381865,-0.0996245,0.1227721,-0.109085  
1,-0.0663737,0.483574,0.0358052,-0.0656982,-0.4751159,0.2632882,-0.148  
3521,0.391391,-0.1881882,0.1944974,-1.3080313,0.3952594,-0.2561276,0.5  
610179,-0.3615734,0.235727,-0.4048702,0.2488251,-0.2409878,0.7592638,-  
0.2658334,0.1763725,-0.0212662,0.0680584,-0.0904324,-0.0424993,-0.0715  
47,0.0324328,0.0619683,0.1224053,-0.1117509,-0.1684646,-0.4432517,0.44  
3814,0.1497219,0.4222303,-0.3530446,-0.0588292,-0.2097445,0.1934652,0.  
3029899,0.5084682,-0.4724995,-0.2665005,-0.4331438,0.416165,-0.3855266  
, -0.4726888,0.4393821,-0.4817216,-0.5328021,0.3539315,0.4473604,0.3524  
97,-0.5301094,1.6138365,0.3386047,-0.4060166,-0.755468,1.3640239,-0.89  
97021,0.5739851,-0.9836079,1.1297652,-2.3618446,0.3778995,-0.17577,0.7  
833405,-0.4841523,0.1261009,-0.5385763,0.1576103,-0.3742938,1.3210128,  
-0.1056124,0.0156923,0.1966941,0.2511725,0.0357692,-0.2548358,0.059295  
9,0.2750184,0.0748842,0.0403936,-0.050122,0.0142953,0.1931364,-0.27204  
3,-0.026853,-0.274279,0.1394145,-0.5283388,0.098371,-0.0665771,0.87170  
89,-1.3810523,0.9471907,-0.7589035,1.0069665,-1.0908682,0.6437646,-0.4  
971084,0.4171712,-0.3456472,0.6573726,-0.3121243,0.2819516,-0.3012896,  
0.5271139,-0.0025994,-0.0155727,0.024625,-0.0206937,0.1062664,0.027440  
8,0.0291995,0.0270529,0.1086583,0.0798351,-0.0282297,0.0289319,0.00299  
26,0.0564594,0.0630839,0.000796,0.0655109,0.0685646,0.0949101,0.015347  
1,-0.0121525,-0.0041181,0.0658607,0.0444951,0.0053182,0.0430121,0.0763  
19,0.0380137,-0.0044783,0.0100858,-0.0328286,0.0803801,0.0358194,0.035  
5434,0.0336184,0.0846508,0.0344252,0.0312253,-0.0197231,0.0312512,0.08  
69573,0.0462428,-0.0197352,0.0462006,0.1014498,-0.0247669,0.0311806,-0  
.018095,0.0618111,0.0437395,0.0464562,-0.0454819,0.0488417,0.0609072,-  
0.0637013,0.0067508,-0.0505011,-0.081096,0.0683706,-0.0202896,0.099432  
6,-0.0430743,-0.0807681,-0.0619405,0.046849,0.0050065,-0.1130098,-0.06  
72107,-0.0493315,0.0767368,-0.0458421,0.0530651,0.0139566,-0.0035079,0  
.0122604,0.0267659,0.1185628,0.0106505,-0.0149988,0.0130737,0.1221273,  
0.0009699,0.0376232,-0.0239052,0.0201437,0.1140862,0.0119965,-0.008097  
1,0.0105412,0.1203403,0.0365376,-0.0291051,0.0317469,0.0150959,0.03575  
01,0.0630065,-0.0080554,0.0665603,0.0481561,-0.0323057,0.0696784,-0.10  
65917,-0.0297016,-0.0505384,-0.0353578,-0.0358608,-0.0026406,0.0484255  
, -0.0230349,0.1168565,-0.0592209,0.0388466,0.0397339,0.0095344,0.02882  
19,-0.0364303,-0.0510319\Polar=229.798073,-17.6518823,135.6265566,2.39  
80967,-68.8264193,118.7283989\PG=C01 [X(C13H13O2)]\NImag=0\

## 23

1\1\MF (MLIB83-EXE) -NEUTRON\Freq\RB3LYP\6-31G(d) \C13H14O2\THEIS\28-Aug-  
2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\dimet\0,1  
\C,-3.5608220897,-0.330217995,0.0068022172\C,-3.0064086319,-1.47485116  
6,0.6278378853\C,-1.6444411526,-1.5895427159,0.7834119618\C,-0.7708949  
861,-0.5659238265,0.3229055462\C,-1.3260289901,0.6000785007,-0.3038135  
68\C,-2.7394161566,0.6783885801,-0.4445653291\C,0.637135605,-0.6797222  
577,0.4839022498\C,1.4712750049,0.3405116957,0.0443574452\C,0.91390669  
5,1.4815047076,-0.5818282899\C,-0.4482625888,1.6290719292,-0.762776947  
\C,-0.9861385705,2.8703619038,-1.4351096814\O,2.8136063119,0.169009706  
6,0.2545532548\C,3.7004457904,1.2087449004,-0.1237550127\O,1.134409327  
4,-1.7859183625,1.1342943947\C,1.8936619921,-2.6889673169,0.3265644061  
\H,-4.6380438823,-0.2474414802,-0.1107351688\H,-3.6617997825,-2.264890  
4526,0.9852618292\H,-1.2082590747,-2.4560750264,1.2676789957\H,-3.1761  
659565,1.5533610973,-0.9158287879\H,1.5720004434,2.2708404467,-0.92857  
37759\H,-1.5439722355,2.6299294651,-2.3491259541\H,-0.1723835731,3.547  
2145477,-1.7125930874\H,-1.669846732,3.4245913577,-0.7796228397\H,4.69  
65598366,0.8680341248,0.1654486444\H,3.4739078402,2.1459505624,0.40117  
11567\H,3.6823463071,1.3886384172,-1.2070989343\H,2.1466374314,-3.5326



09994,0.9734819239\H,2.8116490399,-2.2197841035,-0.0402270616\H,1.2991  
736969,-3.0491113514,-0.5236154362\\Version=HP-PARisc-HPUX-G98RevA.11.  
3\HF=-654.2454575\RMSD=4.209e-09\RMSF=2.941e-06\Dipole=0.5082362,0.447  
4787,-0.6682092\DipoleDeriv=0.0697037,-0.1195102,0.0748407,-0.0405934,  
-0.1003228,-0.016204,0.0332543,-0.022551,-0.1097647,0.0027628,0.093382  
3,-0.0380632,0.0333858,0.1156708,-0.1131864,-0.0087477,-0.1092866,-0.0  
609707,-0.1126069,-0.0670378,0.0363688,-0.0133795,0.0159542,-0.075281,  
0.0145237,-0.0813862,-0.0752003,0.2637193,0.142323,-0.0509869,0.034248  
6,-0.1617817,0.0602488,0.0049057,0.0677399,0.0129271,-0.052438,-0.0104  
326,0.0017116,0.1918106,-0.1839486,0.1063635,-0.0965055,0.0919347,-0.0  
42807,0.0487121,0.0443494,-0.0076699,-0.0885283,0.0241647,-0.0847598,0  
.0601349,-0.0665149,-0.0886006,-0.0017539,-0.3317436,0.1216096,-0.6771  
749,0.7971099,-0.2811241,0.4013924,-0.5172749,0.1475695,1.6558043,0.17  
46766,0.101434,-0.0231725,-0.1081009,0.0706619,0.1406662,0.1640086,0.0  
813189,-0.2237121,-0.0234506,-0.0013316,0.1030775,0.0068262,-0.0781,-0  
.0566046,-0.0939879,-0.1389311,0.0382869,0.0147587,0.0052786,-0.054783  
9,0.218341,-0.1401445,0.0298136,-0.1272469,0.0319565,0.0641421,0.03913  
45,-0.0210158,0.0122737,0.1091285,0.0056583,-0.0088559,0.0049526,0.107  
4762,-2.0227618,-0.5210467,0.0432866,-0.217747,-0.4741417,0.052635,-0.  
0853284,0.0113887,-0.2857727,0.8421333,0.2869345,-0.0656147,0.6182724,  
0.5994052,-0.0437978,-0.233597,-0.0925402,0.3726007,-0.7683907,0.62739  
7,-0.0751545,0.6354607,-1.1903957,0.0979887,-0.1093767,0.20788,-0.4716  
804,0.56851,-0.4027265,-0.0040997,-0.3206353,0.715051,0.0986538,-0.217  
1262,0.3341892,0.363827,-0.1469039,0.0075709,-0.0205055,0.0172133,0.06  
75566,0.0239119,-0.0271731,0.022789,0.0993746,-0.0226937,-0.0876343,0.  
0373775,-0.1010719,-0.0367657,0.0690507,0.0406343,0.0691488,0.0780322,  
0.0791104,0.0462881,-0.0334401,0.022502,-0.0143037,0.0579271,-0.013605  
4,0.0607494,0.0749141,0.035727,0.0407633,-0.0234581,0.078336,-0.037053  
3,0.074887,-0.0434521,0.0720386,0.0635182,0.0150453,-0.0748376,0.03094  
12,-0.093417,-0.0203807,0.0532681,0.046297,0.0585117,0.0881995,0.00525  
21,0.0362953,-0.1128657,-0.0057874,-0.0122501,-0.0230927,-0.0869402,0.  
0239652,-0.0833024,-0.0522531,-0.138181,0.059339,-0.0443812,-0.0364842  
,0.0491087,0.0130344,0.0429282,0.0496512,-0.0194835,0.1227576,0.043199  
,0.0706379,-0.0474659,-0.0044998,0.0614922,-0.0379656,-0.0217248,-0.15  
74514,0.0009712,-0.0315796,0.0552444,0.0422969,0.0234891,-0.0504604,0.  
0184024,0.0616775,0.0053216,0.0537507,0.0402727,-0.1202978,-0.146716,-  
0.0678808,0.0583807,-0.0637169,-0.015535,0.0053419,-0.0068956,-0.03777  
63,-0.1277616,-0.0169438,0.019962,0.0842082,0.0576553,-0.1613587,0.030  
8269,0.065316,-0.0162828,0.1016681,-0.1241157,0.0819025,-0.028566,0.09  
38458,-0.014018,-0.105161,0.0180152,0.0444728,-0.0661723,0.0335405,0.0  
196789,0.087251,-0.0398634,0.0175763,-0.0447936,-0.0311894,-0.1002866,  
0.0207724,-0.0338768,-0.0373247,-0.0096493,-0.1497934,-0.0809541\Polar  
=206.4471246,11.3102463,152.976296,1.4880144,-37.2560236,82.7688762\PG  
=C01 [X(C13H14O2)]\NImag=0\

### 23<sup>+</sup>

1\1\MF(MLIB83-EXE)-LEPTON\Freq\RB3LYP\6-31G(d)\C13H13O2(1+)\THEIS\20-A  
ug-2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Pos lad  
et\1,1\C,1.6800623076,1.1866383115,-3.0114137209\C,1.8618301403,-0.20  
1688688,-2.9123759703\C,1.3145399342,-0.8900372839,-1.8467844304\C,0.5  
726235744,-0.2010042721,-0.8564925271\C,0.3869745048,1.2082582814,-0.9  
550153556\C,0.9547072722,1.8773003455,-2.0480243006\C,0.0078713366,-0.  
9349196695,0.2492731137\C,-0.7537656761,-0.2520503822,1.272545319\C,-0  
.9270926,1.1018825077,1.170178657\C,-0.3882859282,1.8924412966,0.09006  
43194\C,-0.6290170829,3.2306669414,0.1004073421\O,-1.2373407763,-1.031  
5761118,2.2618174091\C,-2.0028942658,-0.4211979939,3.3105020969\O,0.24

