

Electronic Supplementary Information

Tryptophan: Antioxidant or Target of Oxidative Stress? A Quantum Chemistry Elucidation.

Adriana Pérez-González, Leonardo Muñoz-Rugeles, Juan Raúl Alvarez-Idaboy,*

¹Departamento de Física y Química Teórica, Facultad de Química, Universidad Nacional Autónoma de México, México DF 04510, México.

Table of Contents

Figure 1S'. Tryptophan in zwitterionic form and protein model, with and without numbering.	3
Figure 1S. Optimized geometries of the OH radical (A) and the OH anion (B) with 4 explicit water molecules.	4
Figure 2S. Optimized geometries of the OOH radical (A) and the OOH anion (B) with 3 explicit water molecules.	4
Figure 3S. Optimized geometries of the transition states corresponding to Tryptophan in zwitterionic form + $\cdot\text{OH}$ reaction.	5
Figure 4S. Optimized geometries of the transition states corresponding to Tryptophan protein model + $\cdot\text{OH}$ reaction.	6
Figure 5S. Optimized geometries of the transition states corresponding to Tryptophan in zwitterionic form + $\cdot\text{OOH}$ reaction.	7
Figure 6S. Optimized geometries of the transition states corresponding to Tryptophan protein model + $\cdot\text{OOH}$ reaction.	9
Optimized Geometries in cartesian coordinates corresponding to:	10
TrpP, (0,1)	10
TrpP-cr, (+1,2)	10
TrpP-n7-HT, (0,2)	11
TrpP-c10-HT, (0,2)	12
TrpP-c2-RAF-OH, (0,2)	12
TrpP-c3-RAF-OH, (0,2)	13
TrpP-c4-RAF-OH, (0,2)	14

* To whom correspondence should be addressed. E-mail: jidaboy@unam.mx

<i>TrpP-c5-RAF-OH, (0,2)</i>	15
<i>TrpP-c8-RAF-OH, (0,2)</i>	15
<i>TrpP-c2-RAF-OOH, (0,2)</i>	16
<i>TrpP-c3-RAF-OOH, (0,2)</i>	17
<i>TrpP-c4-RAF-OOH, (0,2)</i>	18
<i>TrpP-c5-RAF-OOH, (0,2)</i>	18
<i>TrpP-c8-RAF-OOH, (0,2)</i>	19
<i>TrpZ, (0,1)</i>	20
<i>TrpZ-cr, (+1,2)</i>	21
<i>TrpZ-n7-HT, (0,2)</i>	21
<i>TrpZ-c10-HT, (0,2)</i>	22
<i>TrpZ-c2-RAF-OH, (0,2)</i>	23
<i>TrpZ-c3-RAF-OH, (0,2)</i>	23
<i>TrpZ-c4-RAF-OH, (0,2)</i>	24
<i>TrpZ-c5-RAF-OH, (0,2)</i>	25
<i>TrpZ-c8-RAF-OH, (0,2)</i>	25
<i>TrpZ-c2-RAF-OOH, (0,2)</i>	26
<i>TrpZ-c3-RAF-OOH, (0,2)</i>	27
<i>TrpZ-c4-RAF-OOH, (0,2)</i>	28
<i>TrpZ-c5-RAF-OOH, (0,2)</i>	28
<i>TrpZ-c8-RAF-OOH, (0,2)</i>	29

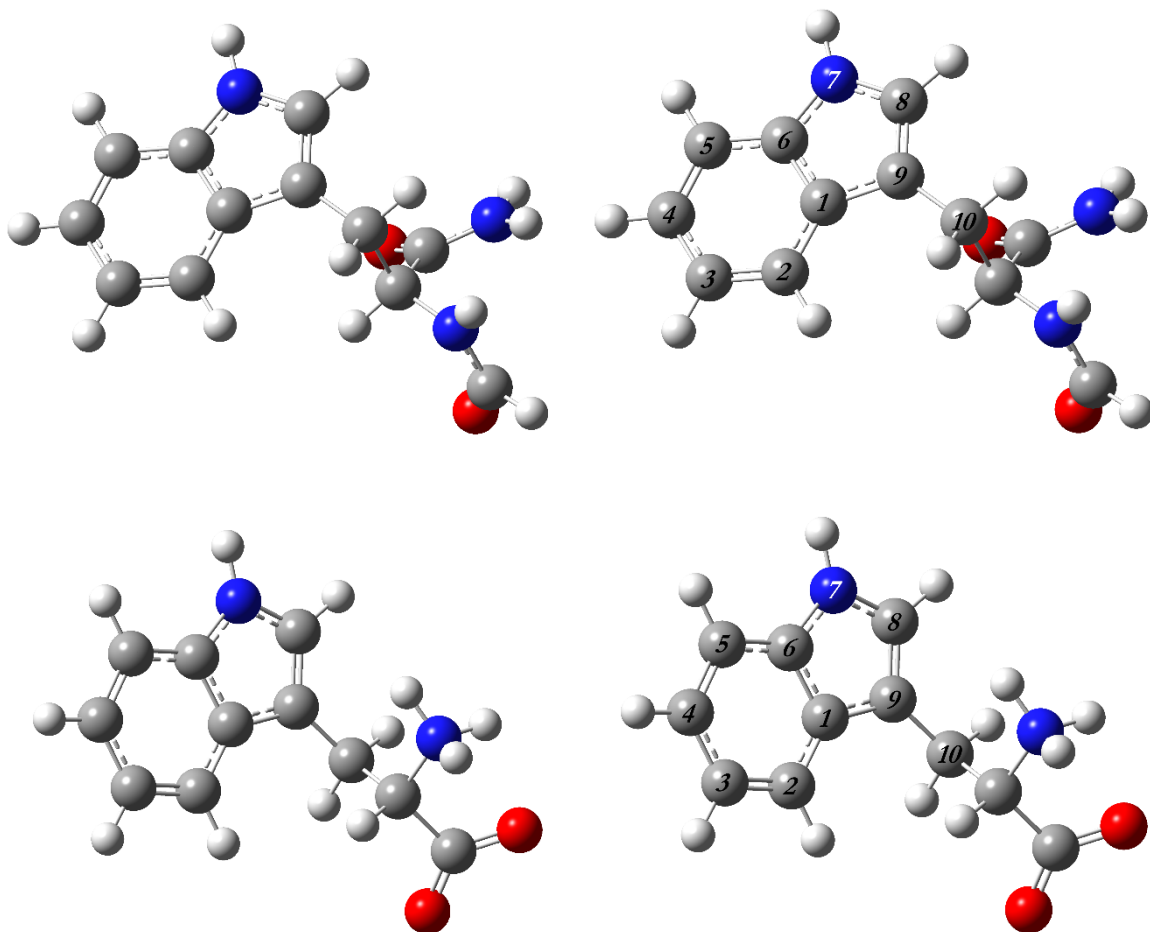


Figure 1S'. Tryptophan in zwitterionic form and protein model, with and without numbering.

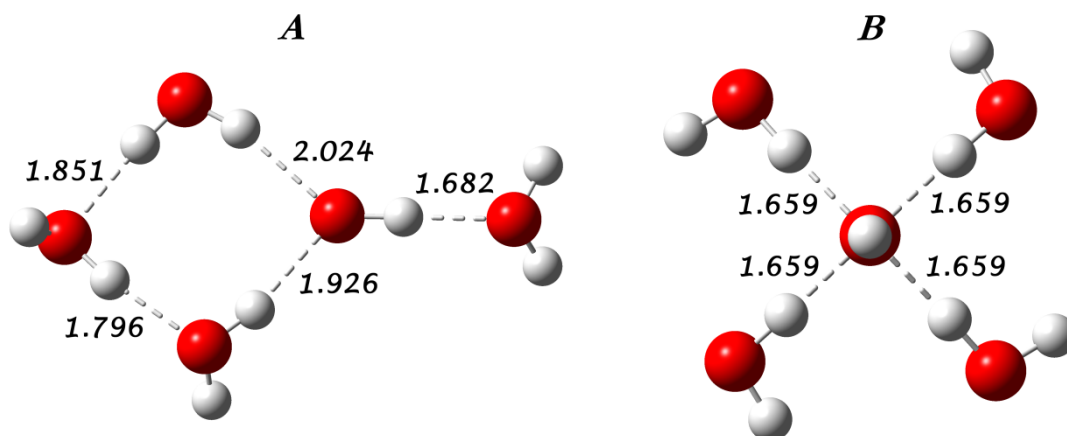


Figure 2S. Optimized geometries of the OH radical (A) and the OH anion (B) with 4 explicit water molecules.

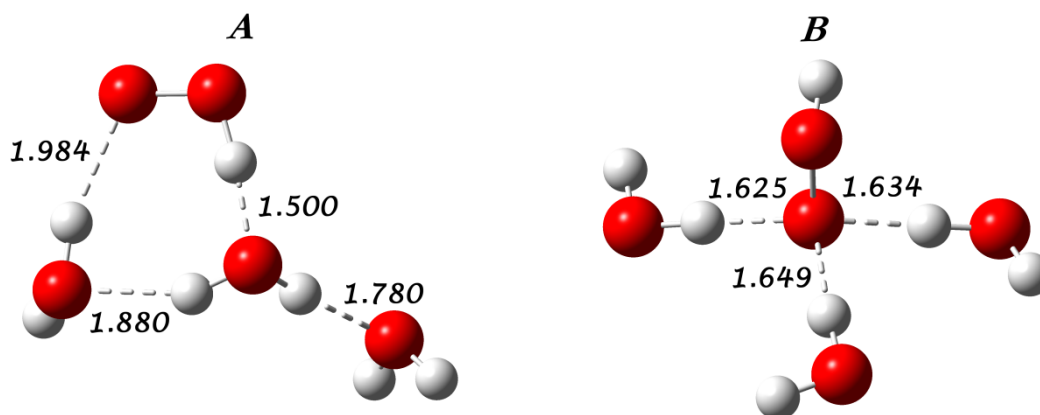


Figure 3S. Optimized geometries of the OOH radical (A) and the OOH anion (B) with 3 explicit water molecules.

