

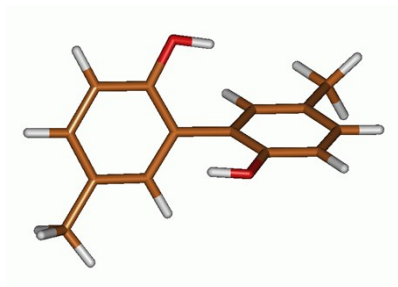
Electronic Supplementary Information

**Chain-breaking antioxidant activity of hydroxylated and methoxylated
magnolol derivatives: the role of H-bonds †**

Andrea Baschieri,^a Luana Pulvirenti,^b Vera Muccilli,^b Riccardo Amorati^{a*} and Corrado Tringali^b

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Results from calculations at the M06-2x/6-31+g(d,p) level: cartesian coordinates, enthalpy and free energy	
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Compound 1, conformer a

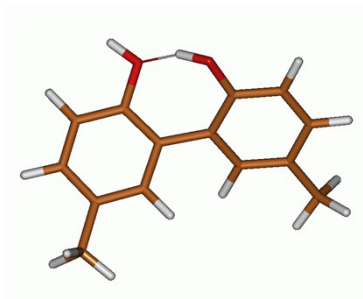


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1.0357361154,-1.9892125845,2.9546601484\H,3.3491185979,-0.1073025697,1.8974824604\
H,3.3251429632,-0.0320842393,-0.5858266119\H,-0.9619297564,0.0410424933,-0.5227735024\H,-
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Sum of electronic and thermal Enthalpies= -691.866825

Sum of electronic and thermal Free Energies= -691.925827

Compound 1, conformer b



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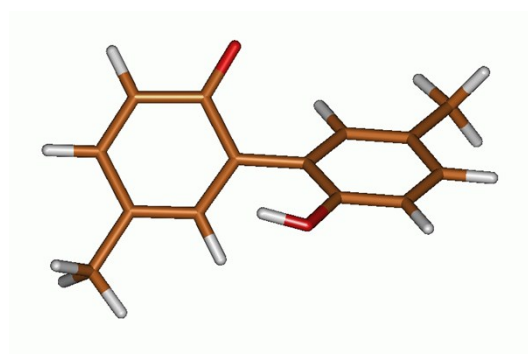
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 7613,-0.0837173318,3.2565865937\C,-2.9183253179,0.8115462219,3.7203238
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 07,-2.715516705\H,0.165276071,-0.3201950134,-2.6517422443\H,1.23236044
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Sum of electronic and thermal Enthalpies= -691.864189
 Sum of electronic and thermal Free Energies= -691.922834

Phenoxyl radical formed starting from 1a



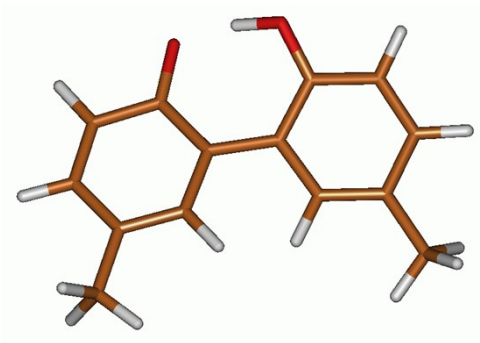
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Sum of electronic and thermal Enthalpies= -691.230469

Sum of electronic and thermal Free Energies= -691.289259

Phenoxyl radical formed starting from 1b



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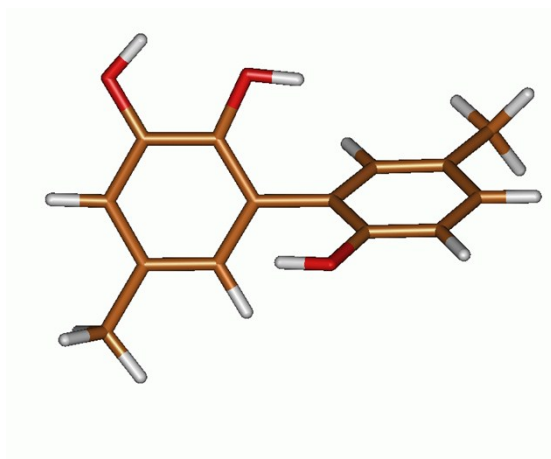
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 3712977\H,-0.937919738,0.2116557515,1.6914622452\C,1.0432985584,0.4046
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 54001,-2.0810439758\C,-2.7997134678,-0.8048474085,-2.6437648012\C,-3.7
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 ,2.6244889038,-1.4117729239\H,-5.3430604717,1.4243119061,-0.298796043\

Sum of electronic and thermal Enthalpies= -691.238331

Sum of electronic and thermal Free Energies= -691.295604

Compound 2, conformer a



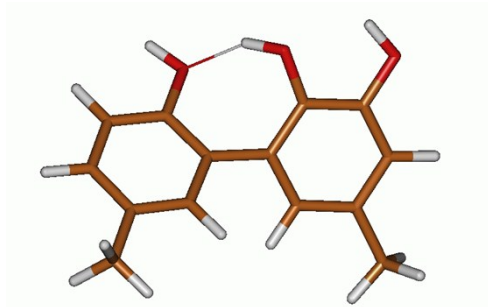
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Sum of electronic and thermal Enthalpies= -767.065280

Sum of electronic and thermal Free Energies= -767.126200

Compound 2, conformer b

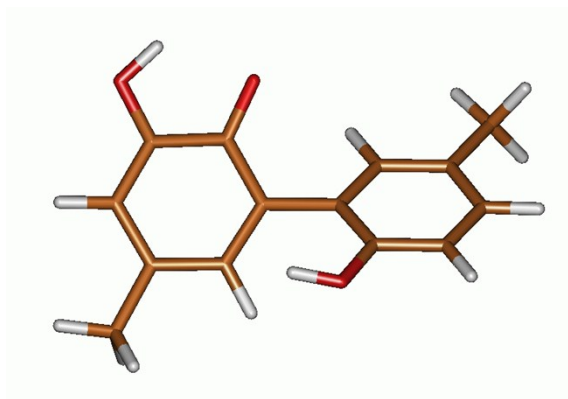


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,2.0032529591\C,-3.4291070596,-0.7814396279,2.8602709717\C,-3.47838644
32,0.1128004767,3.9178815316\C,-2.4183782806,0.9995583561,4.1383237087
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Sum of electronic and thermal Free Energies= -767.124308

Phenoxyl radical formed starting from 2a

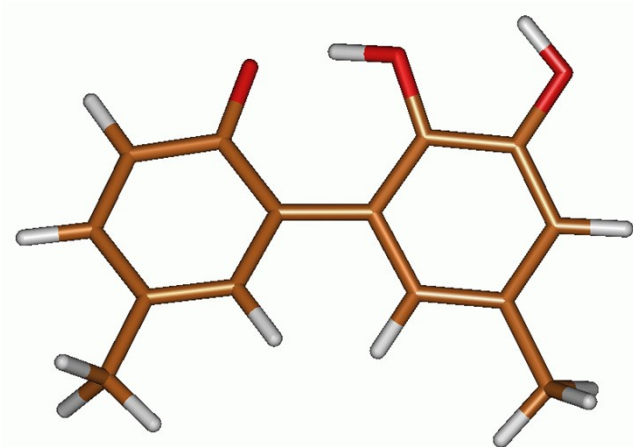


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Sum of electronic and thermal Free Energies= -766.502393

Phenoxyl radical formed starting from 2b



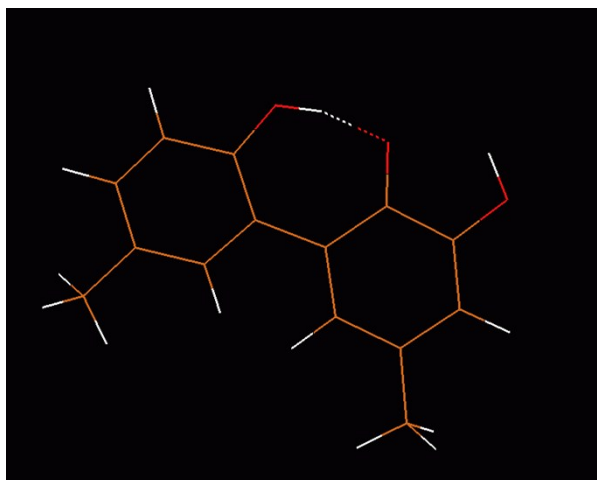
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386305\C,-1.3132681474,-0.0350370024,2.0872965238\C,-2.4087770587,-0.6
644796321,1.4397817216\C,-3.6863454458,-0.6679489381,1.9680643668\C,-3
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582560438\C,-1.5547238442,0.5685994328,3.3347342069\C,-4.824491994,-1.
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Sum of electronic and thermal Enthalpies= -766.439331

