Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials for "Excited-State Intramolecular Proton Transfer to Carbon Atoms: Nonadiabatic Surface-Hopping Dynamics Simulations"

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1. OM2/MRCI Active Space

The active space in the MRCI calculations included 12 electrons in 10 orbitals. Figure 1 shows the active orbitals for the most stable ground-state conformer of 2-phenylphenol (enol form).

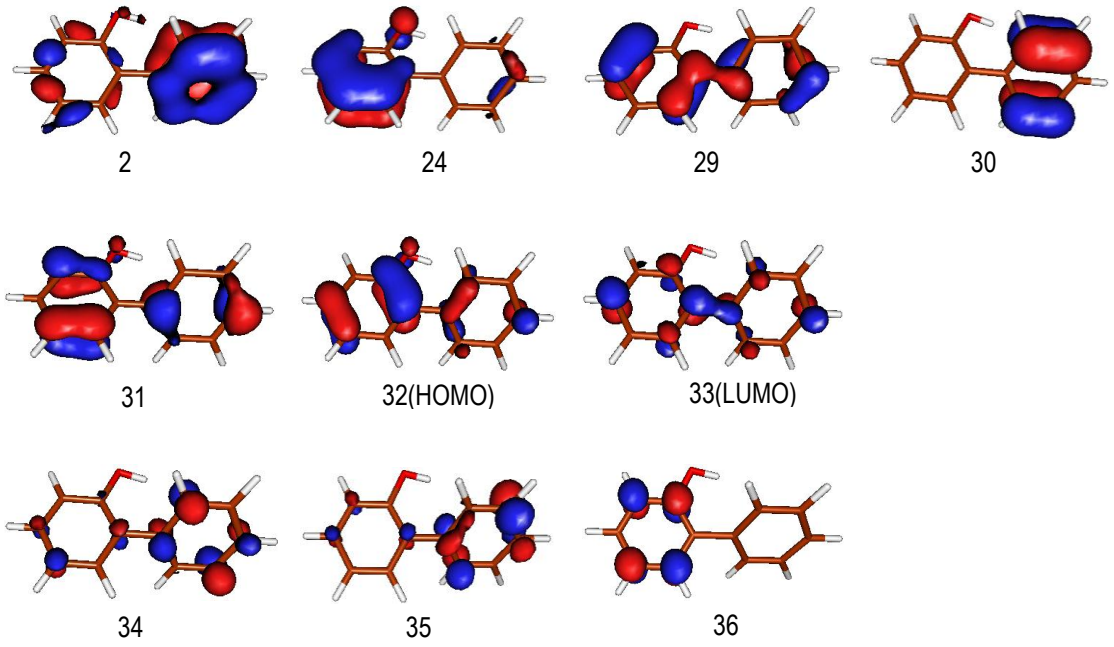

Figure 1: The active space (12e,10o) of 2-phenylphenol (enol form) used in the OM2/MRCI calculations. All orbitals are of p type. See text for simulation details.

2. Cartesian Coordinates of All CASSCF Optimized Structures

S0-MIN-ENOL

C	2.247076000	-1.379371000	-0.375939000
C	0.851273000	-1.346981000	-0.362204000
C	0.155628000	-0.312044000	0.252544000
C	0.899676000	0.706895000	0.881791000
C	2.274255000	0.676363000	0.869847000
C	2.947127000	-0.368518000	0.236092000
H	2.761834000	-2.186439000	-0.864749000
H	0.293875000	-2.127410000	-0.849032000
H	2.811365000	1.465863000	1.361885000
H	4.022607000	-0.375526000	0.235290000
C	-1.339402000	-0.291648000	0.255267000
C	-2.066600000	-1.318652000	0.865618000