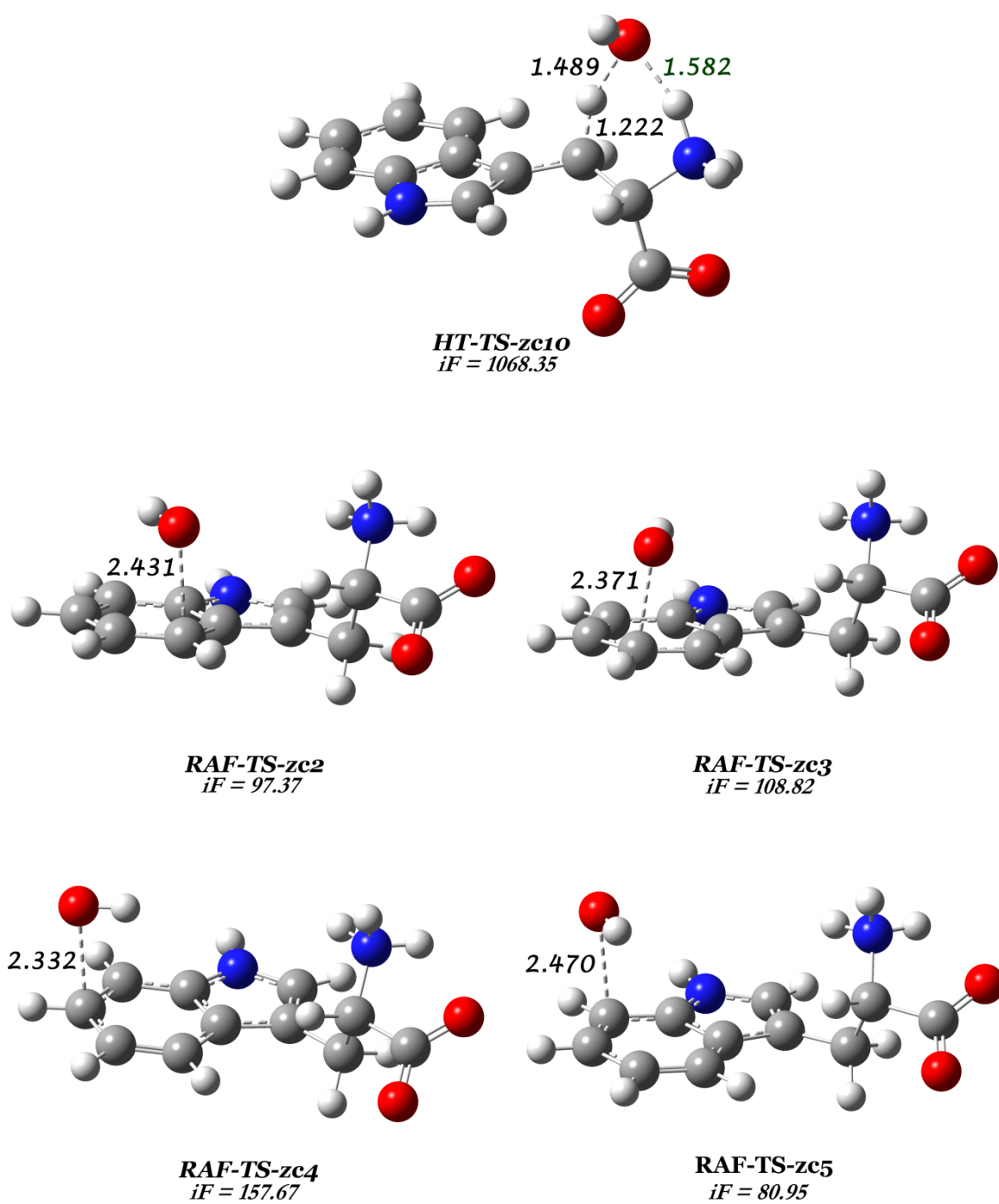


Figure 4S. Optimized geometries of the transition states corresponding to Tryptophan in zwitterionic form + $\cdot\text{OH}$ reaction.

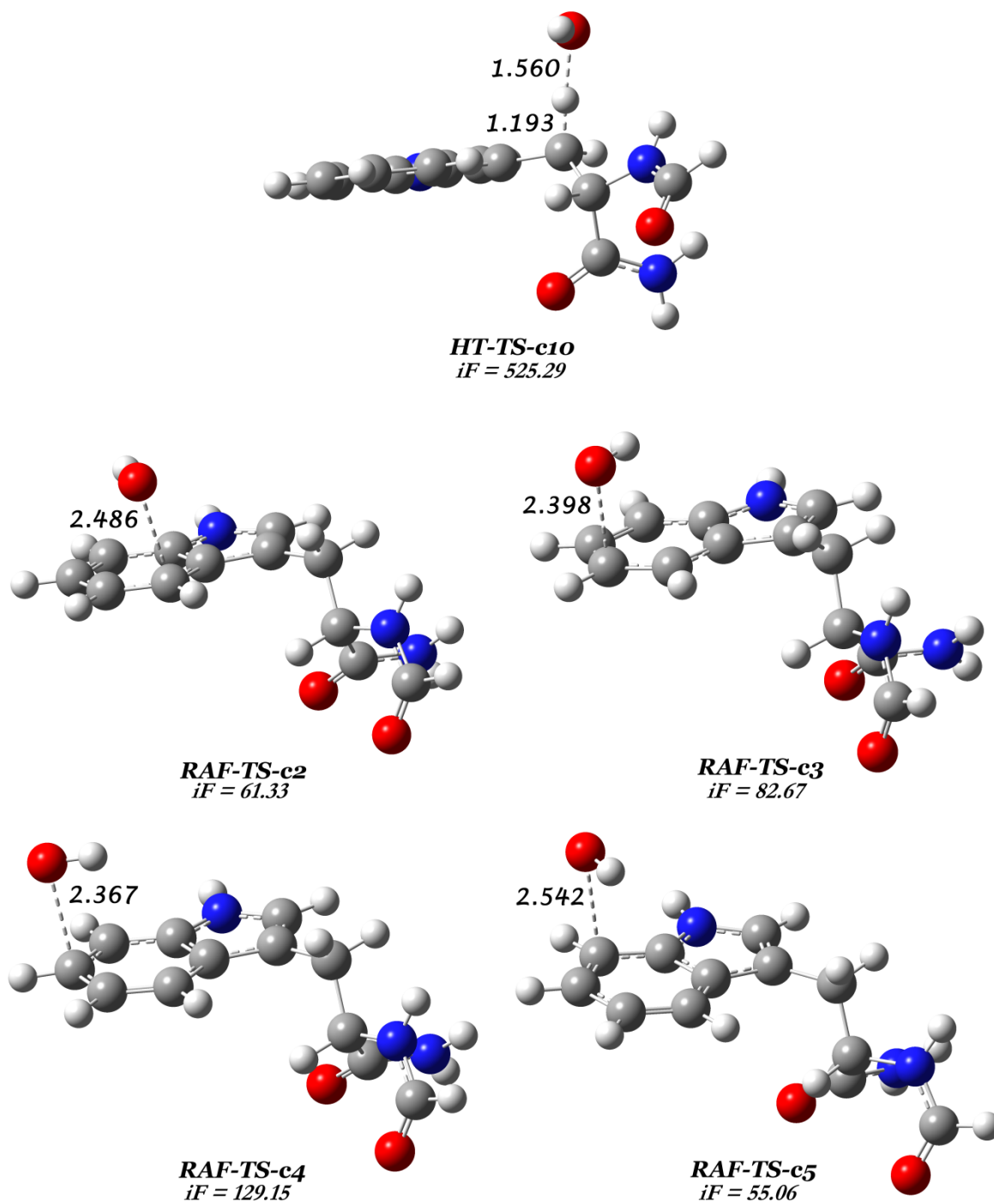
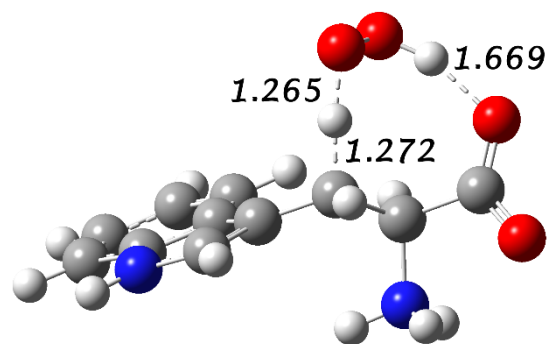
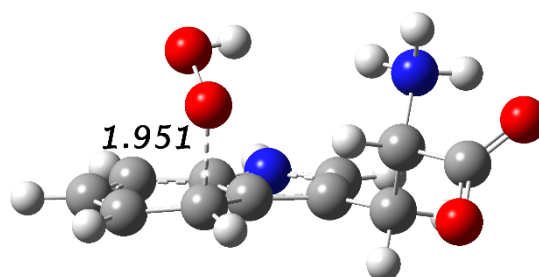


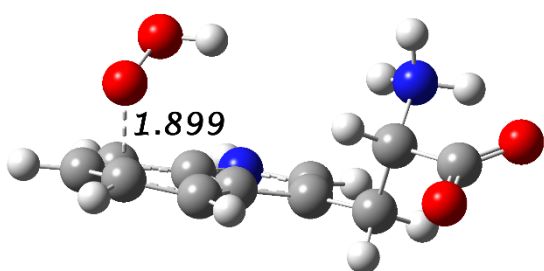
Figure 5S. Optimized geometries of the transition states corresponding to Tryptophan protein model + $\cdot\text{OH}$ reaction.