64724326,-2.2179403967,0.2279548419\C,-0.1725523478,-3.2399434973,1.18  
07283884\H,2.1088873118,1.7302517712,-3.8476773014\H,2.4296617901,-0.7  
329029577,-3.6691748558\H,1.4479314275,-1.9610082316,-1.7596816459\H,0  
.8338155544,2.9491212235,-2.1556731726\H,-1.4952403454,1.6254835531,1.  
9298370304\H,-1.208805391,3.6842655126,0.8982427687\H,-0.2659002826,3.  
9046963413,-0.6665086828\H,-2.2796914719,-1.2355319006,3.9789573657\H,  
-2.9057781763,0.050294999,2.9070823028\H,-1.399206944,0.3146453468,3.8  
530425687\H,0.2464422875,-4.15636011,0.7685889559\H,-1.2592790724,-3.2  
890370233,1.2199058844\H,0.2441030467,-3.0258618393,2.1633231846\Vers  
ion=HP-PARisc-HPUX-G98RevA.11.3\HF=-653.3888768\RMSD=3.652e-09\RMSF=5.  
875e-06\Dipole=-0.4626823,0.2716724,0.6608542\DipoleDeriv=0.0622897,-0  
.0504165,-0.131231,-0.0476695,0.3182811,-0.0210589,-0.1319426,-0.01681  
01,0.1864133,0.0061306,-0.1483762,-0.0890531,-0.0912677,-0.3124152,0.2  
117257,-0.1050285,0.3028964,0.0069801,-0.0077316,0.1855496,-0.1284758,  
-0.0878536,0.0983424,0.0969494,-0.0519961,-0.3390008,0.1220085,-0.1636  
938,-0.2217321,0.2802981,-0.2076985,-0.4455502,0.4483411,0.2764479,0.4  
704924,-0.5992664,0.087691,-0.1571207,-0.0202692,0.1846434,0.2311656,-  
0.3457807,-0.1160054,0.1994395,0.1768293,-0.2422572,0.0825501,0.207137  
,0.0078012,0.1265545,-0.0753992,0.2279701,-0.1945683,-0.4071542,0.5701  
496,-0.5732374,-0.3061782,-0.0123523,2.3279536,-0.5537392,-0.4629334,0  
.3396102,0.921077,0.1023629,0.7024621,-0.2017571,0.7585859,-0.2966766,  
-1.0989372,-0.2176707,-1.0093641,0.7283112,-0.1193033,0.0289842,-0.008  
6744,-0.3819133,0.5374483,0.4252982,0.1061675,-0.2294897,-0.2248389,0.  
0837203,0.1243479,-0.0792882,0.2065505,-0.7641225,-0.1002946,-0.102113  
5,0.0302272,0.2101493,-0.0699363,-0.1072555,-0.0660418,-0.0932815,0.37  
48919,0.0077411,-0.0699434,0.0300958,-0.0271129,-0.6103542,-0.2521723,  
0.6372462,-0.1686215,-0.5633335,0.3551583,0.6139195,0.4887783,-1.37008  
47,0.5299621,0.06427,-0.3636964,-0.1608865,0.1892094,0.2910511,-0.3005  
747,-0.0678643,0.8110621,-0.275473,0.2590258,-0.0081687,-0.1133729,-2.  
2973193,0.7572594,0.0959329,0.1644103,-0.4340628,0.2668089,0.1378588,-  
0.069967,0.0799937,1.0952009,-0.3644463,-0.053774,-0.4565606,0.4603385  
,0.0961441,-0.0141751,0.0438396,-0.0162734,0.060959,0.0428161,0.044451  
1,0.0394675,0.0391986,0.0859993,0.0285234,0.0575619,0.0325838,0.057038  
9,-0.0323469,0.0564444,-0.0258742,0.044325,0.111529,-0.007372,0.008076  
4,0.0141104,0.0281125,0.0019038,0.002061,0.0361426,0.101895,0.1006849,  
0.0516494,0.0100061,0.0148792,-0.02656,0.016212,0.0202725,-0.0424162,0  
.0955795,0.0972304,0.0056377,0.0548325,0.0340365,0.0747865,-0.0381124,  
0.0469007,0.0071442,0.0558288,0.0941225,0.0088597,0.0580487,-0.0071147  
,0.1129419,0.0166809,0.0624723,-0.0087927,0.0349368,0.0999871,-0.01491  
74,0.057368,-0.0076338,0.1079875,0.0192538,0.0553569,0.0309153,0.03647  
,0.0773259,-0.0091516,0.0369943,-0.0330434,0.0155732,0.0759236,0.04366  
,0.0378298,0.0187875,-0.0363038,0.0092098,0.0047087,0.1042475,0.040007  
1,-0.0570874,-0.063635,0.060906,-0.0412906,-0.0443573,-0.082929,-0.007  
5505,-0.0108878,0.0038845,-0.1306721,0.0140094,0.0175286,0.0028686,0.0  
703442,0.0485177,0.0379685,0.0149217,-0.0395136,0.0159241,0.0473413,-0  
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,0.0531979,-0.0172196,0.1072013,0.037852,0.0581006,-0.0743222,-0.02713  
68,-0.0491471,-0.0406346,-0.017561,-0.020569,0.0653929,-0.0248267\Pol  
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24

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4975106,-0.3701468257,0.8281731536\C,-1.2953315019,0.3361684737,-0.412  
8400326\C,-2.5751599453,0.7834810842,-0.8354829392\C,0.0656064747,-0.8  
361074012,1.2775880916\C,1.1967030467,-0.6062218411,0.5299195926\C,1.1  
076508295,0.1178354978,-0.7063390091\C,-0.1056731059,0.5771563405,-1.1  
805207541\C,-0.1754365458,1.3108846807,-2.4978510847\O,2.250882775,0.2  
855185684,-1.4558896668\O,2.4532904847,-1.0258002516,0.8578371077\C,2.  
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, -2.6668554081,1.3220118775,-1.7731664338\H,0.1133265963,-1.3806400842  
,2.2141982984\H,0.8124013361,1.3695200215,-2.9559139329\H,-0.561528724  
8,2.3301831027,-2.3702951085\H,-0.8446361203,0.7996048047,-3.200955145  
6\H,3.6699885595,-2.030661626,2.1078800645\H,2.3160256475,-1.206872333  
7,2.9342068103\H,2.0198467236,-2.7096190587,2.0098744729\H,4.002322023  
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921,-0.1589945,0.0466655,-0.0274453,-0.0101221,-0.0602607,-0.0692563,-  
0.0905461,0.0663242,-0.0913295,0.0288257,-0.3666951,0.0963286,-0.11022  
88,-0.0469096,-0.1782871,-0.0660689,0.1398555,-0.1003402,-0.0696635,1.  
3280764,-0.5117673,0.4261211,-0.4550795,0.2990554,-0.1331341,0.4492827  
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,0.350374,-0.0590799,0.0772547,-0.3086699,0.5520126,-0.2290931,0.49474  
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917,-0.0607401,-0.1384987,0.0769877,-0.0534361,0.0513872,0.0501392,0.0  
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24<sup>+</sup>

1 \1 \MF (MLIB83-EXE) -PROTON \Freq \RB3LYP \6-31G(d) \C13H13O2 (1+) \THEIS \20-A  
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-1.2515724676, -0.3569744012, 0.7461479347 \C, -1.4028629918, 0.3198033573,  
-0.4936177523 \C, -2.6972534955, 0.6093095005, -0.9392432429 \C, 0.054501517  
3, -0.6651758863, 1.225108468 \C, 1.2275956614, -0.349804307, 0.5611965573 \C  
, 1.1378426492, 0.3294730801, -0.6870974883 \C, -0.1823882741, 0.6792395931,  
-1.2416224854 \C, -0.2106129281, 1.3265234834, -2.4344031644 \O, 2.149963304  
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\C, 2.6187807954, -1.3230245473, 2.2607438871 \C, 3.5709647138, 0.4998760952  
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1116797,0.0271305,0.0035094,-0.0613355,0.0187579,-0.1070184,-0.0074768  
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25

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0.0217068,-0.0484303,-0.0448287,-0.0080572,-0.0417692,0.0944431,-0.036

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114,0.0857433,0.0045776,0.0801195,0.0581524,-0.0116864,0.0028016,-0.0111835,0.1306245,0.0390475,0.0964812,-0.0513165,0.0408433,-0.1008031,0.0328906,-0.0505404,0.0788329,-0.0513198,-0.0393508,-0.1099898,-0.041789,-0.0453432,0.0452326,-0.01304,-0.024224,-0.0197913,0.0673098,0.0079311,0.0667629,0.1151496,0.011538,-0.0443458,-0.0301632,0.0842428,-0.0638819,-0.0779334,0.0409078,-0.0361543,-0.0142094,0.0198867,-0.1406873,-0.0580043,0.001115,-0.0642493,0.0623885,-0.0593194,0.1370719,-0.0303487,-0.0102203,0.0278764,-0.0318823,-0.0860435,0.0508573,-0.1180783,-0.0919024,0.1012492,0.1001201,-0.0673988,-0.0038856,0.0826497,0.0695019,0.0350421,-0.0537529,-0.0970467,-0.0663899,-0.0369202,-0.1208962,-0.0266495,-0.0413681,-0.0516494,-0.0354647,0.0625002,-0.0626882,-0.0000494,-0.0081924,0.1437645,0.0224105,-0.0461795,0.0945415,-0.0520482,-0.1338498,-0.0558388,-0.0224396,0.0098722,0.1511828,-0.070281,0.1212061,-0.04292,0.0929466,-0.0493827\|Polar=208.3180405,-4.3131766,162.4859041,14.6556035,26.1409679,73.7615679\|PG=C01 [X(C13H14O2)]\|NImag=0\|

25<sup>+</sup>

1\|GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C13H13O2(1+)\THEIS\18-Jul-2004\0\|#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\|Dimethoxy paa s amme ring\|1,1\C,-3.4350818404,-0.6869388638,0.3984721055\C,-3.5021315881,0.1814543598,-0.6982199762\C,-2.3457528477,0.7368198094,-1.2373690196\C,-1.0851105649,0.4436852751,-0.6993978032\C,-1.0255742928,-0.4381024434,0.4118301144\C,-2.2028928368,-0.9955396586,0.9508796388\C,0.1608258096,1.0181283646,-1.2485406067\C,1.4280124985,0.6362952745,-0.6065141634\C,1.4614834166,-0.2273105962,0.4781748841\C,0.2645080494,-0.7582297232,0.9844781339\C,0.2054559939,1.8703889814,-2.2985306422\O,2.507969961,1.1763074693,-1.1407295106\O,0.2295818127,-1.58217833,2.0113660151\C,1.4307467381,-2.0006652719,2.6947239163\C,3.8214602978,0.8951087544,-0.6155750186\H,-4.341215256,-1.1159722925,0.8133871596\H,-4.4642979386,0.4275393935,-1.1368752004\H,-2.4394715985,1.4038773404,-2.0866153458\H,-2.1321591834,-1.665778327,1.799073315\H,2.4039540565,-0.4923446844,0.9337563599\H,1.1488474296,2.2614697336,-2.6593334278\H,-0.6870297744,2.1965934176,-2.818927391\H,1.0868550594,-2.6673850996,3.4834704156\H,1.9395418947,-1.1359675351,3.1293876548\H,2.0886015446,-2.5399862024,2.0077936115\H,4.5044141407,1.4670269782,-1.2412990748\H,4.0418573044,-0.1730179301,-0.6983992057\H,3.8939951331,1.2303465206,0.4230197153\|Version=SGI64-G98RevA.7\HF=-653.4077\RMSD=2.335e-09\RMSF=9.110e-06\Dipole=1.2874381,-0.0276465,0.2082509\DipoleDeriv=0.0490273,0.2040044,-0.237455,0.1587909,-0.1257833,0.0782749,-0.1813032,0.0848571,-0.209782,0.244294,0.0189424,0.0151472,0.0088094,0.0718582,-0.1342962,0.0270323,-0.1336529,0.1335275,-0.4717441,-0.1364485,0.1196315,-0.0881263,-0.0352817,-0.0951961,0.0601368,-0.1014661,0.034136,0.1737519,0.1233977,-0.135861,-0.2076963,0.089037,-0.0796146,0.2787089,-0.0339906,0.1267695,-0.8599129,0.1963949,-0.3560225,0.2386778,-0.1079633,0.1276409,-0.4101094,0.1218923,-0.238823,0.1992609,-0.2094122,0.2952708,0.1050922,-0.0042875,-0.0504175,-0.0974082,-0.0925203,0.0469854,0.0048848,0.1465186,-0.1796809,0.1406261,-0.2767597,0.3542727,-0.1727143,0.3528891,-0.4681621,1.2995342,0.0621472,0.0533291,0.8570228,0.8171372,-0.5653909,-0.9398061,-0.6694564,0.987139,-0.7020769,-0.3792132,0.417491,-0.6172063,-0.6906163,0.4344306,0.7161252,0.4664688,-0.7657187,1.7622536,0.3898272,-0.2910633,-0.1051385,1.0249921,-0.9318346,0.3273916,-0.8670881,1.4200901,-0.0303183,-0.0329701,0.0489363,-0.0907539,0.0712767,-0.2191259,0.1208127,-0.2118762,0.1830044,-1.9642228,-0.3263719,0.1839113,-0.5255465,-0.4276076,0.1538137,0.4326445,0.1797001,-0.4179904,-0.6187326,0.1366643,-0.2208003,0.329272,-0.9269834,0.8951785,-0.4617695,0.8698968,-1.3964288,0.525052,-0.3839717,0.5129934,-0.1658006,0.4448164,-0.227830

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## 26

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## 26<sup>+</sup>

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-0.3436822, 2.1074124, 0.185632, -0.2369852, 0.0693851, 0.320125, -0.0552436  
, -0.0871509, -0.0135102, -0.1876545, 0.2840517, 0.0551397, -0.0207835, 0.040  
6646, -0.1001726, -2.0498794, -0.283768, 0.237722, -0.6327186, -0.5094125, 0.  
0715861, 0.211878, 0.0215247, -0.2779201, -0.5902856, 0.1656907, 0.0624243, 0  
.5343256, -2.0670993, -0.2127935, 0.0899131, -0.159779, -0.2691253, 0.501883  
2, -0.6106327, -0.0774553, -0.2920928, 0.8119423, 0.08172, -0.05387, 0.127987  
8, 0.2973362, 1.1293498, 0.0790465, -0.1153685, -0.3234269, 0.1890308, 0.0393  
454, -0.1450191, -0.0186486, 0.3062977, -1.5269248, -0.8715781, 0.1157862, -0  
.9415268, -1.0502397, 0.0800379, 0.1105872, 0.0699517, -0.2961261, 0.3325247  
, 0.0933195, 0.0064617, 0.609263, 0.9518631, -0.0424235, 0.0446432, 0.0324719  
, 0.3254936, 0.0320925, 0.0230616, 0.0157125, 0.0196872, 0.0860285, -0.006012  
3, 0.0154676, -0.0065309, 0.1257611, 0.0856716, -0.0513673, 0.0003906, 0.0052  
644, -0.0426445, -0.0124196, 0.0044905, -0.0042354, 0.113673, 0.1233978, 0.01  
51565, 0.001762, -0.0269016, 0.0211094, -0.0039878, -0.0013713, -0.0100429, 0  
.1272689, 0.0171378, 0.0382505, 0.0219937, 0.0299099, 0.0719068, -0.0100482,  
0.021147, -0.0113937, 0.1462464, 0.0558234, 0.0050368, 0.0110313, -0.0014167  
, 0.1209495, -0.0003962, 0.0103571, -0.001596, 0.1279125, 0.0094218, 0.043038  
3, 0.0197818, 0.0241376, 0.1192388, -0.0039156, 0.0186131, -0.0065988, 0.1220  
469, 0.0478922, -0.0445389, 0.0050455, 0.0083657, -0.0236298, -0.0109196, 0.0  
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.0099772, 0.0739878, 0.0406352, 0.0116032, -0.0292701, -0.0248332, 0.11783, -  
0.0275165, -0.010464, 0.0242478, -0.0667026, -0.0443102, -0.0397061, -0.0211  
791, 0.0061345, -0.0180154, 0.0132517, -0.0663895, 0.0190912, 0.0030035, 0.00  
97105, -0.0039459, 0.1059545, -0.0186257, -0.0242868, 0.0433524, 0.1253162, 0  
.0321765, 0.0554648, 0.0079261, 0.0617284, -0.0274674, -0.0318237, -0.032564  
7, -0.048775, 0.105998, 0.049823, -0.0783523, 0.0080371, -0.0431526, -0.03206  
2, -0.0664548, -0.0657951, 0.0187853, -0.0374892, 0.0419181, 0.0013981, 0.020  
8755, 0.0055036, 0.094007, 0.0681173, 0.0695316, 0.0743714, -0.0983023, -0.05  
05027, 0.0020037, 0.0225907, -0.0581279, -0.0894006, 0.0289862, 0.0962836, -0  
.0958993, -0.0873651, -0.0595799, 0.0268492, -0.0700937, 0.0359794, -0.04119  
29\Polar=230.9736557, 23.5152281, 214.9384793, -21.8230037, 7.3864159, 71.9  
042947\PG=C01 [X(C14H15O3)]\NImag=0\