C	-2.046820000	0.747186000	-0.364017000
C	-3.460044000	-1.307367000	0.853413000
H	-1.540529000	-2.119626000	1.353261000
C	-3.427630000	0.761352000	-0.370315000
H	-0.633186000	1.621198000	1.552485000
H	-1.503013000	1.535760000	-0.854411000
C	-4.143646000	-0.263828000	0.236253000
H	-4.005049000	-2.103960000	1.327425000
H	-3.949504000	1.566968000	-0.855471000
H	-5.218669000	-0.250876000	0.227824000
O	0.306630000	1.739512000	1.519984000

S0-MIN-KETO

C	2.636369000	-1.636130000	0.002355000
C	1.290697000	-1.532719000	0.002364000
C	0.589882000	-0.239439000	-0.000058000
C	1.464464000	0.972493000	-0.001564000
C	2.926947000	0.768671000	-0.002203000
C	3.472792000	-0.441906000	-0.000523000
H	3.106257000	-2.602447000	0.005003000
H	0.720935000	-2.438279000	0.005680000
H	3.516403000	1.666902000	-0.004150000
H	4.542401000	-0.558641000	-0.001072000
C	-0.769438000	-0.145502000	-0.001004000
C	-1.625834000	-1.338215000	-0.003671000
C	-1.489463000	1.195149000	-0.000051000
C	-2.956446000	-1.272819000	-0.001914000
H	-1.173007000	-2.307100000	-0.008094000
C	-2.991470000	1.143726000	0.003539000
H	-1.152635000	1.776624000	0.851636000
H	-1.156438000	1.775795000	-0.853955000
C	-3.683503000	-0.003527000	0.002966000
H	-3.525253000	-2.186034000	-0.004456000
H	-3.498532000	2.092720000	0.006496000
H	-4.758040000	-0.015747000	0.005577000
O	1.036112000	2.114502000	-0.002856000

S1-MIN-ENOL

C	-1.334620000	-1.395000000	0.380958000
C	-2.710631000	-1.489614000	0.430285000
C	-3.477868000	-0.375109000	0.120792000
C	-2.868751000	0.808946000	-0.240620000
C	-1.484035000	0.895063000	-0.289936000
C	-0.687736000	-0.206793000	0.033545000
H	-0.734612000	-2.250223000	0.635883000
H	-3.179215000	-2.414880000	0.712025000
O	-0.969737000	2.084731000	-0.675410000
H	-0.036135000	2.017996000	-0.821534000
C	0.793330000	-0.139474000	0.011465000
C	1.561573000	-1.168153000	-0.644990000
C	1.505642000	0.909116000	0.706379000
C	2.995093000	-1.138184000	-0.629974000
H	1.050116000	-1.936618000	-1.191825000
C	2.939341000	0.926502000	0.731514000

H	0.956465000	1.630632000	1.281212000
C	3.684691000	-0.091203000	0.057520000
H	3.548040000	-1.900688000	-1.144249000
H	3.450359000	1.700984000	1.270786000
H	4.757587000	-0.071820000	0.073454000
H	-3.443376000	1.678577000	-0.500206000
H	-4.551289000	-0.430523000	0.155096000

S1-MIN-KETO

C	-0.571650000	1.850610000	0.000000000
C	-1.768590000	2.655780000	0.000000000
C	-2.953700000	1.999930000	0.000000000
C	-2.989250000	0.583290000	0.000000000
C	-1.806130000	-0.245300000	0.000000000
C	-0.541700000	0.483240000	0.000000000
H	0.347440000	2.401530000	0.000000000
H	-1.690180000	3.725090000	0.000000000
H	-3.884450000	2.541000000	0.000000000
H	-3.927450000	0.061640000	0.000000000
C	3.221320000	-0.162030000	0.000000000
C	1.948730000	0.479170000	0.000000000
C	0.769880000	-0.202930000	0.000000000
C	0.823520000	-1.712830000	0.000000000
C	2.195500000	-2.321360000	0.000000000
C	3.336280000	-1.564690000	0.000000000
H	4.100020000	0.459410000	0.000000000
H	1.971180000	1.545590000	0.000000000
H	0.262420000	-2.079450000	0.851010000
H	2.247050000	-3.394940000	0.000000000
H	4.307280000	-2.025600000	0.000000000
O	-1.918710000	-1.467850000	0.000000000
H	0.262420000	-2.079450000	-0.851010000