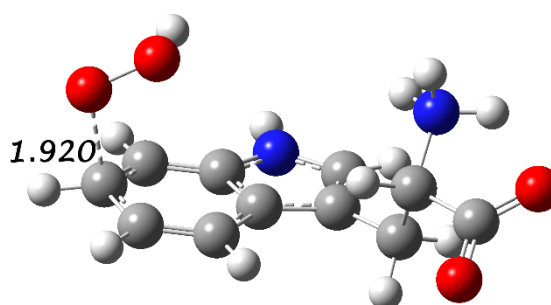
HT-TS-zc10
iF = 2576.55



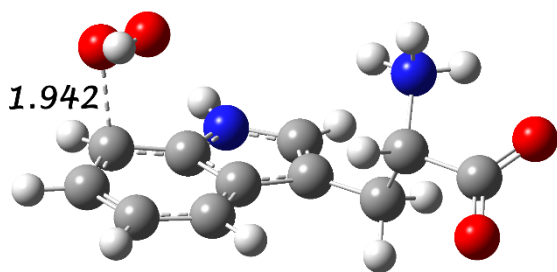
RAF-TS-zc2
iF = 590.89



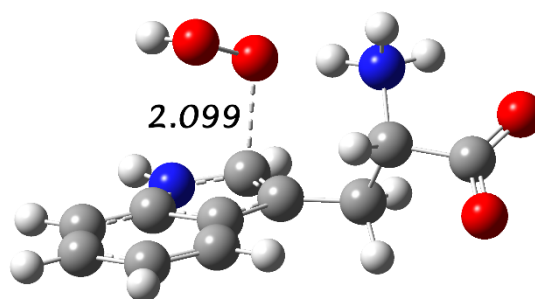
RAF-TS-zc3
iF = 542.95



RAF-TS-zc4
iF = 583.93

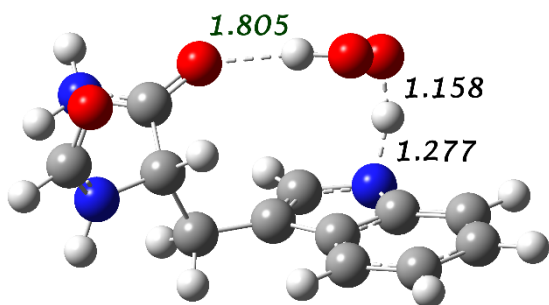


RAF-TS-zc5
iF = 583.44

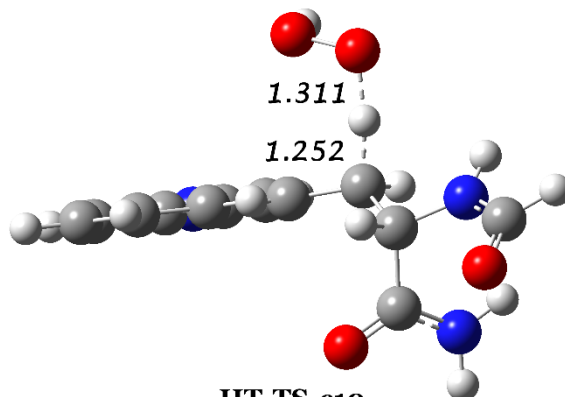


RAF-TS-zc8
iF = 437.33

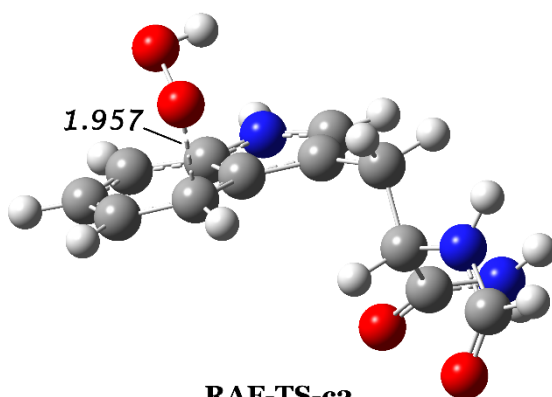
Figure 5S. Optimized geometries of the transition states corresponding to Tryptophan in zwitterionic form + $\cdot\text{OOH}$ reaction.



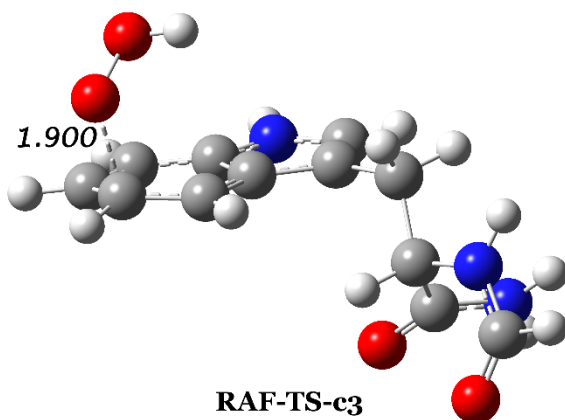
HT-TS-n7
iF = 2958.94



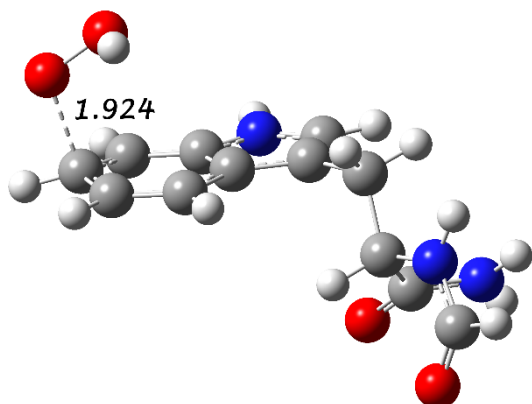
HT-TS-c10
iF = 2032.57



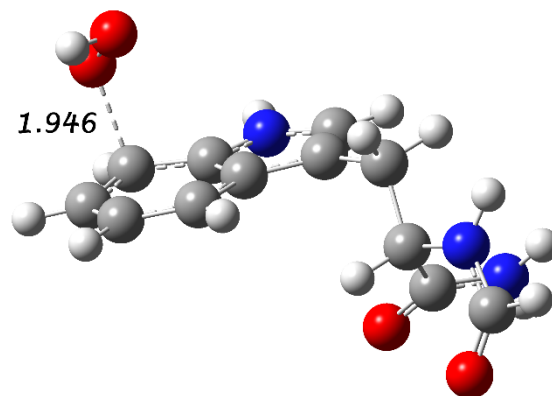
RAF-TS-c2
iF = 600.06



RAF-TS-c3
iF = 536.36



RAF-TS-c4
iF = 566.86



RAF-TS-c5
iF = 578.40

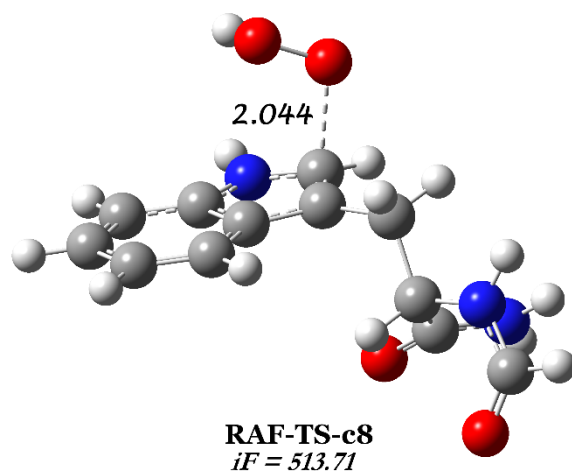


Figure 6S. Optimized geometries of the transition states corresponding to Tryptophan protein model + H_2O_2 reaction.

Optimized Geometries in cartesian coordinates corresponding to:

TrpP, (0,1):

\C,-0.7337555371,0.2787588583,-1.3884
140868\H,-0.6270366444,-0.4989627407,-2.1500499047\H,-1.2096766741,1.1
384922782,-1.8681531805\C,0.6052525737,0.6723619917,-0.8595427465\C,1.
0655369459,1.9386439213,-0.667138728\C,1.6547928185,-0.2070836265,-0.4
178143055\H,0.5799717832,2.882846287,-0.8716337245\N,2.3292295457,1.91
03355641,-0.1365435961\C,2.7134878928,0.6052552278,0.0240198971\C,1.79
44854383,-1.6000993634,-0.3639279453\H,2.8880420761,2.720682583,0.0830
390619\C,3.9044694759,0.0694920151,0.5156408536\C,2.9681085753,-2.1330
791919,0.1199778934\H,0.9905805431,-2.2477913927,-0.699753223\H,4.7110
049934,0.7123796062,0.8517397416\C,4.0147647035,-1.3020108268,0.557720
5293\H,3.0923215003,-3.2099193364,0.1672275506\H,4.9271787711,-1.75189
5321,0.9351966478\C,-1.6779756362,-0.2689805824,-0.3120917424\N,-2.927
8499985,-0.6486029868,-0.9370088178\C,-1.8640651075,0.7548246204,0.800
9686916\H,-1.2308041145,-1.1448688415,0.1620195821\C,-3.8961431785,-1.
2750338846,-0.2637722744\H,-3.0765888429,-0.441058073,-1.915504417\N,-
2.7640407981,1.7169008857,0.5932454508\O,-1.1666473722,0.698933714,1.8
150989701\O,-3.8222669772,-1.5642961176,0.9288162578\H,-4.7790961432,-
1.5155976464,-0.8697273746\H,-3.3296349239,1.7357422712,-0.2416980344\
H,-2.8975756887,2.4302451078,1.2950759739\

TrpP-cr, (+1,2):

\C,-0.7299878086,0.3230677412,-
1.3843268216\H,-0.6504744611,-0.521515026,-2.0722567799\H,-1.131567460
1,1.1765110779,-1.9342433679\C,0.6224261471,0.6381184497,-0.8700093885
\C,1.1853632748,1.9491750349,-0.7554342392\C,1.6116263094,-0.250143318
1,-0.3849699185\H,0.73431109,2.8936470597,-1.0276800289\N,2.3887533583
,1.8727495751,-0.2468225687\C,2.7149889729,0.5271906821,0.00805986\C,1