27

1\1\MF(MLIB83-EXE)-NEUTRON\Freq\RB3LYP\6-31G(d)\C14H16O3\THEIS\20-Aug-  
2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Trimethoxy  
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844579192\C,-1.1443300755,1.5902568129,-2.3292680063\C,-0.821083667,-0  
.7694783915,0.572637815\C,0.4141329658,-0.4049412696,1.088491663\C,1.1  
677450064,0.6301583118,0.4474058846\C,0.6760785112,1.3343034463,-0.638  
1012225\C,1.4288324042,2.5231077464,-1.1885506411\O,2.3824451642,0.964  
5055071,1.023864543\O,0.8012993459,-0.9556751445,2.2861353195\C,2.0718  
494666,-1.595846896,2.3847175811\C,3.5374877649,0.5709111827,0.2813573  
311\O,-1.6408111702,-1.7083589506,1.1351404916\C,-1.0912005426,-2.9316  
280947,1.6214060473\H,-2.7581210958,1.7090339646,-3.7263830403\H,-4.05  
42162464,-0.138823591,-2.659925364\H,-3.1448595822,-1.2852547396,-0.66  
05352883\H,-0.5902726126,2.3890780327,-2.8109743129\H,2.1973127614,2.8  
505977548,-0.4856472949\H,0.7518179409,3.3689820126,-1.3500262328\H,1.  
9118221069,2.3102901955,-2.1521934801\H,2.0054893488,-2.2698549311,3.2  
435215933\H,2.8710363685,-0.8707033955,2.5548018629\H,2.2920497414,-2.  
1864979702,1.4856040956\H,4.4014220887,0.8931321781,0.8681431296\H,3.5  
74075545,1.0478260431,-0.7043331846\H,3.574736767,-0.5179200397,0.1474  
742595\H,-1.9183699211,-3.6469236257,1.6246982199\H,-0.694403903,-2.81  
9949115,2.6327437496\H,-0.2995340643,-3.3012817164,0.9572667514\\Versi  
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313,-0.0178659,-0.2794974,0.417943,-0.1561058,0.1542467,-0.2677578,0.6  
000705,-0.3974366,0.944646,1.0520672,0.148726,0.329772,0.2864659,0.199  
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.0596898,0.1187538,0.0217205,0.0049342,-0.1691197,-0.0291076,-0.176313  
,0.063602,-0.0045414,-0.0553935,0.0056584,0.0875581,0.0134333,-0.02622  
89,0.0384636,0.0816786,-1.5912608,-0.0024669,-0.2550566,-0.190737,-0.4  
077116,-0.0725597,-0.1229445,0.0205159,-0.4941078,-0.9063065,0.2722883  
, -0.5300822,0.3457096,-0.5556408,0.3572093,-0.668034,0.4043298,-1.1018  
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1,0.2544411,-0.2544853,0.1446823,0.068715,0.973351,-0.3524926,-0.08009  
43,-0.2987104,0.4641403,0.0377713,0.0172078,-0.0729063,0.0253904,0.037  
6045,0.0999889,-0.0861274,0.0957578,-0.0591163,-0.0933068,-0.0569522,-  
0.0907146,-0.0686971,0.0683451,-0.0040548,-0.0860724,0.0053467,0.04313  
85,0.0469962,-0.0593874,0.0149395,-0.078057,0.0195709,0.0359473,0.0364  
906,0.0424369,0.080711,0.0308434,-0.0873275,0.0445504,-0.0544547,-0.00  
922,0.0809581,0.0203993,0.0672812,0.0481373,-0.0408374,-0.0774173,-0.0  
430591,-0.0396429,0.0642305,-0.0106787,-0.0785181,-0.0615944,0.0094524  
, -0.0121029,0.1083528,-0.0090801,0.0403319,-0.0772451,0.0470367,0.0104  
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, -0.1286962,-0.018099,-0.0813017,-0.0866158,-0.0170815,-0.0393465,-0.0  
024217,-0.0372512,0.0787143,-0.0388412,0.0469096,-0.0579942,0.0670258,  
-0.025445,-0.0422806,0.0867516,-0.1260118,-0.0637345,-0.143968,-0.0334

645,-0.0771249,-0.0378085,0.0533922,-0.0329185,-0.091821,-0.0378078,0.0062456,0.0034541,0.0105834,-0.0153038,-0.0139109,0.0041213,0.0760808,0.0989433,0.0624458,-0.0964364,-0.0211822,-0.0229452,-0.0060712,0.1071539,-0.1619696,-0.0161416,0.0529308,-0.020061,0.0504736,-0.0599636,-0.1302914,0.0150292,-0.0991641,-0.1138095,0.0706965,-0.0184769,0.0194667,0.05475,0.0516968,0.0899079,-0.1043986,-0.0023112,-0.0172847,0.0069665,-0.0414258,0.0494674,-0.1212766,-0.0414359,0.1526543,0.0368954,0.0020062,-0.0477901,0.0243665,0.0927525,-0.0465947,-0.0494648\Polar=189.3668791,20.8666472,142.2582502,49.5585705,-50.8038543,157.2221253\PG=C01 [X(C14H16O3)]\NImag=0\

27<sup>+</sup>

1\1\MF(MLIB83-EXE)-BOSON\Freq\RB3LYP\6-31G(d)\C14H15O3(1+)\THEIS\20-Au  
g-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\trimethoxy\\\1,1\C,3.4908489307,1.177688047,-1.2039810054\C,3.1848452875,0.1322142461,-2.0825939062\C,1.9523351487,-0.5000033122,-2.0011328666\C,1.0109294379,-0.092075182,-1.036305291\C,1.3066296782,0.984581525,-0.1664866403\C,2.5596127037,1.6006661448,-0.2581007539\C,-0.2601382066,-0.7877508074,-0.9020697769\C,-1.1262846218,-0.5264841046,0.1886740916\C,-0.8413680974,0.5329352108,1.0584771523\C,0.2648290485,1.4561770312,0.7685758512\C,0.2107412028,2.7460430116,1.1734229104\O,-1.6899888844,0.6652724005,2.0646623406\O,-2.2466171866,-1.2816384016,0.3702040341\C,-2.1969348677,-2.2642536923,1.4264849788\C,-1.4037692981,1.3286329752,3.3184442497\O,-0.4690439415,-1.6985782944,-1.8228134052\C,-1.7124840326,-2.4132296679,-2.067795604\H,4.4616610959,1.6612743254,-1.2517212987\H,3.9117209446,-0.1912040326,-2.8205598545\H,1.7084790365,-1.3171959304,-2.6689213212\H,2.8246075929,2.3984965411,0.4279835874\H,-0.5923036129,3.1395773201,1.7823348106\H,0.9487592215,3.4671104396,0.8398701466\H,-3.1481896755,-2.7949186477,1.3757268942\H,-2.0972684391,-1.7847356742,2.4031903523\H,-1.3693226366,-2.9653395638,1.2672274691\H,-1.8998613616,2.3013083799,3.3324337896\H,-0.3293805717,1.4364632521,3.4761172233\H,-1.8411532767,0.6899881271,4.0866419482\H,-1.573006113,-2.8380471325,-3.0611704387\H,-2.5579850795,-1.7281234339,-2.0484825539\H,-1.8402309074,-3.2059481588,-1.3307748483\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-767.9028107\RMSD=4.934e-09\RMSF=3.008e-06\Dipole=0.0325704,0.3114089,0.8250115\DipoleDeriv=0.1923211,0.0644642,-0.0320375,0.0630927,0.1080882,0.0763822,-0.0702983,0.121453,0.0597268,-0.0268652,-0.2166179,-0.1864411,-0.1548873,-0.218533,0.012838,-0.1811943,-0.013047,0.0443162,0.1314298,0.2655292,0.082384,-0.016637,0.0532459,0.1253292,-0.1712903,-0.0620508,0.0319449,-0.6968921,-0.4022732,0.0950077,-0.391937,-0.2251981,0.057492,0.0279607,-0.0172592,-0.0999136,0.1826351,-0.131599,-0.1007883,0.1714074,0.1051335,-0.0443493,0.2169361,0.0744096,-0.0772102,-0.3366842,0.0975289,0.1809486,0.0804118,0.0256459,0.0853272,0.1822311,0.058606,-0.1033705,1.1905573,0.0543556,-0.6292089,0.5813092,1.131462,0.721815,-0.0244755,1.1329363,1.6276275,0.5195223,0.8686439,0.0982449,0.8008265,-0.0434823,-0.8348451,0.3643791,-0.6988973,-1.1104855,0.5493587,-0.0812763,-0.6738124,-0.2847063,0.8451406,0.7811451,-0.7806141,0.4248944,1.5258933,0.0705164,0.0103626,0.0262436,-0.1679249,-0.5258442,-0.1353383,-0.1378238,0.0304643,0.0479816,-0.0492896,-0.0102618,-0.0824536,0.09912,0.1927959,0.0158548,-0.0080574,0.0835477,-0.0830872,-0.767603,0.2507226,0.8889903,0.1767556,-0.4670406,-0.5039505,0.6548553,-0.4582802,-1.6279149,-0.8335617,-0.6256333,0.1878418,-0.5125957,-0.8802214,0.372229,0.2895457,0.4326107,-0.5727368,0.2655466,0.0047321,-0.0145631,0.1922616,0.6835026,-0.3060114,-0.2595787,-0.4710136,0.5431655,0.2101888,-0.0306822,0.0642505,-0.1619899,0.4155353,0.432757,-0.2242064,0.2394271,0.971584,-0.6969124,-0.4368539,-0.2294963,-0.6096051,-1.28123

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0.0159991,0.0959608,0.0344893,0.0039628,0.0589626,0.0096943,0.0895531,  
-0.0415351,0.0628785,-0.0392317,0.0489406,0.1017907,-0.0306721,-0.0269  
748,-0.0180132,0.0537649,-0.0479897,-0.0052334,-0.0291687,0.0853006,0.  
0932233,0.0151487,0.023341,-0.0378666,0.0350051,-0.0598798,-0.0036087,  
-0.0824593,0.0341426,0.0449505,0.0056508,0.0499353,-0.0068911,0.113080  
4,-0.0052243,0.0650217,-0.026761,0.0795054,0.0341909,-0.047249,0.04963  
33,-0.0161109,0.1108435,0.0096164,0.0313784,0.0068969,0.0938426,-0.029  
8355,-0.0726889,0.0006571,-0.078938,0.0106027,0.0395669,-0.0172917,0.0  
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-0.0876332,0.0190674,0.0204441,-0.084186,-0.0335982,0.1264496,0.012770  
1,0.0145154,-0.0569352,0.0376663,0.0849003,0.0001371,0.001574,0.084906  
7,0.0204901,-0.0608633,0.0725515,-0.0527606,-0.0657867,-0.0028755,0.02  
92805,-0.0045665,-0.0509474,0.0070415,-0.0362855,0.0246478,0.0348367,-  
0.0671576,0.0703388,-0.040437,0.0002326,0.085407,-0.0361836,0.0189677,  
-0.0376709,0.0298705,0.0560038,0.0581519,-0.0071182,-0.0450721,0.03970  
28,-0.0314672,0.0331222,-0.0315994,0.0542722,-0.0448537,-0.0131924,-0.  
078793,-0.0373855,-0.0210153,-0.0605592,-0.0605023,0.0341454,-0.041199  
8,-0.0295507,0.0092241,-0.0359366,0.078102,-0.0108187,-0.0804102,-0.09  
37641,-0.0380903,-0.0158602,0.0234712,-0.0054659,0.083509,-0.0048197\p  
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032\PG=C01 [X(C14H15O3)]\NImag=0\

## 28

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C14H16O3\THEIS\19-Jul-2004\0\#\#  
N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Perieffekt er volds  
om\0,1\C,-2.9014559089,-0.3204199887,1.2581032972\C,-3.3702149024,-0.  
1507139966,-0.0579019008\C,-2.4829565922,0.0647204233,-1.0857125191\C,  
-1.0791621389,0.1300257598,-0.8553706562\C,-0.5908107365,-0.0516348714  
,0.4903609247\C,-1.5491845627,-0.2762095454,1.5319543386\C,-0.18895577  
09,0.3783838058,-1.9461197664\C,1.1689590644,0.4497402532,-1.680181909  
2\C,1.6754927953,0.277867632,-0.3701560901\C,0.8270616385,0.0323597005  
,0.6923507557\C,-0.7070835934,0.5684066401,-3.3521755669\O,1.999435280  
2,0.6934250301,-2.7450532226\O,1.288258275,-0.1461766204,1.96346661\C,  
2.6763903206,-0.0165204268,2.2124344489\C,3.3958065719,0.7882544424,-2  
.5329517284\O,-1.1741760172,-0.4026373948,2.8528385543\C,-0.8994226754  
, -1.7345848416,3.2733524161\H,-3.587450215,-0.4745991056,2.0852608693\  
H,-4.4379760065,-0.1871617015,-0.2579177263\H,-2.8572976748,0.19757791  
3,-2.0939339857\H,2.7405014712,0.3362452602,-0.2019392676\H,0.11639905  
66,0.7439430852,-4.0448137753\H,-1.3907439171,1.4245947483,-3.41875749  
96\H,-1.2594823398,-0.3128228277,-3.7033006092\H,2.7989119333,-0.16497  
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07\H,3.8152886169,-0.1478180922,-2.1398805527\H,3.6520032611,1.6119035  
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2,-0.0044125,-0.0744194,0.2810758,-0.2360525,-0.0464474,0.2318834,-0.0  
266254,-0.1646551,-0.0022596,0.1133314,0.0136278,-0.0866745,0.3532187,  
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28<sup>+</sup>

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C14H15O3(1+)\THEIS\31-Jul-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Perieffekt er v oldsom\1,1\C,-2.7732023692,-0.7529972843,1.2303614465\C,-3.2819388345,-0.5411480443,-0.0439262489\C,-2.4576309015,-0.1428172263,-1.0930583558\C,-1.0929041227,0.0573303325,-0.8878417145\C,-0.5363486835,-0.1694333841,0.4121467687\C,-1.4067710711,-0.5755926633,1.4815116624\C,-0.2269318822,0.5017531719,-2.0044739076\C,1.2152667502,0.5937885325,-1.7542622534\C,1.7330741947,0.3603532375,-0.4987983006\C,0.8884482145,0.0046214331,0.5766559951\C,-0.6850918933,0.8578111161,-3.2265701349\O,1.9478228837,0.9276194354,-2.8054088556\O,1.3819819759,-0.1946392141,1.7800299343\C,2.7874415903,-0.0575485826,2.0664027001\C,3.3750809336,1.0787771054,-2.6908441167\O,-0.8670969947,-0.7733628379,2.6911568698\C,-1.6985943911,-1.1840925669,3.7847879915\H,-3.438100523,-1.0607969709,2.0264327773\H,-4.3419040145,-0.691549332,-0.224989024\H,-2.8962730267,-0.