Sum of electronic and thermal Free Energies= -766.498687

Most stable phenoxyl radical formed starting from 2



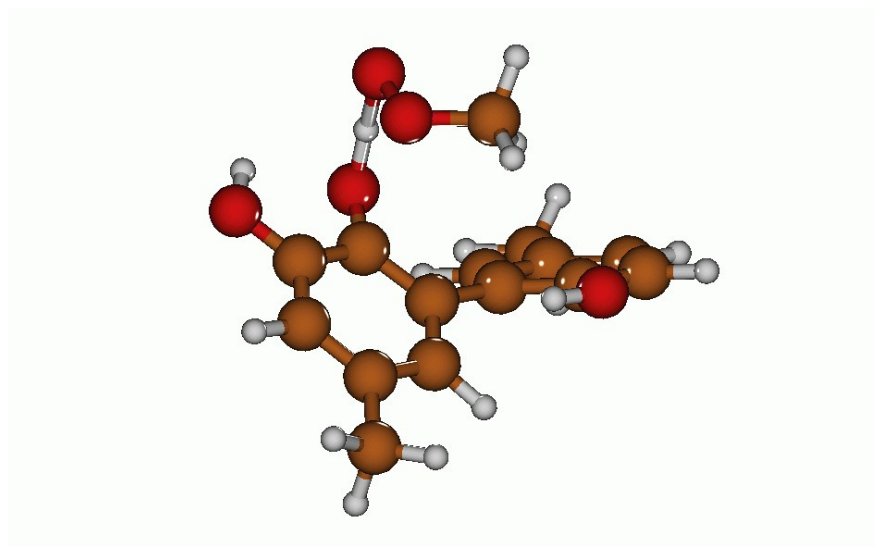
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 676104,-1.7930004986\H,-3.9370937421,3.1033396179,-0.6108573659\H,-3.0
 882694985,-2.342818013,1.033783514

Sum of electronic and thermal Enthalpies= -766.447584

Sum of electronic and thermal Free Energies= -766.507570

Transition state for the reaction of **2a** with CH₃OO*



C,-0.1375274754,0.1359127944,0.1166866335\C,-0.11413059
 52,0.0297788966,1.5057541868\C,1.1482702843,-0.055724145,2.1539772279\
 C,2.3363021441,0.0161538553,1.3715703172\C,2.2782005336,0.1462304541,-
 0.0131417129\C,1.0429986722,0.1921992977,-0.6512107549\C,-1.3650128258
 ,0.0084163068,2.3003290221\C,-2.3676990643,0.9695733275,2.0872898276\C
 ,-3.5440019382,0.932792025,2.8383681175\C,-3.7277156343,-0.0543386491,
 3.7945920188\C,-2.744393275,-1.0229437911,4.0389442351\C,-1.5745021034
 ,-0.9650626044,3.2905512358\O,-2.2489229292,1.9918078089,1.1908990003\
 C,-2.9578526853,-2.0901567455,5.0830415296\O,1.2800867015,-0.235508973
 1,3.4594798644\O,3.524881228,-0.0353468502,1.9825963208\C,0.9567013835
 ,0.2577051406,-2.1528464562\O,1.9750767184,1.9223134555,4.1360033359\O
 ,1.7121435381,2.4838683801,2.9320541165\C,0.4331624187,3.1169606123,2.

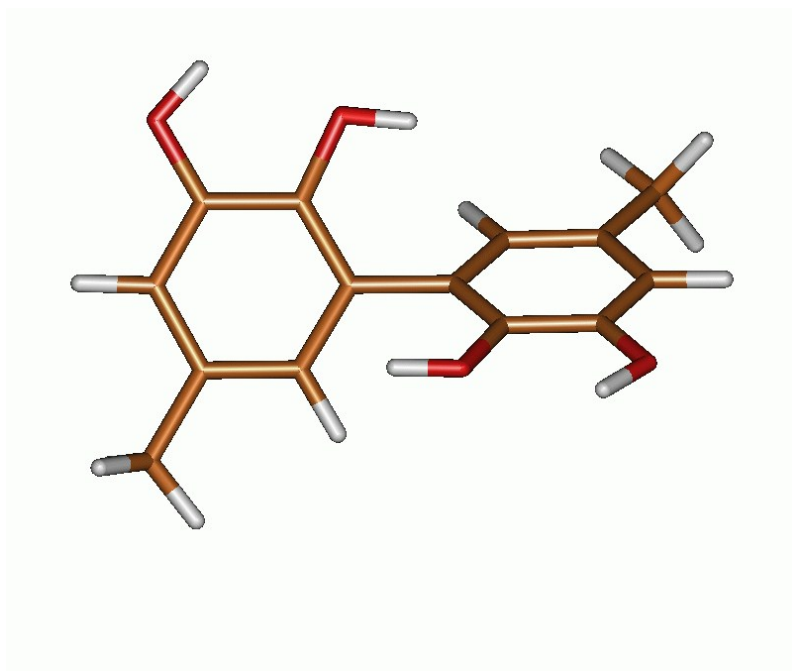
9815878111\H,3.2070673729,0.1983171485,-0.5719458144\H,-1.0968442601,0
 .1254294804,-0.3975908905\H,-4.2957842494,1.6931615568,2.6549883076\H,
 -4.6509492416,-0.0727596905,4.3687554409\H,-0.788388238,-1.6935152451,
 3.4650112321\H,1.5689551282,0.7262826535,3.9441042218\H,-1.390553596,1
 .9419144518,0.7489563138\H,0.7578925737,-0.7374278374,-2.5652984359\H,
 0.1443435816,0.9146178576,-2.4748471479\H,1.890162983,0.6203551139,-2.
 5881008782\H,-3.1831184699,-1.6474583244,6.0581234624\H,-3.7955301515,
 -2.7420942241,4.8153936952\H,-2.0680267812,-2.7138287975,5.1943768492\
 H,3.3787152307,-0.1210663599,2.9387418447\H,0.2553080433,3.5010755302,
 1.9759127742\H,-0.3316484848,2.3872780671,3.267452885\H,0.4657371684,3
 .9323233666,3.7079486775

Sum of electronic and thermal Enthalpies= -957.149850

Sum of electronic and thermal Free Energies= -957.222445

Frequencies -- -1852.0223

Compound 3, conformer a (most stable)



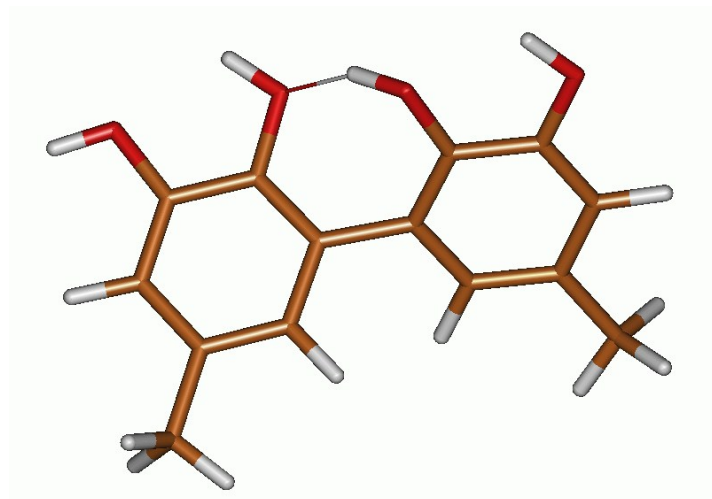
C,-0.0095930545,0.0803141517,0.04455374
O2\C,0.0080057526,0.026936279,1.4364870862\C,1.2484371017,-0.038456427
1,2.0956355776\C,2.448492646,-0.041417842,1.3876437245\C,2.4047994055,
0.0167714667,-0.0107383185\C,1.1915925982,0.0785584815,-0.679486732\C,
-1.2761133819,0.0015343011,2.1859699914\C,-1.5914325175,-1.1046537748,
2.9718193633\C,-2.8097329581,-1.1570210997,3.6647019872\C,-3.710637996
9,-0.1076195671,3.5645053809\C,-3.418253192,1.0133735218,2.7779603676\
C,-2.2044743074,1.0538102135,2.0949521544\O,-0.7882416961,-2.201017392
8,3.1216455822\C,-4.3988895952,2.1565245288,2.6976848411\O,-3.11156267
34,-2.2399428741,4.4230965691\C,3.7767794655,-0.0851685961,2.100824021
9\O,-1.1468635889,0.1201940124,-0.7134712591\H,-4.6461168345,-0.179229
339,4.1119648376\H,-1.9426087359,1.9286479289,1.5036736499\O,1.1656855
715,0.1250548338,-2.0345328539\H,3.3171870104,0.0153584116,-0.60023584
57\H,1.2592935439,-0.0508455067,3.1834101541\H,0.0169999922,-2.0953040
965,2.5943302231\H,-1.9270183384,0.0938148249,-0.1404846344\H,-4.51308
08157,2.642280163,3.6717803445\H,-4.0654743371,2.9116749547,1.98221133
88\H,-5.3875868956,1.8060351085,2.3867600486\H,4.3374021757,0.84085840
61,1.9394660838\H,3.641611959,-0.2133855651,3.1772116781\H,4.393399941
, -0.9113247768,1.734375429\H,-2.3801275636,-2.8710260879,4.3668406624\

H,0.2433024868,0.1522892621,-2.3259016908

Sum of electronic and thermal Enthalpies= -842.263977

Sum of electronic and thermal Free Energies= -842.327043

Compound 3, conformer b (less stable by 1.0 kcal/mol)