.6640048842,-1.6415817407,-0.2471926604\H,2.9928640936,2.6671769755,-0.062239778\C,3.860851028,-0.0092226387,0.5293668483\C,2.8146457002,-2.1997217715,0.2772753275\H,0.825376748,-2.2596339043,-0.5471918114\H,4.7009616629,0.6070482193,0.8259639353\C,3.890928595,-1.3987060143,0.6591995854\H,2.8859351738,-3.2745201332,0.3959362282\H,4.7797624344,-1.8663443199,1.0677141129\C,-1.7083066269,-0.0813330258,-0.2715871672\N,-2.9302538569,-0.5725618509,-0.861297037\C,-1.8989015494,1.0765160847,0.7020270022\H,-1.2695818125,-0.8898176933,0.3175425308\C,-3.6728064223,-1.5390642365,-0.3023585243\H,-3.2348141752,-0.1925804708,-1.7484449251\N,-3.1315957882,1.5285924569,0.9072174506\O,-0.9059684222,1.5488750235,1.2608349355\O,-3.4204332959,-2.0743775417,0.7720497653\H,-4.5492459627,-1.8187077866,-0.90101609\H,-3.9302098534,1.117873129,0.4485813721\H,-3.2740889773,2.2816279628,1.5652731526\

TrpP-n7-HT, (0,2):

\C,0,0.986215,-0.205248,-1.176469\H,0,0.9963,0.749339,-1.709876\H,0,1.498214,-0.944139,-1.797532\C,0,-0.421837,-0.596644,-0.923789\C,0,-1.063338,-1.862233,-1.196043\C,0,-1.433361,0.18998,-0.298997\H,0,-0.583971,-2.711755,-1.672707\N,0,-2.298142,-1.91444,-0.805425\C,0,-2.568439,-0.645429,-0.240532\C,0,-1.482232,1.497665,0.180067\C,0,-3.748659,-0.203704,0.301105\C,0,-2.67865,1.940715,0.728278\H,0,-0.617434,2.152635,0.116515\H,0,-4.617576,-0.85033,0.34026\C,0,-3.788686,1.105427,0.7898\H,0,-2.75119,2.953238,1.108899\H,0,-4.710014,1.480909,1.222151\C,0,1.791957,0.019968,0.123105\N,0,3.009596,0.739241,-0.135029\H,0,1.180701,0.608201,0.813296\C,0,3.000625,2.074859,-0.309144\H,0,3.87022,0.209576,-0.08476\O,0,1.992127,2.752077,-0.311546\H,0,4.004544,2.505441,-0.454399\C,0,2.171656,-1.3049,0.774376\N,0,1.16997,-1.951421,1.403541\O,0,3.304615,-1.738805,0.700835\H,0,0.236615,-1.577361,1.452919\H,0,1.358172,-2.858319,1.798775\

TrpP-c10-HT, (0,2):

\C,-0.5327779259,-0.5996802544
,0.1119207909\H,-0.4469424949,-1.6559690367,-0.1249514004\C,0.62452137
33,0.1767131801,0.2115531969\C,0.7429813682,1.5425612651,0.4638493131\
C,1.992155348,-0.3055623571,0.0702055436\H,-0.0254630894,2.2833247436,
0.6268411279\N,2.0602585714,1.8986421385,0.4908991518\C,2.8421409385,0
.792319562,0.252190619\C,2.5399669172,-1.5616219151,-0.1883979612\H,2.
4042621802,2.8353301032,0.638775954\C,4.2277196417,0.6763938234,0.1839
232472\C,3.912657876,-1.687128135,-0.2582128403\H,1.8986707543,-2.4253
173862,-0.3321316385\H,4.8701773906,1.5383093734,0.327239017\C,4.74692
45303,-0.5752541635,-0.0729897561\H,4.355809886,-2.6567761335,-0.45854
54367\H,5.8227481631,-0.7028550068,-0.1329154835\C,-1.9158236225,-0.04
54164214,0.2293385738\N,-2.7717075064,-0.9934009986,0.9145622315\C,-2.
4087227198,0.3153470448,-1.1740159086\H,-1.9109422441,0.8957945565,0.7
835712574\C,-4.0022928261,-0.6739994474,1.3274846364\H,-2.4085214869,-
1.9094977117,1.1404739994\N,-3.1708248676,-0.5736311365,-1.8093527021\
O,-2.0438057773,1.3776530922,-1.6808283269\O,-4.5302424688,0.418110615
8,1.1312848736\H,-4.5141067582,-1.4822310946,1.8653506941\H,-3.4906693
224,-1.4139615614,-1.3525169208\H,-3.4854538287,-0.3728357386,-2.74767
18523\

TrpP-c2-RAF-OH, (0,2):

\C,-0.8204349131,0.1433702942,-1.3
589500996\H,-0.6590517599,-0.754584084,-1.9596838837\H,-1.3171070147,0
.8783874023,-1.9983990856\C,0.4865704,0.6929620285,-0.885385622\C,0.86
32112245,2.0145235484,-0.942221102\C,1.5576898102,-0.0040331668,-0.270
7117231\H,0.3312505361,2.8682398954,-1.3369157409\N,2.1016117454,2.151
7513185,-0.3926368283\C,2.5462392238,0.9252326043,0.0253288054\C,1.726
5120986,-1.4517059705,0.0547380875\H,2.6101573316,3.0191142278,-0.3060

521662\C,3.7670456778,0.602552842,0.6550276385\C,3.0376273036,-1.71413
33012,0.7358959676\H,0.9124136115,-1.7900929247,0.7051881132\H,4.51414
13359,1.3583571111,0.8650315152\C,3.9682967757,-0.7516137112,0.9948938
623\H,3.2314194307,-2.7463576987,1.0103630627\H,4.8975950948,-1.033906
7697,1.4797432574\C,-1.7714425651,-0.2384311933,-0.2192169341\N,-2.978
5084014,-0.8025464319,-0.7866616738\C,-2.0469301596,0.9665262246,0.671
399265\H,-1.2956685189,-0.9804135875,0.4247795705\C,-3.926392534,-1.35
72546075,-0.0262590361\H,-3.1072303333,-0.7936587557,-1.7897460026\N,-
3.0250220972,1.7900500822,0.2915472901\O,-1.3493884484,1.1702437009,1.
6665797715\O,-3.8718715147,-1.4162585271,1.2003413742\H,-4.7742226428,
-1.7622985607,-0.5934038862\H,-3.6060679365,1.5806922642,-0.505865521\
H,-3.2332309764,2.6037850565,0.8517642946\O,1.5921057983,-2.2921595199
, -1.1094773262\H,2.2905452076,-2.0447505303,-1.7266326343\

TrpP-c3-RAF-OH, (0,2):

\C,-0.9985941001,0.2565444832,-
1.3822086683\H,-0.7656535981,-0.557515206,-2.07482259\H,-1.5706684991,
1.003040792,-1.9403012755\C,0.262401478,0.8665940978,-0.8703873328\C,0
.5628986578,2.193052931,-0.818743273\C,1.4005602575,0.1667466613,-0.32
04703421\H,-0.0225950919,3.0452453856,-1.1336494925\N,1.811006376,2.37
01842551,-0.2717196432\C,2.3384950203,1.1524965439,0.0372072892\C,1.68
22718687,-1.1760580081,-0.1193460432\H,2.2660585812,3.2606063592,-0.13
76448377\C,3.6027384884,0.8307564971,0.6142347506\C,3.007919035,-1.600
3754284,0.424615868\H,0.9708050847,-1.9540963988,-0.3752395132\H,4.294
3359457,1.6210768275,0.8880873767\C,3.9093215022,-0.4631781255,0.81211
62483\H,2.8620449247,-2.2519324913,1.2935454764\H,4.8624134226,-0.7401
708078,1.2516506744\C,-1.8935584225,-0.3291980511,-0.2832207945\N,-3.0
468492264,-0.9442947331,-0.9070748269\C,-2.2720358047,0.7500380052,0.7
233481811\H,-1.3417922093,-1.083137777,0.2818641053\C,-3.9524582124,-1

.6339026785,-0.2088418428\H,-3.1546342524,-0.886590502,-1.9109127202\N
, -3.3124696657,1.5261096182,0.4164164019\O,-1.5968210867,0.9062695081,
1.7420410904\O,-3.9096957409,-1.7811874305,1.0107859148\H,-4.754735442
5,-2.0656284967,-0.8208023958\H,-3.8665254189,1.3578517574,-0.40951040
31\H,-3.5844048478,2.2647836841,1.0487282633\O,3.692604061,-2.46635430
92,-0.5144215596\H,3.8330667358,-1.956017973,-1.3208446458\

TrpP-c4-RAF-OH, (0,2):

\C,-1.1067682999,0.2944476082,-
1.3776975712\H,-0.9241820282,-0.4837681807,-2.1235645012\H,-1.64753652
5,1.1021762896,-1.8782780533\C,0.1926414319,0.805133945,-0.8471885675\
C,0.5412483602,2.1266911757,-0.6820550875\C,1.2925333939,0.039311642,-
0.3978926547\H,-0.0257437042,3.0186064037,-0.9081092258\N,1.797554367,
2.2109390643,-0.151885073\C,2.2979075455,0.9394601411,0.0359881872\C,1
.5445731388,-1.3727747568,-0.322342307\H,2.2903851773,3.0675026729,0.0
48418966\C,3.509720597,0.5401824478,0.5368396018\C,2.7167629358,-1.818
1931859,0.156575122\H,0.7839321025,-2.0732729755,-0.653538916\H,4.2569
377682,1.2504279602,0.8733797005\C,3.8282548173,-0.9178687608,0.615595
4614\H,2.9190185326,-2.8833006544,0.2168630065\H,4.0916768031,-1.18028
16883,1.6468432589\C,-2.0104948355,-0.3155419268,-0.2998143744\N,-3.18
54883307,-0.8719249834,-0.9374517163\C,-2.3539372013,0.7238468712,0.76
07471419\H,-1.4738949154,-1.1090749355,0.2239319994\C,-4.0902131135,-1
.5844986003,-0.2611262279\H,-3.3235918442,-0.7336289471,-1.9296479316\
N,-3.3912755505,1.5239276253,0.5095677284\O,-1.6562789264,0.8271229723
,1.7708286246\O,-4.0193357293,-1.8111972005,0.9448920448\H,-4.91729625
75,-1.958959789,-0.8777427383\H,-3.9658480639,1.3954738359,-0.30949245
24\H,-3.6448821223,2.2335787721,1.1815600871\O,5.0388251362,-1.2214968
404,-0.1143923537\H,4.8792326905,-0.9988776617,-1.0392072788\