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Supplementary Material for Organic & Biomolecular Chemistry  
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1\1\MF(MLIB83-EXE)-NEUTRON\Freq\RB3LYP\6-31G(d)\C14H16O3\THEIS\19-May-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\trimethoxy benzen\0,1\C,-2.7373150068,0.8349187691,-0.2485015057\C,-2.7474273558,-0.5730376146,-0.4019461444\C,-1.5667135019,-1.2919464091,-0.3333946368\C,-0.3211644994,-0.6543353092,-0.1102137332\C,-0.3191365958,0.7717678147,0.0441347692\C,-1.5390980744,1.481473431,-0.0302186403\C,0.8995419617,-1.3980014981,-0.0393918828\C,2.0765192749,-0.6991630023,0.1818917048\C,2.1009473472,0.7139368057,0.3375993404\C,0.9262588587,1.4320231023,0.269696292\O,-3.8828072839,-1.304563797,-0.62139956\C,-5.1236584871,-0.6245039175,-0.7043552035\C,0.9017393208,-2.898381582,-0.2013220006\O,3.230186494,-1.4414485771,0.2444350891\O,0.8510735779,2.7892217113,0.4072376053\C,2.0474701482,3.5132090737,0.6327575237\C,4.4677062843,-0.7925652651,0.4677507159\H,-3.655127611,1.4088525866,-0.3000089989\H,-1.6217537955,-2.3671015216,-0.4563771965\H,-1.5214794327,2.5591805308,0.0884866075\H,3.0409126926,1.2181964288,0.5083644936\H,-5.87514892,-1.3964563375,-0.8821556871\H,-5.1411186701,0.0926467218,-1.5360311902\H,-5.3634150356,-0.0976051615,0.2290371445\H,1.9131025256,-3.2975482722,-0.1186495358\H,0.4989695233,-3.1979697089,-1.1778415976\H,0.2824429752,-3.3861308646,0.5630102393\H,1.7541894868,4.5619247728,0.7098121449\H,2.7536890365,3.3940634312,-0.1998751295\H,2.5360510872,3.2034953944,1.5663498274\H,5.2204212639,-1.5838153646,0.4749260446\H,4.489095914,-0.2707243247,1.4341750114\H,4.7075286072,-0.079049401,-0.3323268445\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-768.7739424\RMSD=5.506e-09\RMSF=7.528e-06\Dipole=0.5014591,0.9319647,0.1611111\DipoleDeriv=-0.3375498,-0.1323572,-0.0325397,-0.3552216,-0.176908,-0.0425025,-0.0564344,-0.0148288,-0.1995074,1.657388,0.324446,0.2197259,0.8867408,0.4381879,0.1394545,0.2796352,0.0694292,0.2095627,-0.7210562,-0.0173445,-0.0660697,0.0962611,0.016512,0.035657,-0.0539162,0.0216066,-0.2080893,0.7488333,-0.0440066,0.0816903,-0.1456358,0.0019507,-0.0233402,0.0706485,-0.0108063,0.0588025,-0.4264969,-0.1811424,-0.0683274,0.0807875,-0.3938296,-0.0289724,-0.0398904,-0.0613494,-0.0447958,0.3961126,0.0714446,0.0677473,-0.0658474,0.0814323,0.0102297,0.0529469,0.0271543,-0.0790437,-0.7635546,0.0958084,-0.067638,-0.080294,0.0929296,0.0145946,-0.0865803,0.0365361,-0.1409074,1.6269423,-0.3090806,0.1513633,-0.6221501,0.4680849,-0.0410667,0.1172607,-0.0023454,0.1494984,-0.3743713,0.2882894,0.0146077,0.1161449,-0.4273956,-0.0057952,-0.0040565,0.0154081,-0.2398164,0.5155068,-0.0804825,0.037821,0.4434203,1.5708218,0.2094549,0.0945144,0.1450349,0.1680237,-2.169152,-0.1653592,-0.2508377,-0.587434,-0.4619517,-0.0908925,-0.2960649,-0.0381948,-0.3351789,1.1885132,-0.0313681,0.0994321,-0.451409,0.3085395,-0.0619312,0.0547803,-0.0097238,0.3684701,0.0368603,-0.0161783,-0.0144823,0.0120463,0.1092537,-0.0017454,-0.0114291,-0.0053286,0.1374658,-2.1140838,0.1652688,-0.2087678,0.5204126,-0.4459463,0.0470204,-0.1700256,0.0030491,-0.3053602,-0.6042926,-0.3394178,-0.0766441,-0.587488,-1.8024369,-0.237039,-0.1034447,-0.2066645,-0.3157775,0.667911,0.6249064,0.1065484,0.2581512,0.6842221,0.0677778,0.0668421,0.1130186,0.3721572,1.1612848,0.034202,0.1032127,0.4214276,0.3016476,0.0460995,0.144995,-0.0018823,0.3760345,-0.0743573,0.0676208,-0.0171433,0.091108,0.0403068,0.0023218,-0.0145288,-0.0005888,0.12139,0.0849872,-0.0032667,-0.0044182,-0.0312464,-0.053692,-0.0224251,-0.0074697,-0.0189765,0.1149618,0.0851123,0.0051776,-0.0019085,0.0199945,-0.0542464,-0.0147388,-0.0003649,-0.0165415,0.1031068,-0.0348944,-0.0835458,-0.0300408,-0.0776599,0.0524246,-0.0185109,-0.0293741,-0.0192304,0.1291175,-0.1140221,-0.0729342,-0.0316371,-0.1271795,-0.0290988,-0.0273277,-0.0375514,-0.0205686,0.0692212,-0.0502756,-0.0253805,0.0166284,0.1530593,-0.0343618,0.1212556,-0.026468,0.0875149,-0.0853778,-0.0596605,-0.0023322,-0.0071341,0.1659535,0.0029249,-0.0626718,0.0730112,-0.0721963,-0.1137741,-0.0500307,0.1164878,-0.0029985,0.0515355,0.038937,0.00247

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34, -0.0100049, 0.0105487, 0.0750578, 0.0511372, -0.0658003, -0.0773835, -0.0146164, -0.0585619, -0.036682, -0.0536177, -0.0831087, -0.0989158, 0.0142882, -0.1021588, 0.0844806, -0.0374314, -0.082013, 0.029872, 0.07322, 0.0619064, -0.0385148, 0.0389246, 0.0458592, 0.0000143, -0.0178401, -0.1579722, -0.0277903, -0.0068606, -0.0199157, 0.0759367, -0.0969081, -0.1341307, 0.0573678, 0.0341746, 0.0283131, -0.0474066, 0.0886309, -0.0017051, -0.0844006, -0.0592954, -0.1187045, -0.0800763, 0.0363927, 0.0148829, 0.0816886, -0.0763766, -0.0038402, -0.1086508, -0.1080843, 0.0734595, -0.0149582, 0.1333901, -0.036727, 0.0041414, -0.0084496, -0.0032781, 0.0757141, -0.0537467, 0.0150439, 0.0209046, -0.1431272, 0.0012217, -0.1029973, -0.0572502, -0.073405, -0.1267081, -0.061987, -0.0030291, -0.0085412, -0.1764212, -0.037459, 0.081794, 0.0336716, 0.0932712, -0.0797086\|Polar=250.0316121, 5.029814, 177.2964757, 22.0250635, 11.4958027, 80.6659576\|PG=C01 [X(C14H16O3)]\|NImag=0\|

29<sup>+</sup>

1\1\MF(MLIB83-EXE)-NEUTRON\Freq\RB3LYP\6-31G(d)\C14H15O3(1+)\THEIS\15-May-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\trimet hoxibenzen\1,1\C, -2.7933653623, -0.5868350366, 0.2468609366\C, -2.7086929014, 0.1223467601, -0.9695192123\C, -1.4758487475, 0.5671960634, -1.403516255\C, -0.304356887, 0.3259512127, -0.6548655702\C, -0.3861188796, -0.3908986642, 0.5758077959\C, -1.6316415337, -0.8329740159, 1.0013172743\C, 0.9717843011, 0.7915141135, -1.1131688784\C, 2.1589207574, 0.5655771022, -0.3867991358\C, 2.1126815947, -0.1259232152, 0.8096014315\C, 0.8467539973, -0.6410251102, 1.3572578917\C, 0.876258784, -1.3081093184, 2.5322633355\O, 3.1792192985, -0.3798404563, 1.5513190949\O, -3.9260212988, -1.068054594, 0.7721769714\O, 0.9579942216, 1.4457692468, -2.2614912878\C, 4.4868321271, 0.0628426055, 1.1417731101\C, 2.1640954107, 1.9739293818, -2.8486856663\C, -5.1702001256, -0.8729541716, 0.0850345422\H, -3.592382751, 0.3208345567, -1.5629735927\H, -1.4006288214, 1.1128282328, -2.3367123014\H, -1.7622347268, -1.3825329502, 1.9257895983\H, 3.1001327393, 0.9333742378, -0.7670491937\H, 1.8077973494, -1.4627513678, 3.0626592076\H, -0.0181010309, -1.7128736989, 2.9909228936\H, 5.1609359313, -0.2782694322, 1.9257335829\H, 4.514576786, 1.154366001, 1.0725731977\H, 4.7614042999, -0.3943816783, 0.186502252\H, 1.841474662, 2.4509357036, -3.7726696766\H, 2.8660235927, 1.16539705, -3.071393929\H, 2.6188399562, 2.7149843148, -2.1852814164\H, -5.9225919275, -1.3507917088, 0.7113257383\H, -5.1508162404, -1.3516731916, -0.8997119536\H, -5.3965828003, 0.1937341159, -0.0159222335\|Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-767.938476\RMSD=5.372e-09\RMSF=7.254e-06\|Dipole=1.3367598, 0.4719179, -0.4516901\|DipoleDeriv=2.0675031, 0.3711021, -0.139398, 0.7446671, 0.4383592, -0.1372053, -0.7920754, -0.2412457, 0.4421386, -0.3804876, -0.1288704, 0.1653248, -0.4210571, -0.2789924, 0.0814594, 0.6759494, 0.162907, -0.2615917, 0.8207558, 0.2221191, -0.1490365, 0.0597624, 0.021759, -0.0869567, 0.1350149, -0.0416496, 0.0729849, -1.497404, -0.3441235, 0.2008059, -0.4732779, -0.2294953, 0.164651, 0.4265003, 0.2006979, -0.2918771, 0.4717171, 0.0193276, 0.0825227, 0.3251275, 0.1598496, -0.0928394, -0.4522462, -0.1781767, 0.2403496, -1.0452275, -0.094342, -0.0832747, 0.0075196, -0.1060746, -0.0839262, -0.261225, -0.1123211, -0.0317866, 2.2228088, 0.0221379, 0.5020839, 0.5412122, 0.7766875, -0.7103287, -0.4059477, -0.8552519, 1.6669345, -0.7633409, 0.19205, -0.4707468, 0.5304802, -0.4043268, 0.3659417, -1.0624322, 0.2716026, -1.0512004, 1.2925399, 0.1149243, 0.0856646, -0.6307332, 0.4897077, -0.5687982, 1.3899457, -0.3608102, 1.2839138, -0.0500293, -0.103498, 0.169596, -0.0443769, -0.1893129, 0.3028069, 0.0661849, 0.2863676, -0.4914647, -0.0326595, 0.0299158, -0.0320396, 0.0629393, 0.007994, -0.1809362, -0.0897772, -0.1902224, 0.2021612, -2.0776777, -0.0336883, -0.4501977, 0.1662697, -0.2988515, 0.1269518, -0.7999894, 0.0711628, -0.6004555, -2.468058, -0.3739233, 0.043278, -0.6384755, -0.4161952, 0.0627977, 0.5055283, 0.136462, -0.3760164, -0.6786765, -0.192896