C,0.0075969316,0.0411751223,0.011740957

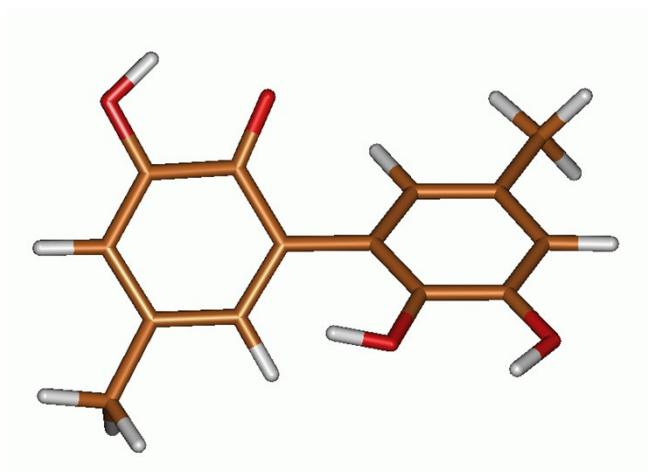
1\C,0.014651945,0.0030981884,1.4181550788\C,1.2461622079,-0.0572860379
,2.0718623172\C,2.4365845216,-0.1053402168,1.3275805669\C,2.4057395824
, -0.079210343, -0.0574444536\C,1.1819251437,0.0020695616, -0.7320132701\
C,-1.2814333986, -0.0270568508,2.1440483633\C,-1.546130405,0.7805915681
,3.247096442\C,-2.7957635608,0.7402463543,3.8750089987\C,-3.7956385825
, -0.0972705307,3.4133479511\C,-3.5577445207, -0.9238738193,2.306725062\
C,-2.3107566974, -0.8740665654,1.6948094368\O,-0.5885983361,1.637032759
6,3.7307435335\C,-4.6383351486, -1.8525543188,1.8124265663\O,-2.9237707
396,1.5918216049,4.9431897584\O,1.4119220758, -0.1443598268,3.430530136
1\O,3.623746151, -0.1848910637,1.9794279559\C,1.1535155374,0.0559756053
, -2.2392795522\H,3.3467214421, -0.1140928224, -0.5990405537\H, -0.9484090
149,0.119393182, -0.4989191099\H, -4.7610700983, -0.115320736,3.915732813
6\H, -2.1041836937, -1.5235740505,0.8491046655\H,0.8245116257,0.49821592
24,3.8638318736\H, -0.973101135,2.1555890856,4.4526890729\H,1.648708063
1, -0.8182776464, -2.6730004882\H,0.1270832306,0.0840001264, -2.612593485

1\H,1.6722655883,0.9456385828,-2.610023862\H,-5.5425561956,-1.29767336
 76,1.5436900815\H,-4.3058289863,-2.4036598281,0.9302220545\H,-4.913066
 9722,-2.581543904,2.5812116773\H,3.4323415951,-0.1855368121,2.92932780
 34\H,-3.8156688114,1.5553827571,5.3052870217

Sum of electronic and thermal Enthalpies= -842.262975

Sum of electronic and thermal Free Energies= -842.325411

Phenoxyl radical formed starting from 3a



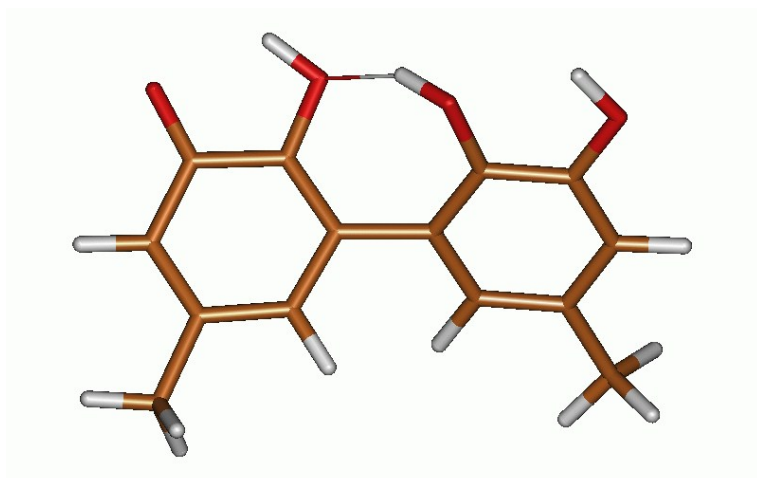
Sum of electronic and thermal Enthalpies= -841.639175

Sum of electronic and thermal Free Energies= -841.702458

C,-0.0055036207,0.002423321,0.006090
 9602\C,-0.0027026831,-0.0033566007,1.386304824\C,1.2820943719,-0.01239
 42863,2.0723265585\C,2.4868272495,-0.010794067,1.2408352661\C,2.430976
 5376,0.0011561827,-0.1440373812\C,1.1865594369,0.0023280878,-0.7710350
 498\C,-1.2532594173,-0.013873591,2.1740825148\C,-1.4197135581,-0.89963
 65518,3.252920539\C,-2.6093182166,-0.9548751777,3.9695191221\C,-3.6526
 930555,-0.0886795745,3.6181735576\C,-3.5000205976,0.8129651152,2.57739

374\C,-2.301685802,0.8508659244,1.8526111999\O,-2.2650186742,1.7959403
 191,0.8563356262\O,-4.5104640862,1.6656123774,2.2641052229\C,-2.786864
 1619,-1.9222341842,5.1130292636\O,1.4418683141,-0.0131228924,3.3119690
 721\O,3.6429024977,-0.0156050224,1.8941319548\C,1.0778323648,-0.023801
 4687,-2.269269729\H,-4.5939522956,-0.0942287087,4.1605899099\H,-0.5948
 310921,-1.5513793654,3.5203968299\H,3.3530509937,0.0011788588,-0.71614
 13327\H,-0.9580286974,-0.0393797314,-0.519093672\H,-1.3538000051,1.942
 006147,0.5705049087\H,-3.5964898353,-2.6294851744,4.9074539336\H,-1.87
 29702483,-2.4942165654,5.2875875331\H,-3.0370428221,-1.3935826639,6.03
 78776055\H,0.6091684445,-0.956346989,-2.601670759\H,0.4515548785,0.798
 4940765,-2.6294775862\H,2.0579984324,0.054309527,-2.742660535\H,-4.212
 2646684,2.245782397,1.5498727545\H,3.4155194116,-0.0196260755,2.845877
 4113

Phenoxy radical formed starting from 3b



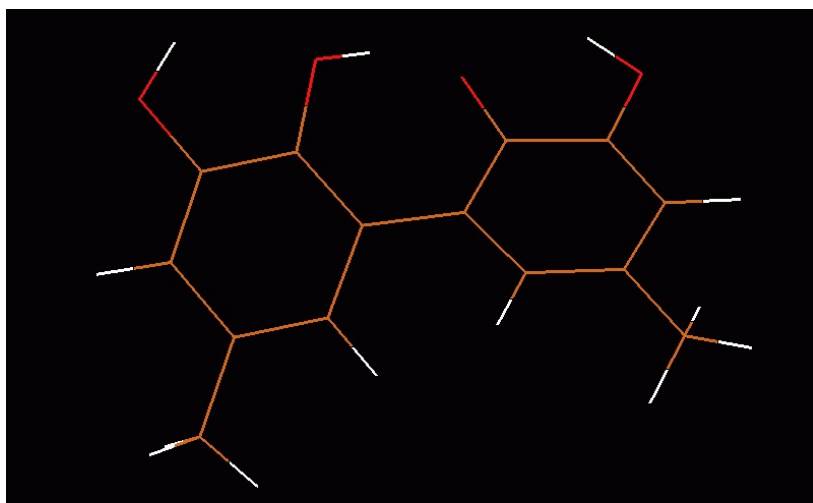
C,-0.007276212,0.0090853215,0.033904
 4471\C,0.0234347849,-0.0032234703,1.4272180001\C,1.2920669353,-0.01107
 80955,2.0136056925\C,2.5134985894,-0.0005502236,1.2733063635\C,2.47126
 70206,0.0152008839,-0.0953535442\C,1.2064243069,0.0193261464,-0.782199
 4878\C,-1.1964377353,0.030457439,2.2732037842\C,-2.2865727332,-0.80950
 07118,2.0445073531\C,-3.3850376001,-0.7876333543,2.9195345668\C,-3.404
 9013537,0.0747135512,4.0048082285\C,-2.3305224319,0.9404636877,4.23794
 87424\C,-1.242970126,0.9075459055,3.3712153667\O,-2.3602466666,-1.7472

008459,1.0450135834\C,-2.3702062955,1.8951375083,5.4049074455\C,3.8151
 383884,-0.0163084615,2.0306956548\O,1.0569882159,0.0386807561,-2.02377
 9272\O,-1.1544981155,0.0215381666,-0.6587427733\O,-4.4278400033,-1.624
 3098201,2.7002818243\H,-4.2730895319,0.066695611,4.657482322\H,-0.4108
 224131,1.5886512227,3.5291985461\H,3.3705413929,0.0222522307,-0.703020
 6579\H,1.3483472471,-0.04286149,3.099044559\H,-2.092744457,-1.34812310
 83,0.2018524301\H,-0.8883861876,0.050838554,-1.6031997282\H,-2.4971223
 666,1.3557413919,6.3484208401\H,-1.4484869298,2.4780979445,5.468703614
 8\H,-3.2065937205,2.5945062508,5.3101973559\H,4.6671199797,-0.00897346
 35,1.3485379675\H,3.8934151078,0.8557100975,2.6873907023\H,3.886194822
 4,-0.9092642529,2.6594434962\H,-4.2276572224,-2.1406078687,1.905130390
 5