TrpP-c5-RAF-OH, (0,2):

\C,1.0724452746,-0.2773891383,-
1.3853337595\H,0.9797480542,0.5001220954,-2.148725843\H,1.5211846004,-
1.1510206,-1.866010247\C,-0.2728580746,-0.6350343729,-0.8451696757\C,-
0.7584094059,-1.8944288212,-0.6414999663\C,-1.2977971285,0.2697269213,
-0.4086647586\H,-0.3052728938,-2.8554199941,-0.837983424\N,-2.01698247
78,-1.8088142093,-0.1040469332\C,-2.3559440012,-0.5019032192,0.0363307
515\C,-1.377999576,1.6904879845,-0.3650019073\H,-2.6091553756,-2.59584
03216,0.1183467815\C,-3.6423725871,0.0222345875,0.5641617815\C,-2.5537
517211,2.2692106871,0.1470354872\H,-0.5621288296,2.3104907576,-0.71799
84937\H,-3.8279379373,-0.3673847805,1.5711910748\C,-3.6061638027,1.521
0217787,0.5974126753\H,-2.6280834221,3.3515475474,0.1895492572\H,-4.49
51819157,2.0071101932,0.9864427821\C,2.0406744543,0.2482260656,-0.3196
031069\N,3.2960480678,0.5839724557,-0.9585187764\C,2.2051111271,-0.772
3774474,0.7999637861\H,1.6236790521,1.1407972268,0.1510542154\C,4.2920
3578,1.1818616968,-0.3000114012\H,3.4222854037,0.3783212559,-1.9404427
22\N,3.0773879428,-1.7601649419,0.5945682459\O,1.5157410706,-0.6891149
957,1.8176951715\O,4.2444740766,1.4756764563,0.8927115389\H,5.17326553
08,1.3933096615,-0.919080629\H,3.6408663229,-1.7978357543,-0.241358788
7\H,3.1964564479,-2.4710737598,1.3014884271\O,-4.7725323111,-0.4524126
354,-0.1924760119\H,-4.6844394855,-0.1154322299,-1.0924463314\

TrpP-c8-RAF-OH, (0,2):

\C,-0.7455142849,0.3334839207,-1.2
131689698\H,-0.6436571447,-0.3051513805,-2.0952856565\H,-1.1665410493,
1.2862138299,-1.5468999264\C,0.5894307606,0.5557542943,-0.6000457141\C
,1.0535996035,1.8866134213,-0.0740435681\C,1.6003622136,-0.3868659074,
-0.3817665762\H,0.4516200196,2.230164363,0.7736145889\N,2.4231762326,1
.631287088,0.328909255\C,2.6903724803,0.275036277,0.2435209981\C,1.684

2053799,-1.7653605234,-0.6429517031\H,2.7852268384,2.1430941994,1.1204
370529\C,3.81424082,-0.415291436,0.6441313527\C,2.8192467308,-2.451144
3157,-0.2507605645\H,0.8633200621,-2.2801796665,-1.1314208114\H,4.6376
437702,0.0934725475,1.1336693716\C,3.8666348834,-1.7874498178,0.393175
5358\H,2.8969962017,-3.5169346133,-0.4370563526\H,4.7434005798,-2.3479
200387,0.7001583084\C,-1.7558549603,-0.3527234865,-0.2818665229\N,-2.9
890242622,-0.5545215573,-1.0119496925\C,-1.9467132654,0.4593708448,0.9
933925378\H,-1.3608043838,-1.318804097,0.038357814\C,-4.0128224601,-1.
2439583371,-0.5009399185\H,-3.0801681579,-0.1766757837,-1.9454871092\N
, -2.8599670104,1.4300383824,0.9680069414\O,-1.2334422299,0.2318859062,
1.972141086\O,-4.0086896381,-1.7464163501,0.620612803\H,-4.8746308773,
-1.3283393088,-1.1752594929\H,-3.4509133672,1.5741824395,0.1631417913\
H,-3.0063306991,1.9939997781,1.7927055726\O,0.9436158305,2.9380024266,
-1.0212149665\H,1.4020933839,2.6646049014,-1.8255244642\

TrpP-c2-RAF-OOH, (0,2):

\C,0.8964101709,-0.0823185856,-1.3
427080338\H,0.6201015818,0.8582169394,-1.8252874597\H,1.4504864738,-0.
6736463011,-2.0771012606\C,-0.3280512817,-0.8282384508,-0.9198664503\C
, -0.5721915002,-2.1622165159,-1.1497213881\C,-1.4437375083,-0.33787665
98,-0.1959382137\H,0.0291586615,-2.8950239501,-1.6683192623\N,-1.77311
08681,-2.4996370875,-0.6034336715\C,-2.3254866883,-1.3944034634,-0.014
1471322\C,-1.7620380903,1.0243989357,0.3108636913\H,-2.1927019222,-3.4
172988976,-0.6342131117\C,-3.5492498913,-1.2858915314,0.6796558152\C,-
3.055180149,1.0624045715,1.0634052478\H,-0.9520956974,1.4188808734,0.9
357592959\H,-4.2088235714,-2.1366320403,0.8008284966\C,-3.8704752742,-
0.0203497955,1.2124531446\H,-3.3361166068,2.0214172544,1.4864353618\H,
-4.798877056,0.0913381919,1.7634401376\C,1.8362472356,0.2599768983,-0.
1814819762\N,2.9762328533,0.9823295246,-0.7060776332\H,1.3161329348,0.

8858868401,0.5461027751\C,3.9004814996,1.5281904434,0.08873707\H,3.080
4151084,1.0833586414,-1.7069784684\O,3.8772600809,1.4554301988,1.31563
75693\H,4.6974048466,2.0564532903,-0.4501985148\C,2.2372025823,-1.0046
067236,0.5693260403\N,3.2421224755,-1.7169324223,0.0579849844\O,1.6120
049109,-1.3517267888,1.5726425106\H,3.7511119719,-1.3989171384,-0.7527
56288\H,3.5275405574,-2.5706418999,0.5151356717\O,-1.7554578016,2.0138
106044,-0.7527723358\O,-2.7500909373,1.6945530537,-1.7009884357\H,-2.2
97058151,1.0871066507,-2.3056991464\

TrpP-c3-RAF-OOH, (0,2):

\C,-1.336310281,0.3056787252,
-1.372339869\H,-1.0018305998,-0.4752300019,-2.0612092784\H,-1.99879864
77,0.9702642107,-1.9336233781\C,-0.1589877504,1.0683516502,-0.86632796
52\C,-0.0194114843,2.4207301779,-0.8144330718\C,1.0603128302,0.5104772
389,-0.3292310579\H,-0.7049084569,3.1968812689,-1.1238536784\N,1.20395
42751,2.7460140836,-0.2783840119\C,1.8772176688,1.6016909518,0.0228009
341\C,1.4982653129,-0.7876398185,-0.1228627643\H,1.5478944885,3.684360
3209,-0.1391211331\C,3.1661680419,1.435944714,0.6096619826\C,2.8629729
205,-1.0382283969,0.4195820579\H,0.881495125,-1.6473308611,-0.36269758
18\H,3.7512457507,2.3040817333,0.8955920058\C,3.6268481314,0.189256582
3,0.8092963902\H,2.8193759492,-1.7334557079,1.2673963543\H,4.600621753
4,0.0268627935,1.2597966458\C,-2.1486951394,-0.3866402014,-0.270673676
4\N,-3.1889915509,-1.1799150765,-0.8911117623\H,-1.4970668854,-1.03973
17446,0.3127863554\C,-3.946591101,-2.0318424981,-0.1945365616\H,-3.349
1789367,-1.0940805734,-1.8860200412\O,-3.8423878366,-2.207710493,1.017
3582716\H,-4.6844202847,-2.5719489183,-0.8016383798\C,-2.6973398807,0.
6400738102,0.7119440411\N,-3.8741395911,1.1935474949,0.4155207585\O,-2
.0370765062,0.9578856603,1.7025333256\H,-4.4141648062,0.8810940771,-0.
3773324207\H,-4.2672359684,1.8849686376,1.0373328178\O,3.6546023696,-1

.8505300971,-0.5012699753\O,3.8778230807,-1.1287176329,-1.6940005081\H
,3.1192986495,-1.3683877097,-2.2472157753\

TrpP-c4-RAF-OOH, (0,2):

\C,-1.4806677514,0.2482967239,-1.38
51571587\H,-1.2791151968,-0.5372586615,-2.1182851159\H,-2.0402042052,1
.0349021523,-1.898682819\C,-0.1944499175,0.8018387337,-0.8656861343\C,
0.1197041855,2.1359837564,-0.7343406409\C,0.9258229754,0.0777566432,-0
.3995587588\H,-0.4700473549,3.0064993436,-0.984235585\N,1.3726531351,2
.2679200131,-0.2083749876\C,1.9085799624,1.0161450755,0.007014794\C,1.
2033744169,-1.3243860916,-0.2672367072\H,1.8442283143,3.1433990646,-0.
0406247309\C,3.1299203869,0.6609702133,0.5154871944\C,2.3892488842,-1.
7297370352,0.2137486185\H,0.4456965817,-2.0503670002,-0.5457125666\H,3
.8608245635,1.3954164332,0.8343830596\C,3.4852238598,-0.7825463968,0.5
975014658\H,2.6100742795,-2.7866898963,0.3263110622\H,3.8568053693,-1.
030161137,1.5993006589\C,-2.3711682768,-0.3642028502,-0.2978136763\N,-
3.5468327964,-0.9290862588,-0.9271318129\H,-1.8257633213,-1.1523950022
,0.2252884526\C,-4.4528600816,-1.632717374,-0.2432411824\H,-3.67215102
75,-0.8252744784,-1.925065348\O,-4.3927830856,-1.8336085811,0.96783684
66\H,-5.2726494332,-2.0235016635,-0.8596010432\C,-2.7117493465,0.67805
04006,0.7605483332\N,-3.7413430791,1.4862600465,0.5051504691\O,-2.0172
469631,0.7770820099,1.7733639875\H,-4.3104570307,1.3670801698,-0.31904
20431\H,-3.9868028361,2.2028216822,1.1727712012\O,4.6889955829,-1.0742
074771,-0.1745505527\O,4.4552124695,-0.7985844976,-1.5391765327\H,4.14
52370872,-1.6464956201,-1.8903585673\