4, 0.2178374, -0.5137907, -0.7740876, 0.7729085, 0.7792967, 0.8625181, -1.5414008, 1.1867736, 0.047656, 0.1668707, 0.2553759, 0.2866801, 0.0769816, -0.1965384, 0.0190445, 0.2018413, 0.6282183, 0.3622803, -0.537684, 0.2209685, 0.471121, -0.2650296, -0.2905435, -0.2256127, 0.5979015, 1.2840127, 0.1091291, 0.0795437, -0.1002037, 0.2857087, 0.0216882, 0.4451892, 0.0799957, 0.2983175, -0.0028377, 0.0019423, -0.0417297, 0.0067931, 0.1219694, 0.0239741, -0.0502065, 0.0226085, 0.0810602, 0.1007326, -0.0123275, 0.0179589, -0.0022485, 0.088811, 0.0427941, 0.0003512, 0.039991, 0.0438151, 0.0883289, 0.0085542, -0.0252399, -0.0101122, 0.0920556, 0.0551184, 0.0074195, 0.0603276, 0.0217698, 0.0085248, -0.0350418, 0.0216785, -0.0307892, 0.1256682, 0.0346763, 0.0140916, 0.0334865, 0.0957817, 0.0599614, -0.0033648, -0.0134766, -0.0080125, 0.1274215, 0.0012247, -0.005335, 0.0025515, 0.1234497, 0.0009944, -0.0373642, 0.0311096, -0.0221116, 0.1159812, 0.0074224, 0.0043969, 0.0031875, 0.1194086, 0.0044669, -0.0022982, -0.0243997, 0.0223275, 0.0872253, 0.0396779, -0.0674284, 0.0328174, 0.0302309, -0.0373882, 0.055174, -0.0138053, -0.0599173, -0.0678823, -0.0166109, 0.0921719, 0.0235881, 0.0837154, -0.0275233, -0.0231912, -0.042222, -0.0587717, 0.0299816, -0.0635494, 0.1153333, -0.0617372, -0.0240003, 0.0449611, 0.0116748, -0.0375079, -0.0160146, 0.0725889, 0.0545046, 0.0109071, 0.062139, 0.0005435, -0.0470446, -0.0303029, 0.1175831, 0.0428574, -0.0580603, -0.0014723, 0.0127111, 0.0249387, 0.0638433, -0.025146, -0.0916453, 0.0915865, -0.044336, 0.0117941, -0.0185446, -0.0142742, -0.0785843, -0.0279809, -0.0425719, -0.0344675, 0.0209518, -0.0557052, 0.0682311, 0.0375856, 0.0581416, 0.0435053, 0.038673, -0.0559987, 0.0156977, 0.0498423, 0.0511339, 0.0326192, -0.0520072, -0.1258326, -0.0851673, -0.0634486, -0.0502433, -0.042344, -0.0034754, 0.0924975, -0.0889421, 0.005041, -0.1252839, -0.0091946, 0.0523816  
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PG=C01 [X(C14H15O3)]\NImag=0\

### 30

1\1\MF(MLIB83-EXE)-PROTON\Freq\RB3LYP\6-31G(d)\C13H14O2\THEIS\31-Jul-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Nyt derivat  
\0, 1\C, 1.9137013585, -2.0721451366, 0.1055100271\C, 2.51335746, -0.8014641605, -0.1212973054\C, 1.6806519813, 0.2978812673, -0.2287970277\C, 0.2600333993, 0.1784978395, -0.1443076829\C, -0.3164763294, -1.1117085068, 0.0922832073\C, 0.5544157268, -2.2295077014, 0.2195079338\C, -0.6058978723, 1.2880219822, -0.3000143706\C, -1.9749808867, 1.1472945128, -0.2115562394\C, -2.5427766031, -0.1287615839, 0.0377247908\C, -1.7218080884, -1.2328854445, 0.1821923903\O, -3.8874557492, -0.3553064657, 0.1438293334\C, -4.776193452, 0.7378698367, -0.0147576136\C, 4.0126220916, -0.6778294759, -0.2445379552\O, 2.2089287983, 1.556580519, -0.46941352\C, 2.5857782388, 2.2693138828, 0.7083700406\H, 2.5640939044, -2.9403368718, 0.1884663121\H, 0.1267901319, -3.2133907655, 0.3951273611\H, -0.1735144564, 2.2603495867, -0.5103910858\H, -2.609087411, 2.0171189949, -0.3403275772\H, -2.1756845306, -2.2032132113, 0.361608802\H, -5.7797851254, 0.3253780935, 0.1062235497\H, -4.6914105765, 1.1908139656, -1.0116291608\H, -4.6116061056, 1.5116597809, 0.7471380025\H, 4.2872822383, 0.2258437315, -0.794452455\H, 4.4321127549, -1.5433565782, -0.769576002\H, 4.501007642, -0.6331397841, 0.7389271346\H, 2.9507947539, 3.244674151, 0.3767289142\H, 3.3841925217, 1.7509409413, 1.2550555034\H, 1.7284677201, 2.4090016691, 1.3798530235\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-654.2494159\RMSD=2.432e-09\RMSF=1.230e-05\Dipole=-0.145299, 0.5419924, 0.4033955\DipoleDeriv=-0.017523, 0.0003588, 0.0038028, 0.0065009, 0.2260108, -0.0465102, -0.0141854, -0.054841, -0.114684, 0.1891824, 0.1057324, -0.0498414, -0.0484422, -0.3056917, -0.003265, 0.0453269, 0.0119416, -0.0599679, 0.4498551, 0.1947589, 0.0435322, 0.5272866, 0.957888, 0.0644789, -0.1028358, -0.1714881, -0.002943, -0.1588226, -0.0334914, 0.0057048, -0.0541902, -0.2790371, 0.0054821, 0.0177276, 0.0348619, 0.0061478, 0.3800007, -0.0460324, -0.0

126113,-0.140597,-0.0786487,0.0288328,-0.008821,0.0201627,0.0498183,-0.1967484,0.0078876,-0.0090365,0.0526638,0.1158112,-0.0522802,-0.0033207,-0.033615,-0.1413518,0.1427276,-0.0868874,0.0031624,-0.0494829,0.1291186,-0.0479438,-0.020322,-0.0582915,-0.0951745,-0.3433955,0.0627285,-0.0040499,-0.2215432,0.0760733,-0.0334284,0.0528815,-0.0442231,-0.1661313,1.9095361,-0.1851463,-0.0379017,0.2492576,-0.0085282,0.0168297,-0.1359725,0.039329,0.1585443,-0.4719323,0.0543416,-0.001775,0.3499876,0.0292016,-0.0517079,-0.0466832,-0.0314438,-0.1850686,-2.2366894,0.4648057,-0.0096839,0.1359483,-0.4316242,0.0202388,0.0725398,0.0022762,-0.2983524,0.8902345,-0.2493142,0.0265137,-0.6936329,0.5832567,-0.0138449,0.0988486,-0.0284077,0.3638281,0.0755173,-0.0258476,0.0172484,0.0011755,0.072579,0.0203998,-0.0739059,0.0473805,0.1181117,-0.6846578,-0.3996183,-0.1121765,-0.5576999,-1.1822142,-0.2395248,-0.1118079,-0.1606468,-0.5172498,0.4321334,0.1788508,0.0927922,0.2046932,0.5982345,0.2022411,0.2998519,0.4231208,0.5801086,-0.0251373,0.1079448,-0.0071693,0.0916507,-0.0604216,0.012436,-0.001981,0.0155834,0.101476,0.013754,-0.0884009,0.0191593,-0.0347537,-0.0804634,0.0313783,0.0138881,0.0304173,0.1064435,0.0690836,-0.0522501,0.0188122,-0.0378475,-0.0402352,0.0217358,0.0087057,0.0287165,0.0982976,-0.0014888,0.0810395,-0.0110104,0.1061322,-0.0216056,0.0212807,-0.0121907,0.0210168,0.1171409,0.0351059,-0.032638,0.0079373,-0.0749939,-0.0411552,0.0296468,0.0181025,0.0269216,0.1183526,-0.1728596,-0.0178106,0.013786,-0.0646172,0.0329056,0.0111643,0.0233996,0.0088877,0.0750189,0.0067186,-0.0118248,0.047033,0.1518176,-0.0368049,0.0632207,-0.0452932,0.0824229,-0.131928,0.0034024,-0.0379775,-0.0483366,0.149056,-0.0991454,-0.0878945,-0.0190968,-0.0932097,-0.0682112,0.011241,-0.0167672,-0.0029667,-0.0881182,-0.0253554,0.0743516,0.0424118,0.0527118,0.0321203,-0.0387801,0.0353881,0.0268752,0.0927527,-0.0639173,-0.0894998,0.0712142,-0.0748556,0.0302382,-0.1298659,0.0169804,-0.00493294,-0.0266027,0.0802632,-0.0130018,-0.1016011,-0.0142723,-0.0992348,0.0275997,-0.0802556,0.0040227,-0.1086276,-0.1463598,0.0163676,0.0082048,0.0376694,0.02475,-0.0845147,0.0105048,-0.0875733,0.0875631,-0.0154458,0.0546653,-0.103074,-0.0367776,-0.039556,-0.0736906,0.0429448,0.1130802,-0.0053333,0.0153079,-0.0158488,0.027989,-0.0813477,-0.0605479\Polar=226.0176817,-16.3447112,153.1830206,-1.2422278,-7.5482421,67.6327912\PG=C01 [X(C13H14O2)]\NImag=0\

### 30<sup>+</sup>

1\1\MF (MLIB83-EXE) -BARYON\Freq\RB3LYP\6-31G(d)\C13H13O2(1+)\THEIS\18-Aug-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\Nyt derivat\1,1\C,2.5701500279,0.7424899881,-0.9049036751\C,2.6205616472,-0.0287871262,0.3363836995\C,1.3508317537,-0.5744370438,0.8428401799\C,0.1309482276,-0.1590587699,0.2633867736\C,0.140589799,0.681450359,-0.9061122422\C,1.4040973477,1.0873804998,-1.4842640662\C,-1.1221163561,-0.5836036876,0.7928786641\C,-2.3094684834,-0.1901227769,0.2260715921\C,-2.2916915091,0.6444117029,-0.9245306383\C,-1.0636885706,1.0612343336,-1.4769734628\O,-3.378137661,1.0779931646,-1.5530078013\C,-4.6905573439,0.7167042928,-1.0858127851\C,3.7927946572,-0.0888233184,1.020627284\O,1.2368853697,-1.4284800512,1.8425113505\C,2.2553451099,-2.3156561564,2.3542079722\H,3.5181179753,1.0710135943,-1.3191699359\H,1.3891285071,1.6887339328,-2.3878103862\H,-1.1320431548,-1.2199657261,1.669887957\H,-3.2474584049,-0.518294222,0.6563727863\H,-1.0878444105,1.6851071901,-2.3643194449\H,-5.3805328322,1.2014117984,-1.7748037036\H,-4.8543681728,1.0906895497,-0.0705879344\H,-4.8280834044,-0.3682608898,-1.123362515\H,3.912638348,-0.5465674445,1.991892175\H,4.6763797459,0.3930844829,0.6119798812\H,2.7543395833,-1.8509446507,3.2076946898\H,2.9708940665,-2.5821226175,1.5738247645\H,1.7120726415,-3.1990836871,2.6895774987\

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277661,0.0987207,-0.0129758,0.0814207,0.0904792,-0.0103634,0.0222083,-  
0.0001226,0.1036662,0.0459654,0.0322522,0.0468509,0.0365949,0.1076568,  
-0.0200624,0.0175431,-0.0289622,0.0970607,0.0407357,0.0339953,0.054498  
7,0.0600142,-0.0092566,0.0587632,-0.1091222,-0.0201916,-0.0230355,-0.0  
42163,-0.0324873,-0.0245438,0.0209416,0.0005051,0.0784345,-0.0151885,0  
.0064834,0.0460383,0.0546148,0.0084261,0.000991,-0.0623107,0.0322525,-  
0.0449447,0.0012512,0.0094563,-0.0155447,0.0756956,-0.0147085,0.036450  
4,0.0790408\Polar=285.1740623,-21.5545223,95.0674543,50.8388518,-48.87  
57798,128.2505656\PG=C01 [X(C13H13O2)]\NImag=0\

### 31

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C13H14O2\THEIS\21-Jul-2004\0\#\#  
N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\dimethoxy dev\0,1\  
C,2.2517764571,0.0880296125,0.0124101613\C,2.001839469,1.5005062425,0.  
0185848011\C,0.6950417163,1.9247393189,0.0137384584\C,-0.4026967605,1.  
0198331085,0.0030448875\C,-0.1353301859,-0.3862942798,-0.0028410889\C,  
1.2196747655,-0.8253423536,0.0020951441\C,-1.7491305188,1.4515604156,-  
0.0018930965\C,-2.7977195479,0.5539637516,-0.0121006561\C,-2.527414023  
2,-0.8377668376,-0.0178311791\C,-1.2193019077,-1.2923988419,-0.0133458  
424\O,-3.4996603224,-1.8009404783,-0.0279393534\O,3.5783808204,-0.2421  
96433,0.0176723952\C,-4.8575536579,-1.3951288504,-0.0327206463\C,3.927  
9415138,-1.6162479301,0.0122065914\C,3.1625126672,2.461243939,0.030014  
4948\H,0.4849508652,2.992738668,0.0182608297\H,1.4148861593,-1.8919583  
353,-0.0023224079\H,-1.9577606719,2.5191281013,0.0024200881\H,-3.81768