S1S0-MIN-ENOL

C	2.034366000	-0.546642000	-0.802185000
C	0.928429000	-1.316095000	-0.584288000
C	0.030816000	-0.982351000	0.528773000
C	0.832059000	-0.290527000	1.501366000
C	1.554704000	0.924357000	1.104621000
C	2.236065000	0.687250000	-0.020853000
H	2.708959000	-0.753400000	-1.612868000
H	0.662106000	-2.087319000	-1.288098000
H	1.641093000	1.810241000	1.704231000
H	2.945921000	1.411208000	-0.383575000
C	-1.330293000	-0.509707000	0.288241000
C	-2.099749000	-0.001014000	1.323803000
C	-1.938606000	-0.570629000	-0.997030000
C	-3.402252000	0.469787000	1.110292000
H	-1.703714000	0.013521000	2.325401000
C	-3.228971000	-0.134800000	-1.193850000
H	0.908234000	-1.801854000	2.528395000
H	-1.376530000	-0.943028000	-1.833150000
C	-3.975967000	0.405403000	-0.129605000
H	-3.955842000	0.869546000	1.942339000

H	-3.662343000	-0.188550000	-2.177406000
H	-4.979526000	0.754893000	-0.292873000
O	1.332040000	-0.942176000	2.509151000

S1S0-MIN-KETO

C	2.348163000	-1.237512000	-0.494777000
C	0.945987000	-1.331061000	-0.537832000
C	0.168671000	-0.471189000	0.208431000
C	0.750684000	0.615119000	0.983736000
C	2.162019000	0.662655000	0.993697000
C	2.923998000	-0.252719000	0.277504000
H	2.953655000	-1.936302000	-1.042091000
H	0.479010000	-2.094810000	-1.136842000
H	2.629082000	1.419330000	1.597003000
H	3.997407000	-0.181251000	0.326245000
C	-1.303905000	-0.450708000	0.206646000
C	-2.101124000	-1.327838000	0.925189000
C	-1.911067000	0.759904000	-0.361063000
C	-3.486799000	-1.154355000	0.948504000
H	-1.653738000	-2.159184000	1.436253000
C	-3.367114000	0.854861000	-0.349664000
H	-1.460662000	1.475700000	0.411039000
H	-1.441106000	1.100126000	-1.279202000
C	-4.118833000	-0.057465000	0.303066000
H	-4.096984000	-1.874527000	1.462692000
H	-3.831172000	1.679130000	-0.860535000
H	-5.189347000	0.025864000	0.332579000
O	0.000590000	1.445393000	1.551834000

3. Cartesian Coordinates of All OM2/MRCI Optimized Structures

S0-MIN-ENOL

C	2.233181488	-1.434832090	-0.309958375
C	0.841130539	-1.420865118	-0.318199376
C	0.148265228	-0.338322390	0.238273365
C	0.883538713	0.717526279	0.810409952
C	2.283492275	0.708361385	0.836239291
C	2.946272090	-0.375298200	0.260726261
H	2.771937520	-2.271712090	-0.761766980
H	0.281881938	-2.243444371	-0.776811218
H	2.819481279	1.535519212	1.297716540
H	4.042653673	-0.397655542	0.262798402
C	-1.332271370	-0.300562500	0.229994224
C	-2.052690123	-1.392698819	0.730152872
C	-1.997859343	0.819774301	-0.285552347
C	-3.445979821	-1.355810677	0.726221269
H	-1.523188939	-2.261834832	1.130990008
C	-3.392758788	0.840524466	-0.294860730
H	-0.675514671	1.634948874	1.479617048
H	-1.433614904	1.656800276	-0.704447224
C	-4.113299475	-0.240227210	0.215671020
H	-4.018160709	-2.196383738	1.132042424