TrpP-c5-RAF-OOH, (0,2):

\C,1.3303932655,-0.2593095814,-1.36
28971393\H,1.2779915093,0.5180174425,-2.1301152889\H,1.7037925765,-1.1

665193228,-1.8460305324\C,-0.0263043404,-0.5161166728,-0.7959829344\C,
-0.5924183295,-1.7372889765,-0.5689194893\C,-0.9842615128,0.4605617276
, -0.3641699564\H,-0.2062184366,-2.7286890799,-0.7568225188\N,-1.836681
209,-1.5617078872,-0.0209827778\C,-2.0853612268,-0.2338851493,0.102310
4786\C,-0.9719876646,1.8829875866,-0.3425375681\H,-2.4783110015,-2.304
3040571,0.2170819322\C,-3.3218194769,0.3885732394,0.6281662283\C,-2.09
65571605,2.5469619472,0.1805608218\H,-0.1212498783,2.4425431987,-0.713
7054734\H,-3.5734590378,0.0044862632,1.6241572746\C,-3.1917246323,1.87
83121418,0.6524248822\H,-2.0920867458,3.631846624,0.2193189383\H,-4.03
7016592,2.4259105456,1.0565363654\C,2.3599866892,0.2006096994,-0.32447
98486\N,3.6240274948,0.4175669832,-0.9973780414\H,2.0293016031,1.13312
62,0.1372970691\C,4.6786038409,0.9578630232,-0.3819192484\H,3.70819586
33,0.18016016,-1.9767819171\O,4.6872012875,1.2866237126,0.802437206\H,
5.5555986138,1.0853855827,-1.0293612295\C,2.4630110872,-0.8100372071,0
.8112879161\N,3.2468851764,-1.8698429561,0.6088827081\O,1.8067318889,-
0.6501943072,1.8416856112\H,3.7873350499,-1.9697009721,-0.237084524\H,
3.32145559,-2.5755554265,1.3270804099\O,-4.5028433759,-0.0316448146,-0
.1050173925\O,-4.3663281219,0.324062874,-1.4638163871\H,-4.7902899136,
1.1938045591,-1.5129872046\

TrpP-c8-RAF-OOH, (0,2):

\C,-0.7129149384,0.2562199639,-1.11
63363192\H,-0.611716561,-0.2998744028,-2.0525823926\H,-1.0982159078,1.
248896254,-1.3654584062\C,0.617885396,0.3746171584,-0.4680902067\C,1.1
290710162,1.6324574211,0.1694564231\C,1.6039019931,-0.6110994383,-0.34
10869193\H,0.5088910879,1.9907398159,0.9985504319\N,2.4695145562,1.305
4904199,0.5767511833\C,2.7093013996,-0.0429726852,0.3435244524\C,1.651
6606351,-1.9587794896,-0.735621895\H,2.8222579594,1.7202527131,1.42713
93851\C,3.8175918284,-0.7940576331,0.6675852156\C,2.770352885,-2.70705

77389,-0.4184587117\H,0.8172747661,-2.4021227865,-1.2690193931\H,4.654
3336865,-0.3560495176,1.2007378344\C,3.8359171311,-2.1353759475,0.2812
534107\H,2.8215300421,-3.7507190924,-0.7093237717\H,4.6999934504,-2.74
39220225,0.5260082077\C,-1.7553440101,-0.4833905269,-0.2646649675\N,-2
.970187565,-0.6282843116,-1.0375944293\H,-1.3752174238,-1.4728934396,-
0.003568733\C,-3.9717367051,-1.4194446509,-0.6413522558\H,-3.056629129
6,-0.1493265567,-1.9243512029\O,-3.9662197991,-2.0536023635,0.41098984
96\H,-4.8145575983,-1.4577292562,-1.3434628514\C,-1.9697798054,0.23940
28366,1.0595034063\N,-2.9258940701,1.1664659286,1.1040136296\O,-1.2370
642094,-0.0169353788,2.0167938244\H,-3.5245017631,1.3421441068,0.31147
54826\H,-3.0764368396,1.6813291854,1.9594901944\O,1.0903684849,2.77273
75986,-0.7012824996\O,1.7801963078,2.4788225654,-1.8954628856\H,2.7107
605203,2.6062996809,-1.6540854603\

TrpZ, (0,1):

\O,3.5024692083,-1.6742595551,-0.648151
7983\N,-2.0247143504,1.9729463543,-0.2152911969\N,1.9948840227,0.87155
48767,1.3679031644\C,-0.2002594723,0.7267256457,-0.5988114097\C,1.2071
56681,0.3255527355,-0.8996509784\C,-1.298423647,-0.1456366776,-0.27265
46522\C,1.9488480117,-0.190541174,0.3323159437\C,-2.4177779167,0.67180
30546,-0.0419038041\C,-0.695965492,1.9952747722,-0.5461900519\C,-1.434
003001,-1.5361407854,-0.1655247625\C,-3.6651215417,0.1450022926,0.2957
125552\C,3.3815255356,-0.5967500023,-0.0265615376\C,-2.6625978744,-2.0
603885394,0.167809469\C,-3.7693053637,-1.2236453818,0.3977391158\H,1.2
303266106,-0.47278825,-1.6440157483\H,1.7558779525,1.175410193,-1.3159
754257\H,1.4261899522,-1.0433775922,0.7629612582\H,-0.1937075072,2.934
9191814,-0.7310967009\H,-2.614739097,2.7850457619,-0.1176191507\H,-0.5
847161083,-2.1881987278,-0.3438495527\H,-4.5178295453,0.7925215603,0.4
694784708\H,-2.7844465033,-3.1349451405,0.2550553279\H,2.1882384308,0.

4783955312,2.2900540932\H,-4.7243967716,-1.6672651904,0.6591753322\H,1
.1090474389,1.3842864822,1.4098055937\O,4.2975898001,0.1910835682,0.30
53090224\H,2.7615195475,1.5138830066,1.1413204237\

TrpZ-cr, (+1,2):

\O,-3.2913616386,1.6203173125,-0
.8637446276\N,2.0591278097,-1.9820906113,-0.2469834845\N,-2.1490271168
, -0.9766969848,1.3538705635\C,0.2357919327,-0.7122457976,-0.5676377196
\C,-1.1812042774,-0.3732899401,-0.8486015218\C,1.3070722132,0.15526907
46,-0.2700413756\C,-1.9470396941,0.1216806975,0.3749757103\C,2.4504034
368,-0.641777133,-0.0680603994\C,0.7835483783,-2.0359469971,-0.5344922
594\C,1.4098602874,1.5494554303,-0.1602671472\C,3.6766713346,-0.125476
4192,0.2401966926\C,-3.3168901195,0.70594302,-0.014758404\C,2.64381588
25,2.0874587214,0.1527235748\C,3.7540217143,1.2669920622,0.3494334523\
H,-1.2061766476,0.4376968504,-1.578587534\H,-1.6949018669,-1.234403880
8,-1.2822355481\H,-1.3855325156,0.9025730445,0.8896839983\H,0.27351537
85,-2.972962081,-0.7150514873\H,2.6733928836,-2.7866303708,-0.16880015
12\H,0.5435182998,2.1813742217,-0.3188761653\H,4.5451218727,-0.7550198
171,0.391343861\H,2.7551320315,3.1611873606,0.2463417134\H,-2.72678731
41,-0.6471555107,2.1304626698\H,4.7092092973,1.7184535526,0.5930852052
\H,-1.2633055701,-1.3259727092,1.7292411836\O,-4.3191898805,0.22875209
65,0.5600664242\H,-2.6493021117,-1.758078192,0.9219887762\

TrpZ-n7-HT, (0,2):

\O,-3.3368009951,1.60122538
37,-0.7943806524\N,2.0835453326,-2.0495128434,-0.2982268936\N,-2.10975
16115,-1.0677864642,1.288157496\C,0.2413991143,-0.7155789376,-0.609294
4296\C,-1.1722448247,-0.3598855068,-0.8904368756\C,1.3173769495,0.1500
614835,-0.2572051408\C,-1.9450740305,0.0740364766,0.352069579\C,2.4314

402805,-0.6930113869,-0.0735989674\C,0.82061175,-2.0353431829,-0.60416
62924\C,1.4344422527,1.5277327616,-0.0936150495\C,3.6591501366,-0.1866
653342,0.2733871715\C,-3.3310888767,0.6367881943,-0.0011062451\C,2.676
3044237,2.0400775715,0.258649334\C,3.7683446366,1.1974200719,0.4395494
871\H,-1.1999000015,0.4831669121,-1.5835619365\H,-1.6876763872,-1.1999
0033,-1.3637741445\H,-1.3964480589,0.8464267006,0.8928930308\H,0.27812
9378,-2.9463296751,-0.832844778\H,0.5825315377,2.1837440041,-0.2383249
933\H,4.51759322,-0.8343653413,0.4135747215\H,2.7987711351,3.108951683
5,0.3944001563\H,-2.677436117,-0.7849027275,2.0897644155\H,4.727750810
8,1.6227830192,0.7142274466\H,-1.210166739,-1.4153174092,1.629840693\O
, -4.3201719418,0.0957821591,0.5410459525\H,-2.6029133743,-1.8388722826
,0.830906915\

TrpZ-c10-HT, (0,2):