Sum of electronic and thermal Enthalpies= -841.641024

Sum of electronic and thermal Free Energies= -841.702653

Most stable phenoxyl radical formed starting from 3



C,1.5288432258,-0.9643166246,-0.4086

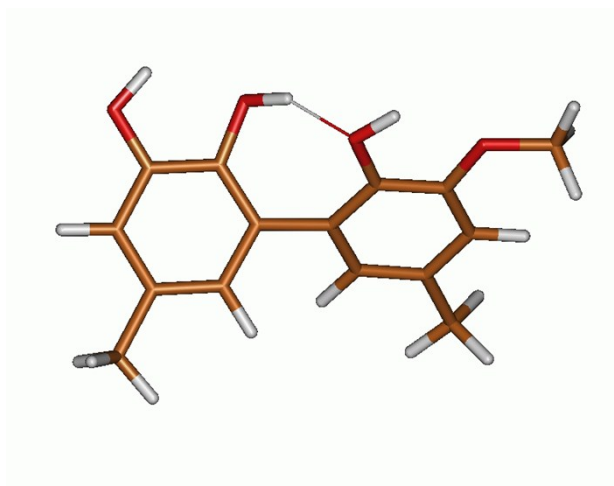
871024\C,0.7309172251,0.1683190581,0.025780822\C,1.4082273458,1.297447
 6493,0.4358663377\C,2.8261302966,1.4082885537,0.4245189134\C,3.6112229
 691,0.3473918879,-0.0210930107\C,2.9833639895,-0.8164769757,-0.4314069

06\C,-0.7493531921,0.1574235792,-0.0188828593\C,-1.5251117783,-0.94522
 59358,0.3543146365\C,-2.9278994894,-0.8390624333,0.3749421155\C,-3.557
 4472375,0.3367732554,0.0035344843\C,-2.8008340167,1.4412756329,-0.4086
 73513\C,-1.4165966446,1.3367002081,-0.4137295807\O,-1.0411607847,-2.14
 73868678,0.7782109295\C,-3.4921283052,2.7069215694,-0.8502589806\O,-3.
 6622929623,-1.9082045497,0.7664143827\C,3.4558223517,2.6837341233,0.90
 53721847\O,3.6720715687,-1.8691448725,-0.8552142587\O,1.0757777013,-2.
 080260689,-0.7797222198\H,-0.8225867327,2.1778762836,-0.7596212942\H,-
 4.6429366368,0.3731575185,0.0231476191\H,4.693921405,0.4095077174,-0.0
 442884993\H,0.8353457067,2.1458694401,0.8001423379\H,-0.2710122295,-2.
 3834344759,0.2174826612\H,-4.1277097238,2.5232795509,-1.7221051654\H,-
 4.1309268195,3.1029154702,-0.0548168891\H,-2.7669201226,3.4789719121,-
 1.118134132\H,3.0962611978,3.5354222321,0.3187851069\H,3.1852477699,2.
 8728556039,1.9494620522\H,4.54387134,2.6470623009,0.8316848726\H,3.017
 0244446,-2.5587340291,-1.0802953741\H,-3.0443081534,-2.6301743835,0.95
 81303336

Sum of electronic and thermal Enthalpies= -841.648432

Sum of electronic and thermal Free Energies= -841.710225

Compound 4, conformer a (most stable)

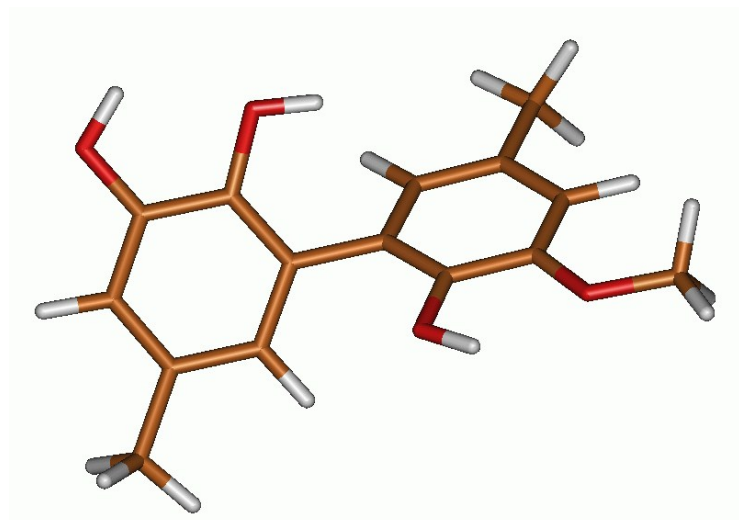


C,0.0615840947,-0.0020523335,0.07810754
43\C,0.0543340119,0.001145842,1.4677756352\C,1.3003292671,-0.003443193
7,2.1247118477\C,2.5043577563,-0.0082503606,1.4356621126\C,2.484140870
2,-0.0066420759,0.0311116594\C,1.2707579687,-0.0074270349,-0.636659903
6\C,-1.1968186235,0.0453327897,2.2683721626\C,-2.2829295494,-0.7944294
581,2.0185248828\C,-3.4074355544,-0.7612898028,2.859917702\C,-3.459650
7065,0.1100622074,3.935850971\C,-2.3894655416,0.9752459833,4.192017035
\C,-1.2770085682,0.930998081,3.3588741484\O,-2.3353739386,-1.737583730
1,1.0242904314\C,-2.4597899433,1.9394286576,5.3500699588\O,-4.44549709
85,-1.5994986054,2.613072768\C,3.8250200385,-0.0265238704,2.1640567746
\O,-1.1162844378,0.0097999666,-0.6259096076\H,-4.3469842468,0.10989724
86,4.5624520785\H,-0.4457479611,1.6075237627,3.5381587461\O,1.10325447
91,0.0002684328,-1.9945097601\H,3.4194703715,-0.0109789799,-0.51899708
32\H,1.3045450501,-0.024818076,3.2106788432\H,-2.0006457393,-1.3462945
828,0.1993778388\H,-0.9034439184,0.0592888747,-1.5698638012\H,-2.61056
77717,1.4081362145,6.2949137986\H,-1.5396649997,2.5227615676,5.4325997
46\H,-3.2933230865,2.6384555306,5.2290932549\H,4.4337787914,0.84352320
19,1.8984828791\H,3.6749411228,-0.0156116711,3.2457445055\H,4.40125789
67,-0.9225884448,1.9128516662\H,-4.2188524578,-2.1153596338,1.82477564
32\C,2.2680094908,0.0222202516,-2.7983013176\H,1.9238692613,0.03418333
42,-3.8314437498\H,2.8619308542,0.9202741095,-2.5961871252\H,2.8772477
759,-0.8711321709,-2.622956501

Sum of electronic and thermal Enthalpies= -881.514850

Sum of electronic and thermal Free Energies= -881.580450

Compound 4, conformer b (less stable by 2.5 kcal/mol)



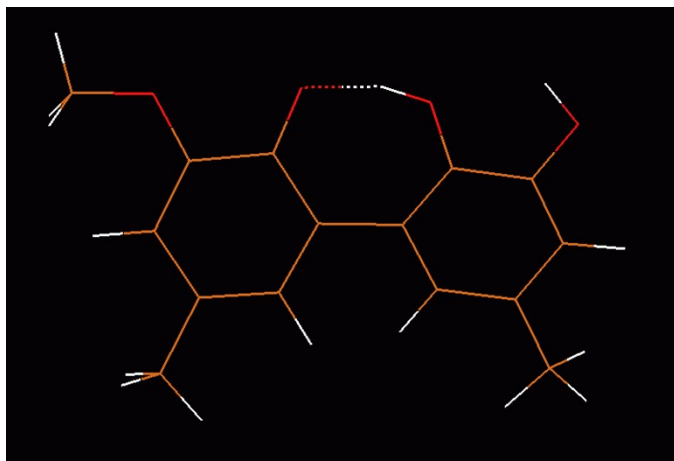
C,0.0582812578,0.0843285733,0.080518462
6\C,0.0440841525,0.0005263441,1.4703353876\C,1.2752859391,-0.083290657
7,2.150609905\C,2.4919302812,-0.0903079784,1.4803798922\C,2.4876698023
, -0.0106518394,0.0784975708\C,1.2867218161,0.0795165941,-0.608161873\C
, -1.2372088331,-0.0068920567,2.2234554255\C, -1.5091877077,-1.044756402
7,3.1121188833\C, -2.6999964494,-1.0533496796,3.851174776\C, -3.61600399
, -0.0251816814,3.7005358034\C, -3.3686982931,1.0224874481,2.8036980682\
C, -2.1855342504,1.0160279756,2.0728051601\O, -0.6857778763,-2.120958305
1,3.3303409948\C, -4.3799425765,2.1304217955,2.6432774705\O, -2.95702574
42,-2.0753542184,4.7107914384\C,3.8012835378,-0.1599619156,2.225863573
8\O, -1.1018112532,0.1618263497,-0.6184177222\H, -4.5298498759,-0.058505
2102,4.2870682057\H, -1.9778479727,1.8136169615,1.3657450986\O,1.151136
6323,0.1598857884,-1.9659080224\H,3.4307368332,-0.0146169099,-0.458565
2259\H,1.2611253569,-0.1107262305,3.2381145955\H,0.0558746052,-2.09909
94607,2.7104356511\H, -0.8855239903,0.1852063357,-1.5612535787\H, -4.544
9692267,2.6536397265,3.5904292407\H, -4.0443222027,2.8633697812,1.90599
84721\H, -5.3456740949,1.7357423467,2.3122040234\H,4.3897167948,0.75050