01656,0.9206145413,-0.0155727595\H,-1.039701931,-2.3636987393,-0.01822  
30359\H,-5.4439345307,-2.3161429901,-0.0405023252\H,-5.1038011249,-0.8  
047551617,-0.9255420491\H,-5.1128482542,-0.8141031102,0.863691199\H,5.  
0191404776,-1.6490711508,0.0175524255\H,3.5521705959,-2.1229679608,-0.  
8865318302\H,3.5431404143,-2.1323813829,0.9017301441\H,2.8078364069,3.  
4964376795,0.0345070483\H,3.8072829312,2.3208482387,-0.8458819161\H,3.  
7987149222,2.3102231231,0.9103780778\\Version=SGI64-G98RevA.7\HF=-654.  
2566592\RMSD=4.585e-09\RMSF=1.314e-05\Dipole=-0.2170824,-0.1329016,-0.  
0017706\DipoleDeriv=1.5902702,-0.4838313,0.0051777,-0.4522805,0.296827  
2,-0.0015181,0.0052159,-0.0016858,0.1363928,-0.1108584,0.2003494,0.000  
8264,0.4229959,0.0087231,0.0025662,0.001832,0.0013258,-0.0552364,0.241  
8873,-0.0459321,0.0017747,0.0931251,0.1418414,0.001971,0.002491,0.0012  
401,-0.1384712,-0.3302998,0.0548446,-0.0015413,0.023366,-0.2620088,-0.  
0013392,-0.0017588,-0.0011369,0.0216258,0.5141391,0.0826511,0.0028629,  
0.0768819,0.0354378,0.0002936,0.0028586,0.0003074,0.0568693,-0.4886761  
,0.0323863,-0.0012331,-0.2257857,-0.021481,-0.0001829,-0.0025434,0.001  
1444,-0.2246456,0.4009922,-0.0244509,0.0025681,-0.0095414,0.1632868,0.  
0013381,0.0027163,0.0011971,-0.1127204,-0.2442663,-0.0654842,-0.000679  
4,-0.4579678,-0.2157454,-0.0025918,-0.0027835,-0.0004713,-0.1856357,1.  
2669618,0.566539,0.0087515,1.196752,0.6737379,0.0089308,0.0120707,0.00  
5577,0.1627954,-0.5437981,-0.2067811,-0.0029151,-0.023355,0.0601688,0.  
0012685,-0.001878,0.0004264,-0.2003547,-1.9772024,-0.5029638,-0.011358  
2,-0.9338678,-0.7110597,-0.0070632,-0.0136789,-0.0048232,-0.2962023,-1  
.7524783,0.487792,-0.005264,0.7548036,-0.7913965,0.0012894,-0.0037217,  
-0.0001559,-0.2789682,1.2632572,0.1674528,0.0055001,-0.2607413,0.24632  
85,-0.0019904,0.0032357,0.000204,0.3648244,0.4775085,-0.1497899,-0.000  
1338,-0.684845,0.7669736,-0.0014669,-0.0031285,0.0013789,0.3532256,0.0  
30847,-0.0297572,-0.0006474,0.044219,0.1552973,0.0005421,0.0000306,0.0  
002544,0.105645,0.0448216,0.0456503,-0.0000667,-0.0029631,-0.1218396,-  
0.0012003,-0.0003313,-0.0009646,0.0993245,0.0545453,0.0023795,-0.00037  
4,0.0683934,-0.0877413,-0.0007611,-0.0000431,-0.0010751,0.1257702,0.04  
58941,0.0037295,-0.000304,0.0497328,-0.1130912,-0.0008441,-0.000057,-0  
.0010767,0.1052175,-0.1015429,0.0380316,-0.0009704,0.0570767,0.0695711  
,0.0000097,-0.0008354,-0.0000681,0.1244026,0.060398,0.0425185,-0.00010  
36,-0.0038207,-0.0766592,-0.0010535,-0.0003459,-0.0008669,0.1206153,-0  
.0725205,-0.0841415,-0.0011987,-0.1390365,-0.0749325,-0.0014957,-0.001  
487,-0.001208,0.0767016,-0.0792172,-0.0286094,-0.0063002,0.1503371,0.0  
127799,0.0969301,-0.0644817,0.0707543,-0.1034107,-0.0799004,-0.0279598  
,0.006235,0.1506345,0.0145256,-0.0941319,0.066313,-0.0697863,-0.104391  
8,-0.1711828,0.0577989,-0.0009769,0.0239523,0.0385736,-0.0000569,-0.00  
11331,0.0001024,0.0764153,0.0474248,-0.060217,-0.0791809,0.1072705,-0.  
0675078,-0.0459846,-0.018398,-0.0757249,-0.0971477,0.0463252,-0.061800  
9,0.0800155,0.1065963,-0.0688318,0.0474326,0.0210733,0.0754104,-0.0948  
723,0.0134228,0.0933474,0.0002977,-0.0223172,-0.1419871,-0.001391,-0.0  
004229,-0.0007627,0.0687975,-0.0744354,-0.052355,0.0781575,-0.0553617,  
0.0352692,-0.0362207,0.1130757,-0.0014363,-0.0525907,-0.0723368,-0.051  
3982,-0.0789195,-0.0542573,0.0349355,0.0367206,-0.1138853,0.0019196,-0  
.0539807\Polar=242.5824293,16.3595378,150.8315198,1.0263557,0.5338985,  
65.4413514\PG=C01 [X(C13H14O2)]\NImag=0\

### 31<sup>+</sup>

1\1\GINC-ELECTRON\Freq\RB3LYP\6-31G(d)\C13H13O2(1+)\THEIS\22-Jul-2004\  
0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\\Dimethoxy\\1,1\  
C,2.312011245,0.0593147874,-0.0193312948\C,2.0538490342,1.5088551794,-  
0.0284196697\C,0.6822032171,1.9520770305,-0.0201713335\C,-0.3676070441  
,1.0677462596,-0.0050719973\C,-0.0902684715,-0.3642035981,0.0033313787

\C,1.2647674607,-0.8235990415,-0.0042615523\C,-1.7346177572,1.51677132  
24,0.0027314272\C,-2.7703660597,0.6320767099,0.0179356164\C,-2.4873934  
99,-0.7759580079,0.0264522806\C,-1.1645173982,-1.2475626923,0.01882911  
59\O,-3.4271006857,-1.7096785225,0.0417439769\O,3.6085425967,-0.259395  
5707,-0.0273047328\C,-4.8265983306,-1.3648353989,0.0509211181\C,3.9947  
106771,-1.6428900185,-0.0207985149\C,3.0634873746,2.4192103459,-0.0447  
904082\H,0.4942189757,3.022758586,-0.0264422866\H,1.4384309504,-1.8928  
667588,0.0024645745\H,-1.9293135831,2.5855065308,-0.0038835773\H,-3.79  
37295802,0.9857000891,0.0234486017\H,-1.0075736419,-2.3210091515,0.025  
5386934\H,-5.3511801863,-2.3188355857,0.0632640627\H,-5.090809931,-0.8  
063473424,-0.8517223901\H,-5.075406023,-0.7915484625,0.9486461967\H,5.  
0837291492,-1.6395251819,-0.0300949124\H,3.6144689658,-2.1508895054,-0.  
.9129304006\H,3.6298337242,-2.1380917683,0.8848487193\H,2.854754153,3.  
4849353842,-0.0513622296\H,4.1030790479,2.1107886441,-0.0514260018\\Ve  
rsion=SGI64-G98RevA.7\HF=-653.3941888\RMSD=3.208e-09\RMSF=2.964e-05\Di  
pole=-0.1642809,0.6962519,-0.004601\DipoleDeriv=2.2861382,-0.5264047,-  
0.0129371,0.3481331,0.3610442,-0.0043636,-0.0195789,0.0026746,0.198728  
1,-0.934914,-0.4591406,0.0119603,-0.2708003,-0.3255698,0.0051239,0.011  
1108,0.0070834,0.0294992,0.923829,0.6026045,-0.0126112,0.3349741,0.326  
456,-0.0051996,-0.0106291,-0.0077857,-0.0066383,-0.7112421,-0.5264017,  
0.0099995,-0.3245528,-0.5762487,0.0071932,0.0083821,0.0088144,0.008290  
6,1.7061422,-0.0072777,-0.0129005,0.628827,0.4304737,-0.0074525,-0.017  
6038,-0.0021902,0.1341776,-1.4899957,0.1759117,0.0091357,-0.4550185,0.  
040021,0.0016598,0.0135072,-0.0034075,-0.2293208,0.5549521,0.505434,-0.  
.0086822,0.0770328,0.2625071,-0.0029141,-0.0053959,-0.0065069,-0.03302  
38,-0.0170344,-0.1900865,0.0002885,-0.4564016,-0.7877707,0.0086736,0.0  
025535,0.0063791,-0.1597875,2.4810058,0.5472887,-0.02278,1.0335855,1.2  
556094,-0.0162159,-0.0268989,-0.0122226,0.288277,-2.0432356,-0.2845448  
,0.0175052,-0.1823144,0.0472166,-0.0003118,0.0167581,0.0005494,-0.2014  
822,-2.446949,-0.6922065,0.023718,-1.4239608,-0.895554,0.016794,0.0299  
225,0.0108445,-0.2621561,-1.9460214,0.6347521,0.0088787,0.7329668,-0.7  
547811,-0.0024211,0.0082214,-0.0016348,-0.266599,1.4743126,0.3132396,-  
0.0123032,-0.1013445,0.2175753,0.001443,-0.0095968,-0.0021886,0.293859  
4,0.5406769,-0.1948009,-0.0005482,-0.807895,0.7284345,0.0035405,0.0038  
876,-0.001305,0.3068399,0.3362691,0.1509582,-0.0047825,0.2807071,0.333  
2591,-0.0055479,-0.0054715,-0.0041756,-0.0652328,0.0412701,0.0125983,0.  
.0005355,0.020592,0.0096855,0.0006286,0.0003863,0.0006853,0.1149011,0.  
0650739,0.0023937,0.0006225,0.0438885,-0.0084237,0.0008219,0.0002765,0.  
.0011769,0.1434547,0.0708253,-0.0190578,0.0005245,0.0225436,-0.0030903  
,0.0007554,0.0001806,0.0011412,0.1178506,-0.0020298,0.0135728,0.001072  
2,0.021408,0.0819598,0.0002237,0.0009505,0.0003541,0.1383961,0.0617179  
,0.0312495,0.0004341,0.0132887,0.0180254,0.0007379,0.0005842,0.0006911  
,0.1409403,-0.0071456,-0.0310949,0.0011869,-0.068193,-0.0056751,0.0015  
16,0.0015371,0.0011866,0.1047482,-0.0973084,-0.0578244,0.0262429,0.110  
3766,0.0570014,0.0728319,-0.0209575,0.0589445,-0.034353,-0.097263,-0.0  
592063,-0.0242912,0.1094585,0.0548054,-0.0761102,0.0203956,-0.0593502,  
-0.0321024,-0.06069,0.0354473,0.0011277,0.0000487,0.0544443,0.0003767,  
0.0014006,0.0000383,0.1015234,0.0528624,-0.0462606,-0.0815591,0.119606  
2,-0.0269772,-0.0176999,-0.0296211,-0.0426821,-0.0430009,0.0547819,-0.  
044346,0.0805579,0.1203864,-0.026144,0.0155846,0.0262232,0.0431452,-0.  
0457622,0.0684875,0.0703125,-0.0000365,0.052697,0.0530352,0.0001067,-0.  
.000002,-0.0001426,0.1259878,0.1354659,0.0428906,-0.000358,0.0199587,0.  
.0786769,0.0002249,-0.0005218,-0.0001161,0.1319798\Polar=303.32186,52.  
1199278,165.3760604,-2.4543227,-1.2656095,57.5736809\PG=C01 [X(C13H13O  
2)]\NImag=0\\

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1\1\MF (MLIB83-EXE) -LEPTON\Freq\RB3LYP\6-31G(d)\C14H16O3\THEIS\16-May-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\trimethoxybenzen\0,1\C,-2.5701817275,0.3202932136,0.4155343097\C,-2.3737991767,-1.0534693894,0.0638889361\C,-1.0927383026,-1.4759468498,-0.2056015802\C,0.0224636502,-0.5988175015,-0.1450704703\C,-0.1845960927,0.7697524659,0.2067320109\C,-1.5120839778,1.2017856954,0.4846465477\C,1.3531904262,-1.0296946365,-0.4231118487\C,2.422075482,-0.151583079,-0.3561581539\C,2.1904952497,1.2030679762,-0.0044554386\C,0.9159054649,1.656633399,0.2715783703\O,3.1947264174,2.1302909094,0.0824833731\O,-3.872130747,0.6547113639,0.666820109\O,1.4775605223,-2.3496006434,-0.7525072516\C,4.525494164,1.7285679787,-0.1871980787\C,2.7666801718,-2.8598866004,-1.0431263715\C,-4.1633738136,1.995404403,1.0230912482\C,-3.5579689696,-1.9835016461,-0.0001351548\H,-0.9196965172,-2.51289792,-0.4742713935\H,-1.6653119298,2.241445297,0.7514048983\H,3.4248761199,-0.4930931151,-0.5696323694\H,0.7720454344,2.6989926225,0.5377567591\H,5.1392495195,2.622067547,-0.0554431409\H,4.641759666,1.3627917382,-1.2165818374\H,4.8680147141,0.9525818065,0.5109676655\H,2.6253567922,-3.9172248658,-1.2750816034\H,3.4417005579,-2.764566357,-0.1821155902\H,3.2143093582,-2.3552079031,-1.9097319443\H,-5.2435548207,2.0384487854,1.175927143\H,-3.8798688181,2.6941277661,0.2248347729\H,-3.651910129,2.285006797,1.950624581\H,-3.2413751262,-2.9927036951,-0.2805053801\H,-4.2996999907,-1.6388420032,-0.7308419363\H,-4.0765196619,-2.0397721147,0.9646335756\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-768.7791104\RMSD=3.152e-09\RMSF=9.109e-06\Dipole=0.7528149,-0.0639218,-0.1137052\DipoleDeriv=1.5612831,-0.5045925,-0.3073607,-0.4066708,0.3556025,0.1047697,-0.2841071,0.1176849,0.2057516,-0.0893619,0.2419517,0.0609215,0.375559,-0.0503352,-0.0467389,0.0927847,-0.0290047,-0.0815663,0.2474526,-0.1056883,-0.0731065,0.1323834,0.0418594,0.0199673,-0.0166669,0.0513954,-0.1017361,-0.4166471,0.2286286,0.1055918,-0.0409226,-0.350827,-0.0711959,0.0416734,-0.1067687,-0.0584849,0.6293845,0.1136448,-0.0476682,0.2064916,0.1440905,-0.000848,-0.0256752,0.0037721,0.0690677,-0.5559958,0.0204894,0.0482191,-0.2117064,-0.0254231,0.0759184,-0.0068111,0.0452611,-0.2160006,0.6214909,-0.1103949,-0.0887597,-0.5996516,1.379739,0.3711756,-0.2047756,0.3066603,0.2479109,-0.3257479,-0.2167908,-0.0417728,-0.1568228,-0.4888951,-0.0352541,-0.0274013,-0.0273464,-0.2556538,1.4711083,0.5475619,-0.0428586,0.881195,0.772993,0.0278134,0.0358273,0.0716157,0.1772323,-0.7594826,-0.2094021,0.0199899,-0.0022005,-0.0596918,0.0411842,0.0690821,0.0685633,-0.2251506,-1.9716567,-0.5175034,0.0988256,-0.8595974,-0.6973964,0.0177907,0.0177758,-0.0271908,-0.3022162,-1.683357,0.5178359,0.3082671,0.7249783,-0.7960622,-0.2182729,0.3573245,-0.1908868,-0.371837,-0.7740988,0.4575029,0.1734769,0.7565976,-1.4766585,-0.3833151,0.2443442,-0.3439177,-0.3948085,1.203132,0.1719261,-0.0705614,-0.2503525,0.2477958,0.0066471,-0.1702968,-0.0490116,0.37021,0.8169535,-0.5519042,-0.1920892,-0.2412276,0.521602,0.0719246,-0.1183679,0.1128543,0.3946919,0.4452737,-0.1354726,-0.0443069,-0.6489994,0.7730744,0.1853271,-0.1660181,0.1174786,0.4027778,0.0433518,-0.0217732,0.0036297,0.0535978,0.1469588,0.0017878,0.0212334,0.011671,0.1094167,0.0909372,0.0039744,0.0021167,-0.0165717,-0.0609485,-0.0359073,-0.002748,-0.0385999,0.0909836,0.0583884,-0.0046586,0.0077025,0.0583456,-0.0802706,-0.0563719,0.0226372,-0.0480559,0.1106096,-0.0612172,0.05448,0.0389998,0.0559276,0.0864566,-0.0191654,0.0394044,-0.018946,0.1264512,0.0571539,0.0374017,0.0182149,-0.0102904,-0.0662669,-0.0446674,0.0069027,-0.0509725,0.1148387,-0.0749785,-0.0881053,-0.0007856,-0.1370627,-0.0691343,-0.0169299,-0.0124352,-0.0233857,0.0739865,-0.0706269,-0.0323216,-0.0086364,0.1204018,0.0462206,-0.0788174,0.0871128,-0.0335407,-0.1473557,-0.0865406,-0.0128818,