\O,-3.3917334756,0.3803583825,-
1.7194064333\N,2.2628335594,-1.905220863,-0.9325602919\N,-2.1174903938
,0.043899745,1.6390451794\C,0.2317229136,-1.0326991548,-0.4532481779\C
, -1.1689455505,-0.969839211,-0.396605037\C,1.2702072788,-0.1015154236,
-0.0161729447\C,-1.9702929794,0.1580271291,0.1503041959\C,2.5046484626
, -0.6891983459,-0.3393421999\C,0.9208702816,-2.1140385364,-0.999335793
6\C,1.2746074884,1.1456647717,0.6177205915\C,3.7247607841,-0.078194506
7,-0.0648464091\C,-3.3695344215,0.2240514187,-0.4791620874\C,2.4792410
681,1.7589447792,0.8944409893\C,3.6953529828,1.1521605816,0.5538000027
\H,-1.7217993063,-1.8256790039,-0.7711767419\H,-1.4890118877,1.1194496
101,-0.0310964254\H,0.5191334374,-3.0161720694,-1.4374382571\H,2.96968
91191,-2.5399934065,-1.2728046553\H,0.3540549584,1.6429798408,0.899662
949\H,4.6597371609,-0.5594302774,-0.3301056665\H,2.4857400148,2.726541
447,1.3845196643\H,-2.7107999846,0.7951224591,1.9970837941\H,4.6273198
526,1.6578981134,0.7831704479\H,-1.2031257547,0.090430976,2.0936604825

\O,-4.3528115697,0.1251240068,0.2876355386\H,-2.5626800388,-0.84264646
26,1.8837482858\

TrpZ-c2-RAF-OH, (0,2):

\O,-3.516227285,1.6518393455,-0.543
3428452\N,1.9795536191,-1.9413270927,-0.0650185927\N,-2.1572907022,-1.
1529045904,1.2429011003\C,0.208672751,-0.6527554316,-0.4982267434\C,-1
.1900765388,-0.23378522,-0.8298288882\C,1.3238258259,0.1804605388,-0.2
216007483\C,-2.0456601013,0.0636514677,0.3995267018\C,2.4094860426,-0.
6451108274,0.0349508552\C,0.6578974899,-1.9508585075,-0.3900816481\C,1
.4560145152,1.6676116488,-0.211123899\C,3.7128222979,-0.1733355476,0.3
04715239\C,-3.4508936526,0.530449802,0.0058392611\C,2.8740822189,2.091
2291026,0.0387738838\C,3.8963234061,1.2245540532,0.293110493\H,-1.1782
839698,0.6728089585,-1.4367510748\H,-1.6812731299,-1.0130557634,-1.420
3015509\H,-1.5732427588,0.8327077821,1.0090867411\H,0.1279491104,-2.88
13852551,-0.5369703273\H,2.557101931,-2.7599709591,0.0571023068\H,1.11
66236204,2.0824207324,-1.1666730875\H,4.532624588,-0.8533040626,0.5020
140819\H,3.0556258673,3.1613832363,0.0396512106\H,-2.5609150476,-0.930
8031859,2.1543146582\H,4.8873258109,1.6213466772,0.4896149327\H,-1.239
8006193,-1.584443808,1.3854446123\O,-4.4034541694,-0.2442105946,0.2535
337076\H,-2.7822212351,-1.8270621057,0.7927992023\O,0.5819387532,2.290
6264664,0.7512495044\H,0.8300557721,1.9594379302,1.622416033\

TrpZ-c3-RAF-OH, (0,2):

\O,-3.4458952102,1.6536631496,-0.72
31457563\N,2.035015323,-1.9767104843,-0.2066620823\N,-2.0590756993,-0.
9241372649,1.355732286\C,0.1933664147,-0.7583584938,-0.5849838542\C,-1
.2151910924,-0.3676800729,-0.8905736389\C,1.2856859796,0.1354621415,-0
.2717688975\C,-1.967569729,0.1487767859,0.3337024095\C,2.411494155,-0.

6768009364,-0.0464698151\C,0.7010751311,-2.0216632169,-0.5298470146\C,
1.3876471557,1.5158575798,-0.1884577586\C,3.6928866367,-0.1365186554,0
.2720272725\C,-3.380493128,0.6101421861,-0.0378177556\C,2.6775974494,2
.1582041895,0.2078722415\C,3.82102751,1.1978004677,0.3733036621\H,-1.2
361199734,0.4295871539,-1.6362585587\H,-1.7573190696,-1.2200977349,-1.
3101213481\H,-1.4291282208,0.9801173562,0.7878299206\H,0.211627118,-2.
9690538824,-0.7069695302\H,2.6389592689,-2.779375254,-0.1111765634\H,0
.5384537625,2.1643998502,-0.3759533308\H,4.5415201267,-0.796624058,0.4
200986658\H,2.954097602,2.9195534938,-0.5299155956\H,-2.3285686033,-0.
5424236259,2.2639092751\H,4.7832950826,1.6402437873,0.6110120819\H,-1.
1658681223,-1.4140143068,1.4583557703\O,-4.3369050879,-0.0987469774,0.
3512477233\H,-2.7867023778,-1.590243851,1.0805507566\O,2.5109908111,2.
9319910946,1.4218398766\H,2.234699807,2.3206338089,2.1150618482\

TrpZ-c4-RAF-OH, (0,2):

\O,-3.4979022132,1.7139320282,-0.56
50519559\N,2.0064151576,-1.9922719326,-0.1776399483\N,-2.0747472642,-0
.9551444881,1.3364424984\C,0.2002384707,-0.7177354398,-0.5666736411\C,
-1.2052330765,-0.3123114397,-0.8773905848\C,1.2901811687,0.1322224845,
-0.2626715928\C,-1.9783741205,0.1540281269,0.3543580187\C,2.4217993997
, -0.6860333111,-0.0234808642\C,0.6802555521,-2.007763215,-0.5011613234
\C,1.4327152051,1.5590135675,-0.1783087996\C,3.6632720771,-0.192877632
7,0.2856086524\C,-3.3956641662,0.5861748971,-0.0370605533\C,2.62486673
73,2.0946627803,0.1278866267\C,3.8558423189,1.2831783164,0.4162417099\
H,-1.2145505823,0.5127965262,-1.5920187622\H,-1.7409641095,-1.14722991
11,-1.3378474349\H,-1.4628888939,0.9806817042,0.8409244769\H,0.1636851
519,-2.9409655397,-0.6766382999\H,2.5913985036,-2.807410998,-0.0763699
499\H,0.5748067946,2.1969794599,-0.3674247502\H,4.5170815953,-0.841083
2089,0.4495356576\H,2.7446104485,3.1717505316,0.1939945407\H,-2.318544

843,-0.6053424206,2.264484587\H,-1.1952388445,-1.474590313,1.404414515
6\O,-4.3168221496,-0.2367142987,0.1740706743\H,-2.8286293826,-1.583964
3655,1.0392118264\H,4.6567522954,1.6078113722,-0.2580592882\O,4.375582
5951,1.620389803,1.7222908018\H,3.7268186245,1.3287943566,2.3738059025
\

TrpZ-c5-RAF-OH, (0,2):

\O,-3.5754935369,1.5885206458,-0.70
74879598\N,1.993043561,-1.9628451693,-0.2235206357\N,-1.978008717,-0.8
645539052,1.3591741474\C,0.1806211146,-0.7255603485,-0.6173862528\C,-1
.2259449016,-0.3222042389,-0.9225381595\C,1.2751350858,0.1385017566,-0
.2733243666\C,-1.9695422427,0.186690127,0.3116256557\C,2.3699010314,-0
.6721908485,-0.0367513553\C,0.6673498433,-2.0019699374,-0.5674107814\C
,1.394913656,1.5540690228,-0.1713733726\C,3.7252947193,-0.1997586308,0
.3494228059\C,-3.417832393,0.5457403913,-0.0376854813\C,2.6489997099,2
.085303242,0.1815458367\C,3.741200816,1.2979037455,0.4200416704\H,-1.2
486224757,0.4794978751,-1.6629186021\H,-1.7732692007,-1.1706049214,-1.
3434518534\H,-1.4671029815,1.0595501441,0.7258347624\H,0.1721303621,-2
.943224537,-0.7585333049\H,2.5890875563,-2.7693347584,-0.1059843598\H,
0.5484554622,2.2046725257,-0.3571267291\H,2.7543411392,3.1623911177,0.
2681121962\H,-2.1105302649,-0.4624210115,2.2882016739\H,4.6908389637,1
.7477527175,0.69159167\H,-1.1037373371,-1.3990687882,1.3550515274\O,-4
.3085868427,-0.2463390861,0.349492427\H,-2.7739838001,-1.4869257376,1.
1792442696\H,4.4682671157,-0.5426888773,-0.3791929361\O,4.1718605544,-
0.7853989736,1.5858146372\H,3.5739623729,-0.4892873713,2.2829020005\

TrpZ-c8-RAF-OH, (0,2):

\O,-3.1572299054,2.1064374379,-
0.2327494351\N,2.0182265067,-2.0292941674,0.0609011642\N,-2.4638454767

, -1.1269074784, 1.1388053052\|C, 0.2348465125, -0.5994143627, -0.3469607238
 \|C, -1.1306032518, -0.1108529778, -0.6863941296\|C, 1.3966417281, 0.16488535
 79, -0.1841305101\|C, -2.0490547064, 0.1517369892, 0.510055525\|C, 2.48726002
 33, -0.725236104, 0.0023303888\|C, 0.6062146021, -2.0519364531, -0.233222251
 \|C, 1.632166469, 1.5502668224, -0.2191506744\|C, 3.7812723237, -0.2640562365
 , 0.1091369509\|C, -3.3087867121, 0.8989368832, 0.0482950286\|C, 2.9305391211
 , 2.0096135586, -0.0989661369\|C, 3.992677258, 1.1145902992, 0.0551646168\|H,
 -1.0438929693, 0.8341636878, -1.2262486035\|H, -1.6270075248, -0.8215850577
 , -1.3558679671\|H, -1.5330049919, 0.747166841, 1.2616319494\|H, 0.3817451404
 , -2.6072130082, -1.1486371011\|H, 2.5950306053, -2.7719246698, -0.307032899
 3\|H, 0.8066385944, 2.2417771239, -0.351314428\|H, 4.6112567467, -0.950945716
 5, 0.2342177981\|H, 3.1310334569, 3.0751510361, -0.1303070075\|H, -2.70476832
 82, -0.9917810012, 2.1212515639\|H, 5.0042024358, 1.4979064293, 0.1376341973
 \|H, -1.7223210303, -1.8466728555, 1.0684687387\|O, -4.3654333826, 0.23039301
 31, -0.0360249211\|H, -3.3136641808, -1.4433151218, 0.6568910262\|O, -0.13135
 26421, -2.7414727129, 0.7870654865\|H, 0.2477093983, -2.4782769662, 1.637017
 1688\|