48838,2.0737106385\H,3.6347081616,-0.2757204673,3.2991140202\H,4.40699
68887,-1.0052413288,1.8844414247\H,-2.2256659776,-2.7064387845,4.66128
16687\C,2.3308016604,0.1513507267,-2.7465775766\H,2.0083503892,0.21963
23598,-3.7845335586\H,2.9660632118,1.0095457898,-2.5008939399\H,2.8911
969526,-0.7779004839,-2.5950288803

Sum of electronic and thermal Enthalpies= -881.509556

Sum of electronic and thermal Free Energies= -881.576518

Phenoxyl radical formed starting from 4a (having the Ar-Ar dihedral angle most similar to that of 4a)



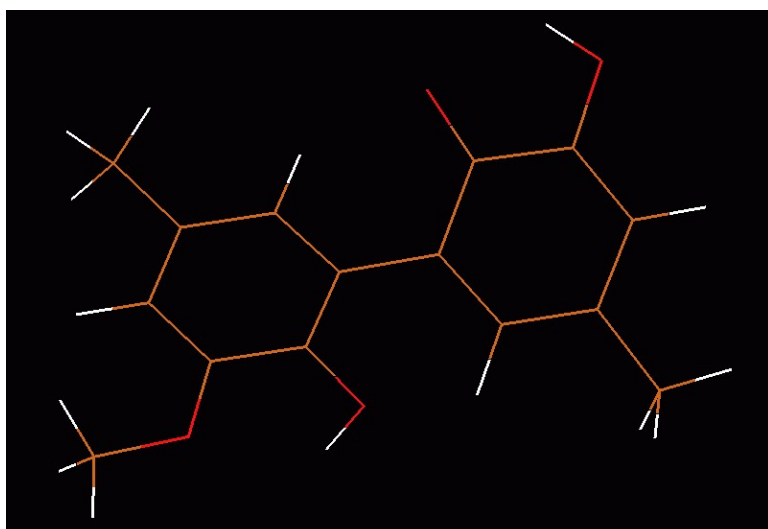
C,1.7586314023,-1.0152276804,-0.3789
392148\C,1.0750641444,0.1453776678,0.0034255596\C,1.8390375696,1.24551
00563,0.4539153898\C,3.2253732224,1.2203672154,0.4947945263\C,3.890081
5843,0.0618988198,0.0696930816\C,3.1664357336,-1.037754599,-0.35611603
02\C,-0.394115469,0.3068548165,-0.089066751\C,-0.9234474721,1.52289753
04,-0.4796981411\C,-2.3096336096,1.7834473712,-0.5063793458\C,-3.22028
10472,0.7931062031,-0.1130583304\C,-2.7537612037,-0.4510790877,0.27579
42794\C,-1.3171137044,-0.7628168369,0.2794690422\O,-0.9507087966,-1.91
49705862,0.5986028004\C,-2.800786847,3.120109309,-0.984707536\C,4.0161
650528,2.401167077,1.0000197695\O,3.8087861981,-2.1609554728,-0.759126
0215\O,1.1833637648,-2.1557777051,-0.844312226\H,1.3160162604,2.128942
8007,0.8087270439\H,4.9743835179,-0.0027543013,0.0834531764\O,-3.51858

55205,-1.4718192875,0.6590148538\H,-4.2816800043,1.0126812662,-0.12792
 29338\H,-0.2467525487,2.3116923683,-0.7957292484\H,0.3567403659,-2.304
 7690066,-0.3250055163\H,4.5898018272,2.1363158496,1.8938080054\H,4.726
 8792431,2.7501937632,0.2445081998\H,3.3582084304,3.2349139955,1.256728
 3589\H,-2.2176968267,3.9326847346,-0.5423033862\H,-2.6912805374,3.1962
 930539,-2.0724742456\H,-3.8537242212,3.2728875935,-0.7397226653\H,3.13
 0174839,-2.8163523019,-0.9833464034\C,-4.9241313362,-1.2883878346,0.67
 57766701\H,-5.3420821579,-2.2341505077,1.0151805307\H,-5.2027653822,-0
 .4886578238,1.3703832581\H,-5.29668735,-1.0561576833,-0.3276920155

Sum of electronic and thermal Enthalpies= -880.887928

Sum of electronic and thermal Free Energies= -880.954562

Phenoxy radical formed from 4b



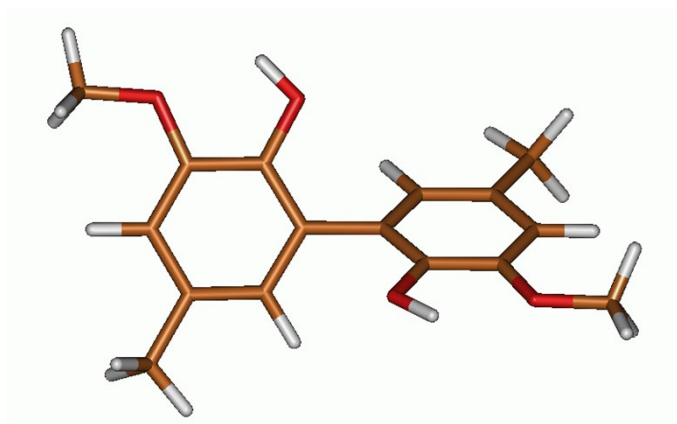
C,0.00077279,-0.0313320893,-0.007626
 7075\C,-0.0035651727,-0.0131343783,1.397440533\C,1.2105424444,0.012158
 1439,2.076054445\C,2.4129403346,0.0447267438,1.3463775456\C,2.40108234
 55,0.0403374564,-0.0399184824\C,1.1818874621,-0.0031257482,-0.73613513
 7\C,-1.2748906231,-0.0324464943,2.1507264505\C,-2.226091311,-1.0017718
 678,1.9444475838\C,-3.460654395,-1.0309543306,2.6541660176\C,-3.745766
 5028,-0.0495967377,3.6012673964\C,-2.8193085916,0.9564024998,3.8305152

76\C,-1.5501735772,1.0274764511,3.1064210092\O,-0.8092024933,2.0065563
 707,3.3334385459\O,-3.0423185592,1.9307145246,4.7075650329\C,-4.433430
 2112,-2.141813104,2.3766352319\O,1.2396760153,-0.0460785179,3.42845139
 06\O,3.5308020415,0.0671325331,2.13425724\C,4.7861963451,0.1310009775,
 1.4879665944\C,1.1776901283,-0.0001172798,-2.2445719288\H,-4.677768769
 2,-0.0546663247,4.1573128021\H,-2.0216215223,-1.7947163501,1.228159764
 7\H,3.3314277384,0.0667478831,-0.5984242719\H,-0.9542252597,-0.0394810
 182,-0.5267166838\H,2.1574781331,0.0469067018,3.7187937534\H,-5.345465
 622,-2.0316847759,2.9661133256\H,-4.7068745154,-2.1610441085,1.3164950
 893\H,-3.9857742376,-3.1130550166,2.6130620007\H,1.7548191257,-0.84008
 22336,-2.6442518405\H,0.1592747788,-0.0769250257,-2.6323499399\H,1.618
 2111781,0.9210827235,-2.6393577903\H,-2.2552514505,2.5106837145,4.6632
 617548\H,5.5346535303,0.1554338872,2.27889908\H,4.9458337874,-0.751276
 8779,0.8576949584\H,4.8648333669,1.0380201953,0.8780323373

Sum of electronic and thermal Enthalpies= -880.888099

Sum of electronic and thermal Free Energies= -880.954583

Compound 5, conformer a (most stable)



C,-0.0134604521,0.0517551931,-0.0062671

783\C,-0.0067946444,0.0128189378,1.3996997045\C,1.2222452192,-0.022802

6663,2.0538903485\C,2.4151883151,-0.0200586585,1.3073779171\C,2.388319

8211,0.0150770358,-0.0768460905\C,1.1564532638,0.0510628157,-0.7508296

504\C,-1.2779789905,-0.0126968019,2.1673760959\C,-2.3120379604,0.86967

29621,1.8641949063\C,-3.5170187534,0.8146537146,2.5890367897\C,-3.6950

157827,-0.1101554008,3.6044567559\C,-2.661323008,-1.0067550116,3.92168

29061\C,-1.4763896316,-0.9422221494,3.2041592047\O,-2.172999623,1.8000

647583,0.8802959602\C,-2.8560364678,-2.0134045118,5.0283203238\O,-4.43

9946457,1.7460039273,2.1884006577\C,-5.6716984008,1.7831326007,2.87931

30213\O,1.2917115451,-0.0477174513,3.4131443277\O,3.5459452601,-0.0488

640508,2.0821533858\C,1.1282999751,0.0898649277,-2.2586773584\H,3.3109

336507,0.0162259931,-0.6485848693\H,-0.9725025399,0.0881241075,-0.5130

029407\H,-4.626431194,-0.1495264447,4.1603506989\H,-0.6656884427,-1.62

27942469,3.4438480314\H,2.2262066117,-0.0263991515,3.6624729549\H,-2.9

797097234,2.3336817413,0.8610089086\H,1.621059467,-0.7887622055,-2.687

6694121\H,0.1006199199,0.1134508426,-2.6280414118\H,1.6433527473,0.977

1665179,-2.6410720987\H,-3.7033538947,-2.6745256298,4.8190267891\H,-1.