-0.0085054,0.1722644,-0.0298325,0.0935271,-0.0242853,0.0927207,-0.0550267,0.0379722,-0.0196606,0.0007109,0.0460065,-0.1423328,-0.0584578,0.0162697,-0.0497887,0.0647593,-0.1123397,0.1148454,-0.0341323,-0.0390565,0.0451749,-0.0364928,-0.0953387,0.0036168,-0.0929966,-0.0751891,0.0905042,0.0820373,-0.0594827,0.0053213,0.1073583,0.0711653,0.0272573,-0.0903326,-0.1683517,0.0599505,0.0464583,0.0246183,0.0381997,-0.0121652,0.0380765,-0.0168304,0.0667592,0.060798,-0.0695532,0.0461739,0.1030854,-0.101385,0.0320757,0.0275654,0.0851326,-0.0802135,0.0343601,-0.0516412,-0.1130486,0.1021593,-0.0467084,-0.0483987,-0.017058,-0.0583286,-0.1084477,0.0186246,0.082415,0.0259476,-0.0288517,-0.1269597,-0.0422126,-0.0003473,-0.0569087,0.0542376,-0.1108722,-0.0273732,-0.0800959,-0.0210121,0.023493,0.0581931,-0.1186307,0.0244834,-0.0157439,-0.0612321,-0.0633879,0.066409,-0.0831317,0.0405301,-0.002618,0.1017864,0.0293138,-0.0821256\Polar=254.6502573,6.3291127,170.2292461,-22.0056942,21.3354797,84.6738883\PG=C01 [X(C14H16O3)]\NImag=0\

### 32<sup>+</sup>

1\1\MF(MLIB83-EXE)-NEUTRON\Freq\RB3LYP\6-31G(d)\C14H15O3(1+)\THEIS\15-May-2004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\trimet hoxibenzen\1,1\C,-1.9118285732,0.4393435809,1.8342236832\C,-0.6145806434,0.4626112652,2.5272402348\C,0.5750647848,0.2480036266,1.7398738363\C,0.5201022179,0.0280011002,0.3910085453\C,-0.7733953676,0.00759326,-0.2838184345\C,-1.9644306022,0.2193053893,0.4855270611\C,1.7283425237,-0.1881006594,-0.3969054289\C,1.6505346957,-0.4078578745,-1.7562746581\C,0.3740824332,-0.4207110423,-2.3785923692\C,-0.815912918,-0.2155578828,-1.648551268\O,0.201788466,-0.6238492521,-3.6792370634\O,-2.9594269235,0.6470027339,2.6392511958\O,2.860217725,-0.1517040002,0.3060327357\C,1.3218667357,-0.8481867431,-4.55306026\C,4.1210489687,-0.3506351887,-0.3544467748\C,-4.2815771575,0.6477285075,2.0819597747\C,-0.5139856973,0.6771058989,3.8650485122\H,1.534199273,0.2644348296,2.2467898112\H,-2.91169682,0.19922745,-0.0395039948\H,2.5430264748,-0.5680804217,-2.3432111414\H,-1.7548613745,-0.2390091117,-2.1902251059\H,0.8873055676,-0.9822308682,-5.5425251015\H,1.8641010761,-1.7524449338,-4.2601452194\H,1.9889015595,0.0193270633,-4.5549814697\H,4.8727544613,-0.2742983607,0.4298208971\H,4.2859175802,0.4272347431,-1.1066442751\H,4.1600423284,-1.343459234,-0.8136209045\H,-4.9505939341,0.8338238741,2.9211099474\H,-4.5091202338,-0.3239181908,1.6311847409\H,-4.3845909246,1.4447240022,1.3381572229\H,0.454116045,0.6902994661,4.3565696533\H,-1.3921236224,0.8409144113,4.47945527\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-767.9278757\RMSD=2.867e-09\RMSF=1.024e-05\Dipole=0.7356082,-0.0620087,-0.0582106\DipoleDeriv=1.1999746,-0.1604951,-0.5381936,-0.2947862,0.2531316,0.2351815,-1.3477117,0.2923914,1.3820465,-0.1783263,0.0648171,0.3026691,0.0465266,-0.0035392,-0.1755317,0.1929062,-0.1679765,-0.9023677,0.0336637,-0.0487471,-0.2830725,-0.0342559,0.0411301,0.1886557,-0.1955936,0.1826213,1.025257,-0.3377796,0.0299285,0.0513532,0.0397138,-0.0658123,-0.1687291,0.109951,-0.1728095,-1.0302852,0.5679318,-0.0626525,-0.1932951,-0.1776536,0.1855969,0.2324453,-0.8868305,0.281422,1.4540303,-0.4012632,0.0727753,0.3678474,0.1732199,-0.2713014,-0.149343,0.9728564,-0.191972,-0.9774167,1.4520022,-0.1359749,-0.298074,0.1089147,0.2425962,0.1222904,1.1793279,0.0176812,0.84039,-0.6751084,-0.0217387,-0.3055917,-0.1176196,-0.2637461,-0.0282914,-0.8837472,0.0125748,-0.568673,1.5698346,-0.1751,-0.508416,-0.1608913,0.3680533,0.4267178,-0.4234594,0.4210851,2.6464542,-0.6335984,0.1920408,0.9814757,0.1980743,-0.2796949,-0.284679,1.0177479,-0.2872485,-1.5171928,-0.5005896,0.0447016,0.1679792,0.117337,-0.3393412,-0.4139371,0.606579,-0.4451895,-2.6899752,-1.8930035,0.2438104,0.7780269,0.2233919,-0.3084399,-0.1444294,0.6552179,-0

.1357618,-0.8078997,-2.0392836,0.1580676,0.19363,0.0295535,-0.2657413,  
-0.0179888,-0.5816791,0.0369412,-0.2862349,0.5087454,-0.136378,-0.7318  
399,-0.0632741,0.3282527,0.1718111,-0.2904682,0.140314,1.0181886,1.113  
7555,-0.0824162,-0.1482922,-0.1162354,0.3064636,0.0072514,-0.3516923,0  
.0216615,0.2774,1.1529555,-0.1137797,-0.3273201,-0.0107197,0.3101534,-  
0.0071047,0.2932,-0.0508656,0.1286971,0.0896366,0.0045327,0.1039573,-0  
.0174312,-0.0760966,0.0807026,-0.0284238,0.0898491,0.4394315,0.0463706  
,0.0047241,0.0016648,0.0001527,0.1081196,-0.0081202,-0.0260417,-0.0061  
775,0.0610935,-0.00905,0.0091016,-0.0097293,0.001558,0.1402868,-0.0131  
081,-0.0552733,-0.0099273,0.0591312,0.0137821,0.0185428,0.0536813,0.01  
60445,0.1465752,-0.0160387,0.038531,-0.0150195,0.0761249,0.0073432,0.0  
063157,-0.0201309,0.0085042,0.1414917,-0.010901,-0.0067888,-0.0118208,  
0.0696889,0.044617,-0.0014673,-0.0338978,0.004367,0.1000381,-0.0239629  
,0.0010302,-0.0263693,-0.0539626,-0.0156889,0.0729771,0.1529544,0.0573  
54,-0.0335701,0.0112731,-0.0071769,0.0699163,-0.029255,-0.0306246,-0.0  
223239,0.1661645,-0.0603016,-0.0469922,-0.0258468,0.002993,-0.0614828,  
-0.0008821,-0.0151193,0.0066295,-0.0103538,-0.0042681,0.1005007,-0.013  
7183,-0.0762334,-0.0090422,0.015058,-0.0220106,0.0414499,-0.0173999,0.  
0130167,-0.0231098,0.0591667,0.124966,0.0659249,-0.0137303,-0.0273638,  
-0.0483,-0.0101399,0.0242063,-0.0574311,-0.0418048,0.1132205,-0.067417  
3,0.0259919,-0.0127787,0.0154179,0.0451197,0.0211551,0.0949227,-0.0195  
023,0.0798825,-0.0219562,0.0010428,-0.0338449,0.0417642,0.0434257,-0.0  
402567,-0.0661435,-0.0307271,-0.1176969,-0.0467429,0.0745646,-0.036063  
4,-0.0262769,0.0614362,-0.0000891,-0.0242664,0.0576947,-0.1137385,0.09  
74173,0.0349095,-0.0100059,0.0079716,-0.0097095,0.0110069,0.1247192,-0  
.0013766,0.0086848,-0.0026235,0.1135696,0.0708654,0.0000836,-0.0259231  
,0.0036878,0.1331842,0.0019492,-0.0045305,0.0006008,0.134789\Polar=202  
.3237625,-18.0858366,76.7188163,-52.0244649,41.7225078,298.028451\PG=C  
01 [X(C14H15O3)]\NImag=0\

### 33

1\1\MF (MLIB83-EXE)-BOSON\Freq\RB3LYP\6-31G(d)\C15H18O4\THEIS\31-Jul-20  
04\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\optimalt der  
ivat\0,1\C,-1.4884114542,-0.0460573973,-2.2539084836\C,-0.2017959025,  
0.4762560783,-2.5079360982\C,0.7180738646,0.5836746453,-1.4751201304\C  
,0.3906127641,0.1723849267,-0.1389953912\C,-0.9304119454,-0.3579052676  
,0.0945169118\C,-1.842857373,-0.4522594916,-0.9862933286\C,1.281975520  
4,0.2503264396,0.9819938953\C,0.8747003896,-0.1717801283,2.2346929734\  
C,-0.4264146988,-0.687922143,2.4358563479\C,-1.3358853829,-0.790241840  
9,1.3967371004\C,-2.7197349444,-1.3445161095,1.6350098571\O,-0.8467200  
54,-1.1112583906,3.6725003924\O,-2.4451273302,-0.180364972,-3.22333397  
59\O,2.5299975797,0.7512459976,0.7628573118\C,0.0393635309,-1.03108286  
75,4.7728873195\C,3.4316038922,0.8403882886,1.8494241511\C,-2.14019665  
79,0.217371028,-4.5480096732\O,1.9676590119,1.0826842774,-1.6836241289  
\C,2.333509247,1.499111992,-2.9855061364\H,0.066162219,0.7921062299,-3  
.5049252972\H,-2.8393448597,-0.8464702767,-0.8365569348\H,1.5563717528  
, -0.1070895979,3.069047701\H,-2.849579442,-1.6203755814,2.6818565794\H  
, -2.9079554007,-2.2375771768,1.0246679956\H,-0.5150932326,-1.420006040  
5,5.6296807296\H,0.3406258609,0.0043620802,4.9820326318\H,0.9383874063  
, -1.6436636937,4.6207461636\H,4.3495798765,1.2637956886,1.4368463712\H  
,3.6501744355,-0.1465049829,2.2799108492\H,3.052325081,1.5013773149,2.  
6408111751\H,-3.0400950553,0.0182431646,-5.1336241904\H,-1.3052454274,  
-0.3607422403,-4.9667842448\H,-1.902871885,1.2882041667,-4.6092998142\  
H,3.3628667459,1.8534970641,-2.9026081163\H,1.6967780976,2.318790207,-  
3.3455516472\H,2.2932955196,0.6700920593,-3.7052414991\H,-3.4976404487  
, -0.6129826013,1.3796988633\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-8