TrpZ-c2-RAF-OOH, (0,2):

\|O, -3.5611090214, 1.6164848374, -0.58
 00191514\|N, 1.9835760812, -1.9650817205, -0.1286879408\|N, -2.1213967173, -1
 .0877099471, 1.2813164494\|C, 0.2066299137, -0.6716751089, -0.5209796468\|C,
 -1.1931219151, -0.254390654, -0.8473754301\|C, 1.3212575234, 0.1559292283, -
 0.2268093312\|C, -2.0392730796, 0.0867194877, 0.3774002462\|C, 2.4101754173,
 -0.6719295172, 0.0054359289\|C, 0.6606861982, -1.970004164, -0.4481549315\|C
 , 1.4560838754, 1.636127506, -0.1637941654\|C, 3.7133353934, -0.2011780591, 0
 .2776621775\|C, -3.4555938635, 0.4922200481, -0.0440270395\|C, 2.8705878768,
 2.0674256661, 0.0682180549\|C, 3.8966602209, 1.19624693, 0.288284794\|H, -1.1
 855846876, 0.632227277, -1.4839040438\|H, -1.6923465659, -1.0511727816, -1.4

066981676\H,-1.583948103,0.8983337406,0.9422416508\H,0.1324237971,-2.8
975484046,-0.6173906286\H,2.5662499414,-2.784246413,-0.0361676988\H,1.
0576019753,2.110098085,-1.0686826431\H,4.5362918116,-0.8835969097,0.45
19202115\H,3.0485470416,3.1377102788,0.0833821345\H,-2.5207966623,-0.8
252378727,2.1843049232\H,4.8914216021,1.5895951987,0.4717208347\H,-1.1
974945748,-1.499728516,1.4383484201\O,-4.3716274433,-0.3386507057,0.15
54484161\H,-2.7427662895,-1.7896502697,0.8690019716\O,0.5781808179,2.2
281962778,0.8312506724\O,0.9180432278,1.7392652581,2.1101229717\H,0.36
9251808,0.9450117744,2.2000687312\

TrpZ-c3-RAF-OOH, (0,2):

\O,-3.4785777451,1.6794092459,-0.64
27724088\N,2.017661098,-1.9862269397,-0.1886897326\N,-2.0531778497,-0.
9419372164,1.337115962\C,0.1865478143,-0.7599549742,-0.591261942\C,-1.
2189264143,-0.3614873106,-0.9007431154\C,1.2829364554,0.1287785676,-0.
2808770301\C,-1.972039305,0.142902697,0.3286959842\C,2.4035979422,-0.6
886139803,-0.0428254224\C,0.6840365232,-2.0261556979,-0.5151724727\C,1
.3948714718,1.508200274,-0.2169449939\C,3.6931804132,-0.1546643543,0.2
511341671\C,-3.3906041475,0.5857610325,-0.0439213118\C,2.6865491283,2.
1322117978,0.1848111689\C,3.8308886857,1.1789998446,0.3416167372\H,-1.
2346248484,0.4430314961,-1.6387151595\H,-1.7628277741,-1.2083984204,-1
.329146206\H,-1.4399682,0.975085446,0.7877464672\H,0.1880716329,-2.972
2651043,-0.6800992301\H,2.6152807912,-2.7924333148,-0.0821293069\H,0.5
561826374,2.1632635322,-0.427253164\H,4.5409750086,-0.8186107631,0.384
8977658\H,2.9606666879,2.9340947219,-0.5114289713\H,-2.3067970611,-0.5
752986451,2.2559986193\H,4.7983297108,1.6201548843,0.5578294028\H,-1.1
605793067,-1.43779055,1.4164917472\O,-4.326923879,-0.1921383621,0.2513
309385\H,-2.7890604641,-1.5980032742,1.0571777536\O,2.5278153272,2.926
5308657,1.401610405\O,2.196755269,2.0767556091,2.4793031989\H,1.229885

3079,2.0275662727,2.4396061196\

TrpZ-c4-RAF-OOH, (0,2):

\O,-3.5040294176,1.6623777052,-0.67

9876106\N,2.0051000228,-2.0091465006,-0.264726966\N,-2.0274731833,-0.8
84153564,1.3600091937\C,0.1831183537,-0.7456192329,-0.6163150777\C,-1.
2295056056,-0.3518470032,-0.9107739001\C,1.2635490319,0.1089858081,-0.
2934923177\C,-1.9679130366,0.1719456265,0.3182743896\C,2.4045162485,-0.
.7036601847,-0.0734322928\C,0.6784287611,-2.0313287397,-0.5828585891\C
,1.3926856148,1.5355872268,-0.1907243549\C,3.639283508,-0.2044181912,0
.2481607379\C,-3.3971139012,0.5934698789,-0.0414619992\C,2.5746029498,
2.0779795594,0.1401901233\C,3.7984447766,1.2649334157,0.4319356791\H,-
1.2574453266,0.4404636384,-1.6609820892\H,-1.7759879974,-1.2066792847,
-1.3192516453\H,-1.43874582,1.0215801501,0.7477314676\H,0.1702085935,-
2.9654991613,-0.7757673407\H,2.5988563201,-2.8199767566,-0.1797570041\
H,0.5331737592,2.1682891835,-0.3893613532\H,4.5042197021,-0.8433012295
,0.3878638914\H,2.6873319884,3.1545253734,0.220239115\H,-2.2655548797,
-0.4862092712,2.2699343852\H,-1.1350611012,-1.3782357563,1.4439471655\
O,-4.3224923918,-0.1750122425,0.3081778172\H,-2.7704374503,-1.54670558
41,1.1156123471\H,4.6393589311,1.6359661087,-0.1670709861\O,4.30509708
39,1.5741846203,1.7630480006\O,3.3454492286,1.2068613569,2.7305931484\
H,3.5678150574,0.2851762307,2.9307753703\

TrpZ-c5-RAF-OOH, (0,2):

\O,-3.5544147408,1.5774346479,-0.76

60640631\N,1.9987468743,-1.9519181552,-0.2466660967\N,-1.9920858995,-0
.8627028455,1.3577867192\C,0.1717211692,-0.7302182414,-0.6259502848\C,
-1.2393843509,-0.3379614154,-0.9262479242\C,1.2608916757,0.1433174486,
-0.2892931728\C,-1.9805174198,0.1821076387,0.3034877673\C,2.3638850906

, -0.6584759845, -0.0620488\C, 0.6710108611, -2.0017308274, -0.5795260215\C
, 1.3723330495, 1.5588927625, -0.1908555855\C, 3.7058810625, -0.1674963139,
0.3278832835\C, -3.4222991025, 0.5685138989, -0.0396414495\C, 2.6281513601
, 2.1035780348, 0.1343444913\C, 3.7288216336, 1.327156951, 0.3670988968\H, -
1.2698182484, 0.4544456612, -1.6760876205\H, -1.7846371145, -1.1939365362,
-1.3346056701\H, -1.4668101839, 1.0492053294, 0.7176554097\H, 0.1832963911
, -2.94711619, -0.7691105047\H, 2.60189751, -2.7538819213, -0.1331810484\H,
0.5193346181, 2.2028854021, -0.3700651394\H, 2.7291088205, 3.1826943746, 0.
195740517\H, -2.2929900092, -0.477594159, 2.254720093\H, 4.6823098206, 1.78
4772992, 0.610225965\H, -1.0622894908, -1.2765488428, 1.4713148548\O, -4.33
43963675, -0.1607177491, 0.4129011996\H, -2.6603891938, -1.5954145683, 1.10
34303637\H, 4.4845481701, -0.549502289, -0.3430660275\O, 4.1541640018, -0.7
410891157, 1.5835187711\O, 3.2454833185, -0.3992727577, 2.608263365\H, 3.62
94834443, 0.4029830807, 2.9927595217\

TrpZ-c8-RAF-OOH, (0,2):

\O, -3.3883895377, 1.6621169173, -0.84
67662164\N, 2.1523963269, -2.0314667661, -0.1380513687\N, -2.1083904864, -0.
.7546056657, 1.4649985753\C, 0.2361704945, -0.76379133, -0.4850412211\C, -1
.1772240888, -0.4198614717, -0.8054330229\C, 1.294159082, 0.0990762929, -0.
1634472575\C, -1.9551165235, 0.2111205387, 0.3495362678\C, 2.4655622046, -0
.6843393745, 0.0032494377\C, 0.7828344279, -2.1590783663, -0.558841436\C, 1
.3780132731, 1.4968218505, -0.0360402364\C, 3.6888433602, -0.1088925707, 0.
2670861285\C, -3.3496701417, 0.6435004168, -0.1240132418\C, 2.6052582134, 2
.0709164583, 0.2374078849\C, 3.7474734696, 1.2801042405, 0.3835302303\H, -1
.200037144, 0.3037059383, -1.625539734\H, -1.7092535563, -1.3116921223, -1.
1486358385\H, -1.4276484208, 1.0798115282, 0.7397172651\H, 0.6785346843, -2
.611624943, -1.5513633942\H, 2.8364468761, -2.6399647628, -0.5654385179\H,
0.4957328729, 2.1136343355, -0.1678412788\H, 4.5798077677, -0.7167084745, 0

.380128198\H,2.6862756706,3.1483824047,0.3313279283\H,-2.3397895281,-0
.2699353362,2.3334096573\H,4.7008754045,1.7540135586,0.5912910313\H,-1
.2583797037,-1.3194279838,1.6174793163\O,-4.3165158048,-0.0691527633,0
.2310538411\H,-2.8972110498,-1.3722385923,1.2474755334\O,0.0720727317,
-3.1168881367,0.2417216474\O,0.040608206,-2.6800428401,1.5815605611\H,
0.9680451698,-2.7285350107,1.86863601\