9660349269,-2.6348902701,5.1498320713\H,-3.052479342,-1.5170691057,5.9

842861027\C,4.7927001602,-0.0208373947,1.4182497781\H,-6.252048009,2.5

854712742,2.4252324082\H,-6.2088718196,0.8339842654,2.7709472792\H,-5.

5161846976,1.9970403623,3.9428994057\H,5.5537020322,-0.0386535669,2.19

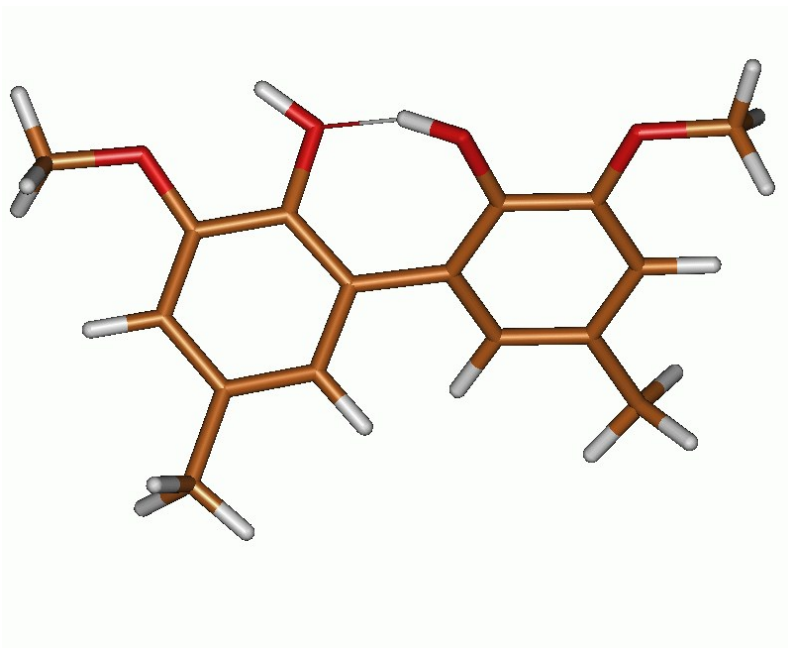
75449417\H,4.9096029029,-0.8968102871,0.7700320513\H,4.8968518638,0.89

29133861,0.8221214587

Sum of electronic and thermal Enthalpies= -920.756739

Sum of electronic and thermal Free Energies= -920.826784

Compound 5, conformer b (less stable by 1.5 kcal/mol)



C,-0.0256019447,0.0576894794,-0.0091314

161\C,0.0056486768,0.0230250495,1.3995716393\C,1.2403197133,-0.0131351

212,2.051099457\C,2.4281808717,-0.0505929105,1.2837472102\C,2.36869304

6,-0.0297291508,-0.1032521005\C,1.1327105623,0.0347609666,-0.766537784

5\C,-1.2891001508,-0.0460797706,2.1286460961\C,-1.5955579488,0.7702245

159,3.2105073918\C,-2.848615975,0.6917490229,3.8410706503\C,-3.8084935

078,-0.2006501618,3.3935230122\C,-3.5227150714,-1.0395884009,2.3036670

562\C,-2.2799293274,-0.9483443195,1.6941694079\O,-0.677706269,1.673511

1562,3.6786398844\C,-4.5595211755,-2.0264521039,1.8277919244\O,-2.9921

268327,1.5668297942,4.8831621463\C,-4.2293316755,1.5700802992,5.569495

8102\O,1.3885433458,-0.0830817757,3.3990076995\O,3.5771810146,-0.10993

59277,2.0038848675\C,1.0909827872,0.0843664068,-2.2734948772\H,3.28022

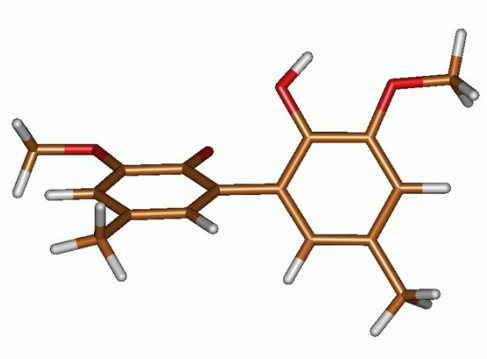
91097,-0.0525096827,-0.6911598463\H,-0.991565057,0.1155970511,-0.50384

09296\H,-4.776913491,-0.2632118501,3.8791070895\H,-2.0417598027,-1.605
 6489069,0.8627166096\H,0.7435248126,0.5072694285,3.8187529991\H,-1.081
 5901668,2.168003672,4.4070991949\H,1.5876091622,-0.7874096586,-2.71155
 22878\H,0.060565842,0.1032963357,-2.6363743898\H,1.5979109016,0.977446
 7688,-2.6532667235\H,-5.485563903,-1.5185041588,1.5403650588\H,-4.1984
 486876,-2.5852309955,0.96161314\H,-4.8076836236,-2.7470217702,2.613601
 3584\C,4.7903463604,-0.1666478755,1.2885952811\H,-4.1428668653,2.32637
 02794,6.3483519858\H,-5.0490503862,1.8307355366,4.890910045\H,-4.42342
 16884,0.5926404274,6.0246445221\H,5.5788965572,-0.216744187,2.03881075
 42\H,4.8354643005,-1.0582268474,0.6509152035\H,4.9312241488,0.72861531
 63,0.6702076373

Sum of electronic and thermal Enthalpies= -920.756221

Sum of electronic and thermal Free Energies= -920.824889

Phenoxyl radical formed from 5a



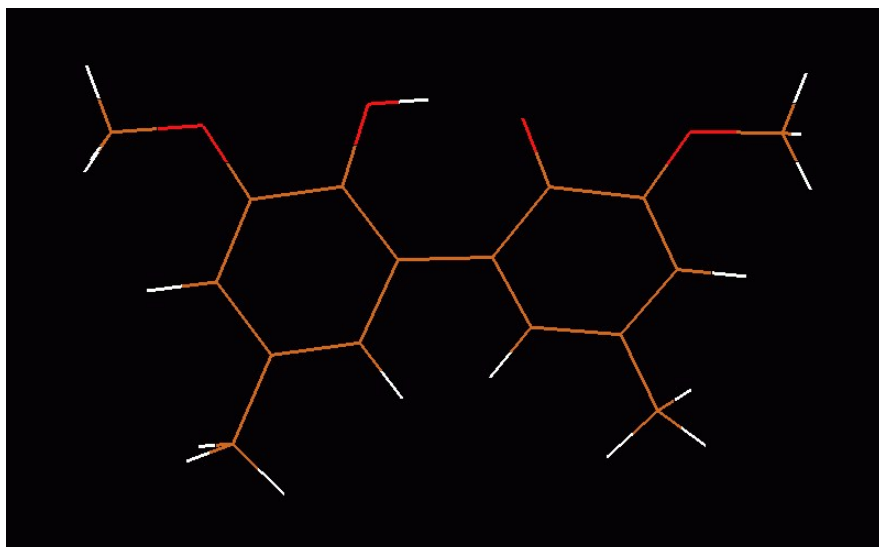
C,-0.0005622965,-0.0292011439,-0.005
 4623763\C,-0.0106353314,-0.0025948639,1.3691672143\C,1.2482926367,0.02
 97773718,2.113258754\C,2.4768183527,0.1060111059,1.3065782733\C,2.4324
 194066,0.0914633489,-0.0805226961\C,1.2028898006,0.0169403497,-0.74799
 09325\C,-1.2772172881,-0.0593467775,2.1288521772\C,-2.1913980508,-1.10
 6640605,1.9250233794\C,-3.3790189231,-1.1916354945,2.6387334187\C,-3.6
 683422078,-0.1944131388,3.5843930626\C,-2.783502866,0.85407839,3.78464
 51425\C,-1.5840178696,0.9331580944,3.054169483\O,-0.7614227645,1.99609

88881,3.2147703529\O,-2.9612215143,1.8903825244,4.6603069191\C,-4.1170
 906374,1.8693514716,5.4726516731\C,-4.3426139407,-2.3337499971,2.43216
 1206\O,1.3032039229,-0.0404425519,3.3487301537\O,3.5947417812,0.166367
 0046,2.0337760164\C,4.8345555714,0.2257702083,1.3541585348\C,1.1456684
 459,0.0126700077,-2.2497689283\H,-1.9360402786,-1.8820233361,1.2071979
 472\H,-4.5916424182,-0.2517638811,4.1522678778\H,3.3442657657,0.135822
 2303,-0.6659755805\H,-0.9468106116,-0.0612486904,-0.5414355486\H,-1.08
 91561612,2.5282282863,3.9526702802\H,-4.4442157329,-2.934939774,3.3415
 362964\H,-5.3393441195,-1.9687256472,2.1643567485\H,-3.9998154575,-2.9
 936087305,1.631750344\H,0.5705579206,-0.8443619986,-2.6146724006\H,0.6
 48641299,0.916493253,-2.6189051392\H,2.1439930697,-0.0303373478,-2.690
 0619531\H,-4.0610688617,2.7547036501,6.1047395316\H,-5.0254902775,1.91
 18023591,4.8608105805\H,-4.137427625,0.9700908172,6.0987120929\H,5.597
 382873,0.2681748439,2.1297214214\H,4.9841267506,-0.6668236037,0.736358
 8917\H,4.8938897178,1.1225541924,0.727311464