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33<sup>+</sup>

1\1\MF (MLIB83-EXE) -BOSON\Freq\RB3LYP\6-31G(d)\C15H17O4(1+)\THEIS\31-Ju

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1-2004\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\tetra op
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94947845,0.2211822117,-0.7315361023\C,-1.5967621504,-0.6616934232,-0.0
788601117\C,-0.2060046753,-0.3342340119,0.0904107627\C,0.2664430636,0.
9134064697,-0.446087444\C,-0.615655618,1.7729691976,-1.0746578939\C,0.
7279560282,-1.1680484668,0.7873915176\C,2.0812378807,-0.7886584765,0.9
792184875\C,2.5625612965,0.3899683493,0.4610650127\C,1.7001554658,1.27
7604019,-0.327714845\C,2.2629505391,2.348626323,-0.92973429\O,3.813580
2132,0.8088706789,0.6033103067\O,-2.7190772197,2.3529242035,-1.8524664
218\O,0.2812805228,-2.3138330272,1.267229388\C,4.7701010622,0.01703032
57,1.3282552821\C,1.1299968536,-3.2238732727,1.9899520007\C,-4.1175005
239,2.1185381629,-2.0562306036\O,-2.0217653078,-1.8330999594,0.4121930
26\C,-3.3958866581,-2.2115917351,0.2782083143\H,-3.5015675658,-0.03423
81829,-0.850610674\H,-0.3065443461,2.7336390042,-1.4653208653\H,2.7348
898528,-1.4411137795,1.5371868462\H,3.3176676449,2.5607991271,-0.80649
49255\H,1.7016175617,3.0255177712,-1.5620595965\H,5.6981302071,0.58552
10984,1.2921733037\H,4.9076981349,-0.9546370939,0.8438231441\H,4.45085
5137,-0.1110071289,2.3671291993\H,0.4847572955,-4.0645216305,2.2404219
565\H,1.5049256165,-2.7582367071,2.9059900242\H,1.9564557269,-3.564826
8406,1.3597663956\H,-4.485086264,3.0002311617,-2.5800536782\H,-4.63959
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1702336,-0.3747062,0.7886964,-0.6516496,0.4874345,-0.6999698,0.3387551
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6722212,0.6006008,-0.6270857,0.9194595,-0.8496948,0.5044966,-0.7807508
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2,-0.3921072,0.5237566,1.1650862,-0.3214387,0.3617479,0.0584832,0.2319
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,0.0283679,-0.0451558,0.0232718,0.0732434,0.0498459,-0.0511652,0.04954
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1983,-0.0360711,0.0030006,0.1186687,0.0373295,0.0574062,-0.0619182,0.0
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879,-0.0677603,-0.0616029,-0.0117535,-0.0110574,0.0057295,0.0789595,0.  
1157673,0.0524423,0.047271,-0.0431705,0.0067621,-0.0659936,0.0282282,-  
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76,0.0790987,0.0269308,0.090086,-0.0970298,0.004219,-0.0415113,-0.0583  
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.025629,-0.032394,0.0623145,-0.0052889,0.066563,-0.0503912,0.0581378,0.  
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96,0.0636717,-0.0661127,-0.0833693,0.0183254,0.014941,0.0696833,0.0227  
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.0896641,-0.0198462,-0.0781847,0.0039933,-0.0641105,0.025464\Polar=271  
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C01 [X(C15H17O4)]\NImag=0\

### 34

1\1\MF (MLIB83-EXE) -PROTON\Freq\RB3LYP\6-31G(d)\C15H18O4\THEIS\14-Oct-2  
004\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\tetramethyl  
\0,1\C,-0.0486669033,-0.0915306706,0.3103687766\C,0.4944473017,0.4882  
398602,-0.8855600467\C,-0.3814183538,0.9381254034,-1.9108795056\C,-1.7  
448155147,0.8390542453,-1.7610094092\C,-2.3232293712,0.2695913356,-0.5  
874294183\C,-1.4797838817,-0.1914921537,0.4093875695\O,-2.066847895,-0  
.7130777352,1.5446584883\C,-2.2301088314,-2.1281765766,1.5347069515\O,  
-2.6568947325,1.2580976589,-2.6888572889\C,-2.1732408092,1.852534617,-  
3.881535382\C,-3.8245342756,0.2047642609,-0.4650362662\C,0.8873502827,  
-0.4957085047,1.3199395451\C,2.2545628285,-0.344871737,1.135848849\C,2  
.7569160955,0.2174588839,-0.0601263085\C,1.8922376918,0.6256022887,-1.  
051843803\O,4.0925664155,0.3909465217,-0.3030652102\C,5.0262564027,-0.  
0042338022,0.6861185122\O,0.3741481355,-1.0353199835,2.4632241774\C,1.  
2570809806,-1.3985729279,3.5091681346\H,0.0591732823,1.3697922066,-2.8  
019283945\H,-2.7321052194,-2.3856215305,2.4709774162\H,-1.2630195501,-  
2.6415076412,1.4920975327\H,-2.8525461836,-2.4498217829,0.6884914821\H  
, -3.0572114062,2.116550148,-4.4653451651\H,-1.5523731944,1.1530765976,  
-4.4568525729\H,-1.5907855758,2.7591449292,-3.670996583\H,-4.258452851  
6,-0.4831666842,-1.2018365617\H,-4.270292159,1.1865033405,-0.659623352  
7\H,-4.1132726888,-0.1196987454,0.5352736102\H,2.9392456321,-0.6586304  
982,1.9096816172\H,2.293884578,1.0630841849,-1.9601394632\H,6.01106476  
75,0.2310625273,0.2773583454\H,4.9722941142,-1.0819400352,0.8921593487  
\H,4.8861589051,0.5491460593,1.6246093677\H,1.951110497,-2.1924791785,  
3.2007014829\H,0.6217927366,-1.7693433691,4.3158156249\H,1.8332370728,  
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916,-0.0472555,0.081365,-0.0361652,0.1358097,-0.039755,0.1627524,-0.57  
69904,0.1149515,-0.2981143,0.0462073,-0.217673,-0.0472815,-0.1066002,-  
0.0283471,-0.1637048,0.8951108,-0.3134624,0.7325021,-0.2497,0.3403929,  
-0.4144449,0.5448664,-0.4479459,1.0666125,0.0827468,0.0308152,-0.11888  
07,0.0325171,-0.1959676,0.1639066,-0.0695817,0.1970816,-0.416656,0.649  
5453,0.1504104,-0.0094273,0.1852704,0.2883845,-0.3303741,-0.3250924,-0  
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### 34<sup>+</sup>

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36438295\O, 0.6397845974, 2.4379289965, -3.1306834253\C, 1.8073173402, 2.53

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Supplementary Material for Organic & Biomolecular Chemistry  
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35

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### 35<sup>+</sup>

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Supplementary Material for Organic & Biomolecular Chemistry  
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36

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36<sup>+</sup>

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04446, 0.0071749, -0.0363786, -0.1006755, -0.0244793, -0.0474745, 0.0543003,  
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### 37

1\1\MF (MLIB83-EXE) -LEPTON\Freq\RB3LYP\6-31G(d)\C18H24O7\THEIS\05-Dec-2  
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1952181, -0.0678882457\C, -1.1189994895, -1.3085751499, -0.057516667\C, 0.1  
61477853, -0.6699736399, 0.0315055505\C, 0.2113116349, 0.7736595476, 0.1268  
622741\C, -1.0190878783, 1.5076820412, 0.0762774913\C, 1.394673436, -1.3997  
174216, 0.0143382742\C, 2.6089324516, -0.7325671334, 0.0849091059\C, 2.6738  
934776, 0.6770285318, 0.246306521\C, 1.4932615034, 1.4004183864, 0.26809867  
7\0, 1.6079449633, 2.7727691405, 0.3889614794\C, 4.0074702652, 1.3634234198

, 0.4205088334\O, 3.767254704, -1.4818128014, 0.1036687245\C, 4.552603428, -1.4476117105, -1.0859409268\O, 1.4134545932, -2.7748960342, 0.0220169045\C, 1.4121509807, -3.413854086, -1.2524483183\O, -1.2542730338, -2.6706564987, -0.2012799365\O, -3.5085362567, -1.1835000505, -0.0720524211\C, -4.038592768, -1.428191183, -1.3783385547\O, -3.3956107816, 1.5674816629, -0.1872948179\C, -4.0749779597, 1.8365282888, 1.0427363054\O, -1.0645750261, 2.8790159592, 0.186271628\C, -1.0010738183, 3.5821913746, -1.056570107\C, 1.4093281601, 3.2822227457, 1.7103117725\C, -1.4161406044, -3.3887692959, 1.0253859156\H, 4.4029416373, 1.7279754337, -0.5368650993\H, 4.7381262193, 0.6714864245, 0.8468970149\H, 3.9234206251, 2.2339299617, 1.0730338929\H, 5.3721842142, -2.1528973091, -0.9281602382\H, 4.9691877658, -0.4517130707, -1.2797393635\H, 3.9691810085, -1.7608078345, -1.9611392418\H, 1.4468025698, -4.4876059801, -1.0517702872\H, 2.2943636742, -3.1319333124, -1.8399883955\H, 0.5003861836, -3.182359262, -1.8121434569\H, -3.377649527, -2.0933692767, -1.9460156062\H, -4.18288802, -0.4874812346, -1.9224558376\H, -5.005611721, -1.9147706653, -1.229471857\H, -3.4481953435, 2.4429773553, 1.7071741433\H, -4.3592346202, 0.9035317503, 1.542974153\H, -4.974845757, 2.3973418042, 0.7785888427\H, -1.0933294242, 4.6428794648, -0.8103832658\H, -1.8286560396, 3.2858709755, -1.7113915898\H, -0.0400144118, 3.40957998, -1.553149121\H, 1.6142111001, 4.3544490697, 1.6558170365\H, 2.1046634669, 2.8147120193, 2.4201542638\H, 0.3791905723, 3.1293284101, 2.0433227176\H, -1.5770400493, -4.4330965676, 0.7462967985\H, -2.2885154438, -3.0202118686, 1.5768956465\H, -0.5128145176, -3.3131876267, 1.6397891539\Version=HP-PARisc-HPUX-G98RevA.11.3\HF=-1226.8122369\RMSD=5.168e-09\RMSF=2.145e-06\Dipole=0.0283012, 0.1693066, -0.4351852\DipoleDeriv=0.9949461, -0.4906521, -0.1593361, -0.4982044, 0.3046249, 0.108688, 0.1340276, -0.0422221, -0.0213314, 1.0653111, 0.4193222, 0.267225, 0.4188267, 0.2776551, 0.1426494, -0.0116756, 0.015066, 0.005402, -0.0080501, 0.0544985, -0.0387796, 0.2951274, 1.0999808, -0.162813, 0.0181656, 0.1216107, -0.0362183, 0.1909094, -0.0360321, -0.0356588, -0.04241, -0.2679693, 0.0133315, -0.037136, -0.0117871, -0.0092733, 0.0741384, -0.0529111, 0.032175, 0.0017339, -0.2961664, -0.0280054, 0.0625568, -0.0164888, -0.0095723, 0.018543, 0.057089, 0.0466902, -0.1937094, 1.1102492, -0.1679909, -0.0093319, 0.0859412, -0.0263942, -0.073056, 0.0811439, 0.015286, -0.1898179, 1.1226204, 0.161752, 0.0197224, -0.046205, -0.0272449, 1.0858297, -0.4888818, -0.145031, -0.4631994, 0.3441346, 0.1281009, 0.0550703, 0.0226899, 0.0096886, 0.1068685, 0.2017032, 0.0463139, 0.1215287, -0.0936542, -0.0533145, -0.0336366, -0.0331582, -0.0727373, 0.1065408, 0.0484482, 0.0473745, 0.1629161, 1.0867378, 0.3396814, 0.0289521, 0.0827803, 0.024883, -0.4209159, 0.0121915, 0.0003208, -0.1139671, -1.3211574, -0.4808288, -0.0856767, -0.3861993, -0.6746574, 0.0734095, -0.0155957, -0.0203389, -0.057006, 0.0412694, -0.0292791, 0.0520615, -0.0121497, 0.1039612, -1.5390738, 0.3480619, 0.3212946, 0.5055042, -0.5320877, -0.1405563, 0.3029212, -0.0980879, -0.5241061, 0.764559, -0.1063219, -0.225013, 0.0230137, 0.3117826, 0.0215882, -0.5446768, 0.1806779, 0.6089241, -0.3927453, 0.0235261, 0.028013, 0.1446266, -1.4270019, -0.3954202, 0.1169607, -0.3136785, -0.5557318, 0.3385415, -0.0016948, -0.0189371, -0.0724712, 0.6162789, 0.2330142, -0.1479964, 0.5123019, 0.6408074, -0.4408756, -0.1664805, 0.0642581, -0.2495885, -1.4483218, 0.337595, 0.1233945, 0.2634614, -0.5431976, -1.4161549, -0.3300621, -0.3729291, -0.5241655, -0.5363468, -0.1867756, -0.4113555, -0.1677761, -0.6216269, 0.5922161, 0.1124733, 0.2231776, 0.1349469, 0.3446546, 0.1037745, 0.5973473, 0.2182685, 0.6967255, -1.4388355, 0.4122318, 0.298606, 0.60038, -0.5992004, -0.1568368, 0.2929998, -0.141451, -0.5443774, 0.6808002, -0.1610178, -0.2297088, -0.1543509, 0.3623547, 0.1047221, -0.5797131, 0.2454209, 0.6162351, -0.3961219, 0.0435265, -0.0118644, 0.1289087, -1.461229, 0.3371486, -0.0904734, 0.3052302, -0.5666854, 0.2909714, 0.0051032, -0.013059, -0.0579468, 0.6564765, -0.2546353, 0.0853471, -0.5518927, 0.6208132, 0.2844233, -0.0791796, -0.0266004, 0.0270798, 0.5308706, 0.2213779, 0.0956723, 0.4899868, 0.7294589, 0.3160253, 0.0962457, -0.0519477, 0.1147008, 0.6575978

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### 37<sup>+</sup>

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3,0.0035285,-0.0060423,0.0488816,-0.078974,-0.0193664,-0.0051205,-0.05  
72064,0.0216782,-0.0365153,0.0339214,-0.0529824,-0.0470237,0.0435241,-  
0.0252585,-0.0433148,0.0372653,0.0413614,-0.0214025,0.0012556,0.093261  
9,0.0523728,-0.0062756,-0.0036332,-0.0009343,0.1061343,-0.0379221,0.07  
99343,-0.0153666,-0.0026004,-0.025757,-0.076351,-0.0162167,0.000692,0.  
0150928,0.0381249,-0.0405,0.0223584,-0.086478,0.0588829,0.0083106,0.03  
66484,-0.0239883,-0.0708837,-0.0168763,-0.0024962,0.0195649,0.0911003,  
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0576541,0.0235264,-0.0753601,-0.0248626,0.0785809,0.0676471,0.0244568,  
-0.020362,0.0641774,0.0492389,0.0073561,-0.016443,0.0256326,-0.0954385  
, -0.0519589,-0.0052076,-0.0133076,-0.017428,0.0926329,-0.0235185\Polar  
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