Sum of electronic and thermal Enthalpies= -920.125349

Sum of electronic and thermal Free Energies= -920.196367

Phenoxyl radical formed from 5b



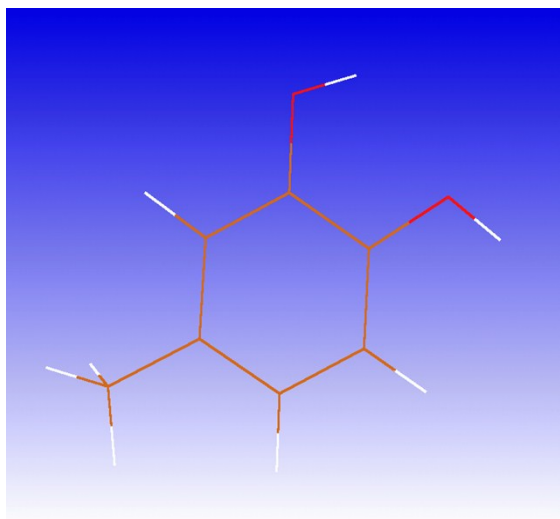
C,1.5620852478,-0.7888733361,-0.3264

618421\C,0.7224285109,0.3400183034,0.0602458085\C,1.3414583797,1.49046
 92951,0.5223101736\C,2.7392094245,1.6242991808,0.6103064482\C,3.576894
 5636,0.571601977,0.2029777664\C,3.0209330339,-0.6061905728,-0.25727726
 45\C,-0.7514182077,0.3205868254,-0.0864480566\C,-1.5568654824,-0.77089
 3298,0.2692373618\C,-2.9679175509,-0.627794592,0.2275767353\C,-3.54653
 58627,0.5546829187,-0.2057461317\C,-2.7476164802,1.6367445918,-0.61581
 0677\C,-1.3749305769,1.506154658,-0.5439729589\O,-1.0933292918,-1.9522
 287536,0.7179328076\C,-3.3972841639,2.8967730921,-1.1299589461\O,-3.66
 10389852,-1.7199941105,0.6336447167\C,-5.0682856174,-1.6425241514,0.61
 3733712\C,3.3436480672,2.8787365764,1.1743910449\O,3.707373944,-1.6750
 890286,-0.6613982501\O,1.1069548846,-1.8847673163,-0.7156707078\H,-0.7
 453793893,2.3272134725,-0.8752095381\H,-4.6262105862,0.6516515488,-0.2
 510540285\H,4.6521649949,0.6971671095,0.2655132013\H,0.7231950447,2.32
 14760922,0.8486440199\H,-0.2669147817,-2.1560609304,0.2292924972\H,-3.
 983416852,2.6985509645,-2.0332282072\H,-4.0757581933,3.3239496285,-0.3
 84482014\H,-2.6473434941,3.6524661121,-1.375801024\H,2.6519537309,3.72
 06289003,1.1028962722\H,3.5887869138,2.7373583242,2.2335475529\H,4.269
 465997,3.1407886207,0.6553045083\C,5.1221358745,-1.6161872186,-0.61885
 28729\H,-5.4264939342,-2.605717749,0.9754835255\H,-5.4328919662,-0.845
 5063804,1.2737230981\H,-5.4435596407,-1.4717619035,-0.4029947016\H,5.4
 704707502,-2.579446665,-0.9867890581\H,5.4973355598,-0.8144935541,-1.2
 643738774\H,5.4735945893,-1.4613444924,0.4071156673

Sum of electronic and thermal Enthalpies= -920.128063

Sum of electronic and thermal Free Energies= -920.197750

Compound 6



C,-0.0229579168,-0.0221159451,0.0016386034\C,-0.

0226911971,-0.003178608,1.3907954051\C,1.1941546658,0.0170644681,2.092

2610923\C,2.3949816156,0.0180292611,1.3893496404\C,2.4125211116,-0.000

9552523,-0.014794415\C,1.1914794157,-0.0209811262,-0.6973752654\O,1.20

82788058,0.035808466,3.4589401344\H,3.3205495065,0.0339076832,1.958022

9304\C,3.729089762,0.0004757332,-0.7586466264\H,1.178086786,-0.0359025

785,-1.7833269873\H,-0.9665607594,-0.037783104,-0.5398256182\O,-1.1575

917407,-0.0023855863,2.1799496495\H,0.2927381877,0.0321422782,3.776533

0508\H,-1.9517712504,-0.016807531,1.6316537295\H,3.5722553907,-0.01567

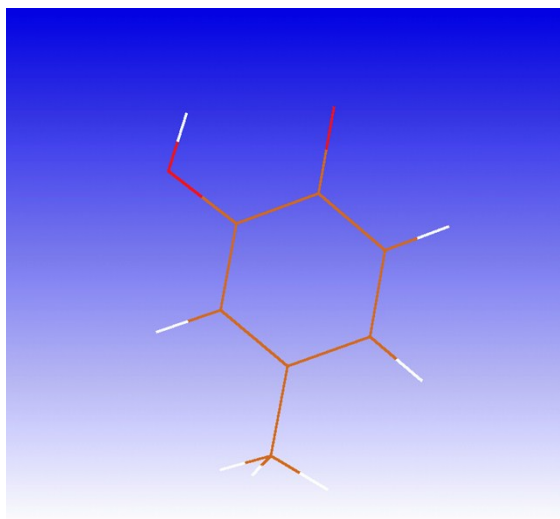
56258,-1.8410375701\H,4.3220412095,0.8913530616,-0.5203959678\H,4.3375

691982,-0.8729955941,-0.4963170525

Sum of electronic and thermal Enthalpies= -421.895351

Sum of electronic and thermal Free Energies= -421.938670

Radical from compound 6

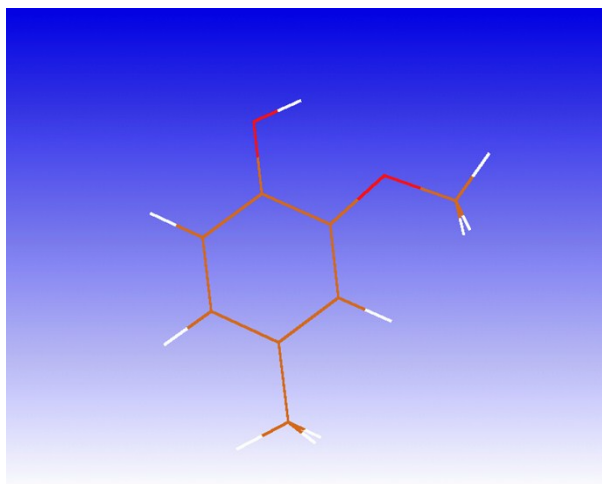


C,-0.0227195038,0.1306486662,0.011917203\C,-0
 .0521657416,0.0321381096,1.4499367012\C,1.2409955528,-0.0826532563,2.1
 299107305\C,2.4404672049,-0.0963214855,1.4265674653\C,2.4251878785,0.0
 015587065,0.0310775247\C,1.1754565002,0.1146986657,-0.6576575343\O,1.1
 981003534,-0.1731576881,3.4630804992\H,3.3761894369,-0.1829837122,1.97
 03191109\C,3.705681595,-0.0102319336,-0.7601810111\H,1.1881124347,0.18
 94865598,-1.742126201\H,-0.9718247216,0.2163025693,-0.5072511004\O,-1.
 0928549159,0.0369542549,2.1614011398\H,0.2427160019,-0.1392235706,3.69
 20625803\H,3.7191360794,-0.845625099,-1.4710848679\H,3.8107213984,0.90
 93695574,-1.3490320549\H,4.5808215279,-0.1009603439,-0.1123104882

Sum of electronic and thermal Enthalpies= -421.281485

Sum of electronic and thermal Free Energies= -421.323867

Compound 7



C,0.0074588914,0.0191879371,-0.024946504

5\C,-0.0137020219,0.0064642924,1.3622535119\C,1.1876301659,-0.04610660

16,2.0919245265\C,2.3929583499,-0.0851071489,1.414157743\C,2.409436399

6,-0.0720951259,0.015545509\C,1.2288673969,-0.0202735746,-0.7178351137

\O,1.1616189024,-0.0583737117,3.4511039566\H,3.3108732852,-0.125463356

,1.9909197873\H,3.3624700404,-0.1030870385,-0.5044919959\C,1.235267227

, -0.0058068822,-2.2263796367\H,-0.9200973152,0.059770924,-0.5875776934

\O,-1.1357890812,0.04128505,2.1456684428\H,0.2382129572,-0.0262215057,

3.7371044288\C,-2.3879902425,0.095028814,1.4926615125\H,-3.1412394766,

0.1158604509,2.2792101742\H,-2.4702307474,1.000151785,0.8802030908\H,-

2.5379316016,-0.7891977918,0.862758904\H,0.6929533003,-0.8651016128,-2

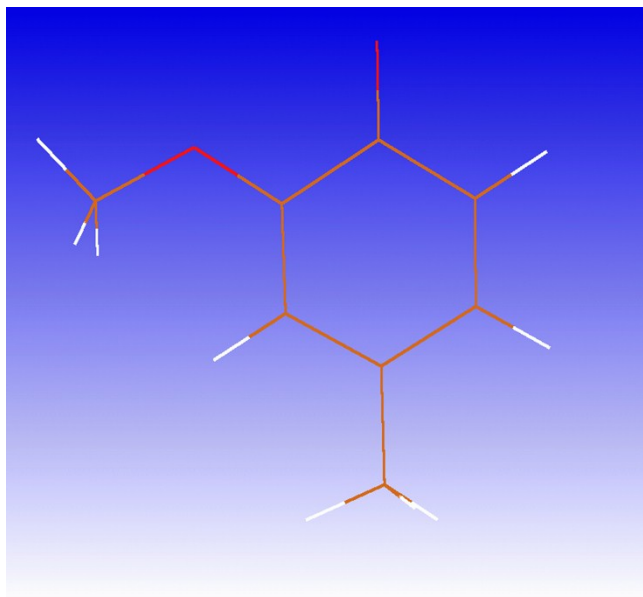
.633876299\H,0.7597584506,0.8997935348,-2.6166677015\H,2.2567279473,-0

.0407084384,-2.6122925304

Sum of electronic and thermal Enthalpies= -460.959662

Sum of electronic and thermal Free Energies= -461.005738

Radical from compound 7

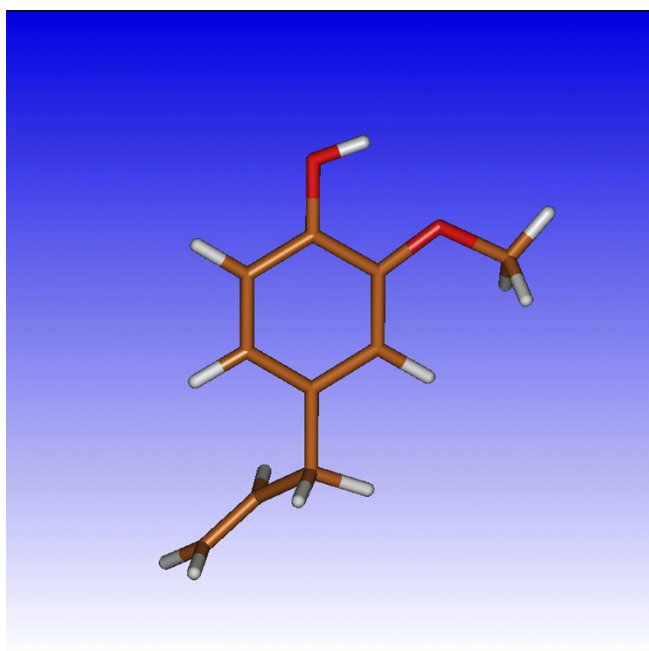


C,0.0003264962,-0.0449140937,0.0018689
04\C,0.0005735041,-0.0123042912,1.4216919792\C,1.2156568571,0.01112170
3,2.115762078\C,2.4256897278,0.0028132303,1.4294244094\C,2.459934872,-
0.0307304477,-0.0403881273\C,1.1720387771,-0.0538949553,-0.7034987562\
C,-1.3066431677,-0.0033581842,2.161992104\O,3.6289376561,0.0233901532,
2.0026239725\C,3.7022184607,0.056316188,3.4166449551\O,3.5358583091,-0
.0383813221,-0.6622405762\H,1.1925187295,-0.0786782207,-1.7881274045\H
, -0.9532700146,-0.062763433,-0.5195208109\H,1.1965859925,0.0359036623,
3.199892414\H,4.7633643192,0.0684140794,3.6587489443\H,3.221996795,0.9
587452719,3.8106199219\H,3.2330352248,-0.8329207967,3.8517679657\H,-1.
1574811889,0.0224221358,3.2432096089\H,-1.9061678171,0.8677930295,1.87
73087897\H,-1.8952840377,-0.8940092687,1.9178161866

Sum of electronic and thermal Enthalpies= -460.328338

Sum of electronic and thermal Free Energies= -460.372273

Compound 8



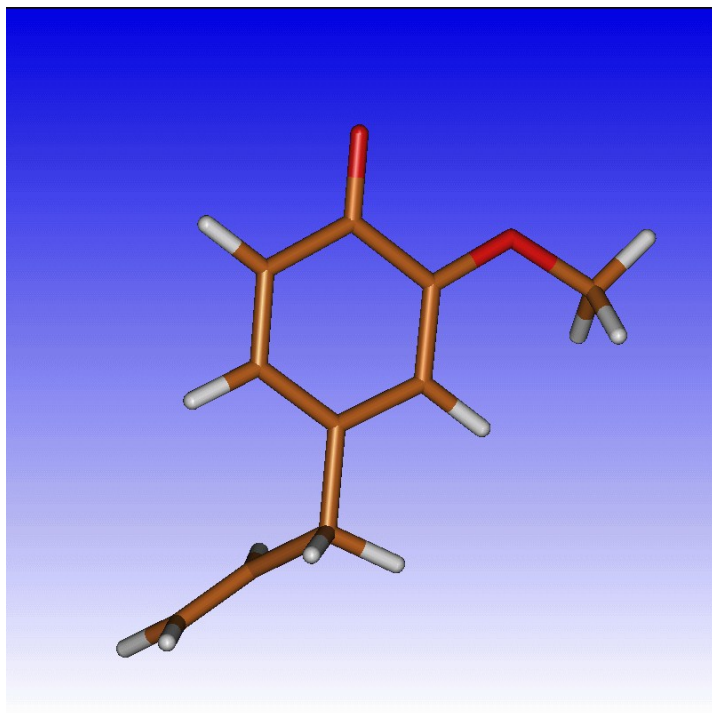
C,-0.1321031458,-0.1058498367,0.0853708

634\C,-0.0574117232,-0.0390960399,1.4834505007\C,1.1779753423,0.012934
1437,2.1182875291\C,2.3630168458,-0.0049530402,1.3657302093\C,2.292338
0533,-0.0755062453,-0.0168248692\C,1.050192526,-0.1274646515,-0.651448
8827\O,1.3796030678,0.0789710662,3.4708680478\C,0.2371056807,0.1050533
013,4.3025515089\O,3.5699398686,0.0423903276,1.9883491003\C,-1.4808181
459,-0.1336163206,-0.6098588184\H,3.2183938039,-0.0915163332,-0.581764
9979\H,1.002764916,-0.1897926681,-1.7349553126\H,-0.9735359322,-0.0262
927692,2.0652139295\H,3.4174971577,0.0860353645,2.9425824251\H,0.60639
71728,0.1610216793,5.3257522607\H,-0.3829501795,0.9825793931,4.0867331
269\H,-0.358821478,-0.8059607246,4.1760364755\H,-2.2625121518,-0.29001
37331,0.143837554\H,-1.6821536518,0.8386026811,-1.0769816912\C,-1.5756
080002,-1.2102144092,-1.655972773\C,-1.8329956614,-0.9896790207,-2.944
2528546\H,-1.4017254022,-2.2285334773,-1.3082220984\H,-1.8886295021,-1
.8029813545,-3.6605310136\H,-1.9982846719,0.0170736521,-3.3211670689

Sum of electronic and thermal Enthalpies= -538.285216

Sum of electronic and thermal Free Energies= -538.336447

Radical from 8



C,-0.1270019782,-0.0249697877,0.0824
86754\C,-0.0590699584,-0.0148180406,1.4797096735\C,1.1718786452,0.0137
358443,2.1279282525\C,2.4278375191,0.032437695,1.3616034839\C,2.291575
5154,0.0179612889,-0.0809634535\C,1.0659918928,-0.0138019786,-0.687087
0219\O,1.3390379163,0.0264196503,3.449832646\C,0.1883880446,0.01103224
48,4.2759221074\O,3.5310182457,0.0586314573,1.9322130749\C,-1.46383582
68,-0.0452165683,-0.6225295481\H,3.2160362029,0.0313377286,-0.64899933
75\H,0.9856275864,-0.0352533063,-1.7706777085\H,-0.9827534208,-0.02587
05779,2.0484694919\H,0.557735314,0.0258066261,5.2996726376\H,-0.433593
8563,0.8942429082,4.0936462759\H,-0.399729097,-0.8976878701,4.10719538
28\H,-2.2645507391,-0.0757690075,0.1252677918\H,-1.5892344515,0.884080
712,-1.1930733599\C,-1.5951542426,-1.2177735845,-1.5597461774\C,-1.800
1763187,-1.1109140156,-2.871234534\H,-1.4982492741,-2.2039068318,-1.10
6542894\H,-1.8851755651,-1.9872877617,-3.5052074618\H,-1.8933392639,-0

.13922584,-3.350773587

Sum of electronic and thermal Enthalpies= -537.652487

Sum of electronic and thermal Free Energies= -537.704044