H	-3.923186760	1.702524940	-0.712750496
H	-5.208912970	-0.215822547	0.211950354
O	0.295676462	1.814125984	1.366710498

S0-MIN-KETO

C	2.234831063	-1.620625751	0.427249410
C	0.870278166	-1.587304063	0.330849045
C	0.146688464	-0.345260813	0.329313176
C	0.929815532	0.894655874	0.435606038
C	2.379843355	0.798310173	0.535581760
C	2.998494233	-0.414846548	0.530782528
H	2.769394667	-2.576192999	0.426849780
H	0.316931858	-2.533810898	0.252887517
H	2.933186404	1.735444717	0.613161715
H	4.090405560	-0.495571614	0.605734869
C	-1.243804826	-0.277387012	0.232458794
C	-2.050739322	-1.460856635	0.126742256
C	-1.914924533	1.055685303	0.238350567
C	-3.407851613	-1.394202524	0.032217906
H	-1.560591119	-2.442431650	0.122118021
C	-3.390106323	1.017660543	0.131130246
H	-1.635761777	1.588774066	1.177098765
H	-1.508091769	1.660915254	-0.605188469
C	-4.094577091	-0.136289274	0.033942108
H	-4.008130506	-2.310547476	-0.047887465
H	-3.900021680	1.990109258	0.133954815
H	-5.185701905	-0.138280011	-0.044316321
O	0.378648659	2.014917428	0.441472257

S1S0-MIN-ENOL

C	2.218371920	-0.682369648	-0.606279572
C	0.878496240	-1.069619100	-0.585469549
C	-0.014355023	-0.484965374	0.347585190
C	0.845876431	0.076988035	1.350448578
C	1.889222890	1.023184209	1.116927092
C	2.692509643	0.407882456	0.153733533
H	2.890141048	-1.135920812	-1.333951767
H	0.478336092	-1.749208482	-1.345485017
H	2.038644451	1.977922228	1.571419045
H	3.669216311	0.849821554	-0.073746761
C	-1.436605443	-0.252857838	0.184465272
C	-2.204095211	0.077281404	1.315117297
C	-2.054923364	-0.390143740	-1.067782570
C	-3.577131089	0.263322597	1.183735297
H	-1.722061893	0.197975811	2.291470989
C	-3.432740834	-0.227742224	-1.178010495
H	0.780685224	-1.704128989	2.210171599
H	-1.457630754	-0.638730875	-1.950795830
C	-4.195509956	0.108433430	-0.057720046
H	-4.175889051	0.538538983	2.060504270
H	-3.920300694	-0.348372590	-2.152611911
H	-5.274986221	0.261787534	-0.156941709
O	1.245727076	-0.820964679	2.274046772

S1S0-MIN-KETO

C	2.303638811	-1.188786733	-0.603407858
C	0.911587269	-1.308035266	-0.629315968
C	0.135789175	-0.528632961	0.215712011
C	0.757879029	0.522107896	1.028034096
C	2.194964918	0.625967906	0.998297059
C	2.934993196	-0.244839424	0.222182890
H	2.915879407	-1.849866908	-1.227204388
H	0.436169213	-2.042191754	-1.285474207
H	2.666032344	1.338631413	1.675762041
H	4.029692392	-0.196526865	0.235611404
C	-1.326746575	-0.465811079	0.198778027
C	-2.132158968	-1.374417493	0.856486908
C	-1.845954679	0.831032917	-0.307840138
C	-3.518880317	-1.184580758	0.880671071
H	-1.696074864	-2.271612520	1.308688709
C	-3.311389701	0.891518202	-0.341503754
H	-1.438133472	1.576956523	0.464996206
H	-1.398114373	1.103503333	-1.294264637
C	-4.096826655	-0.075315167	0.237302008
H	-4.162515803	-1.905259561	1.396039688
H	-3.768560204	1.742278341	-0.861381697
H	-5.189435503	-0.001476614	0.188453755
O	0.015671043	1.366096439	1.584066290

4. Cartesian Coordinates of All DFT Optimized Structures

S0-MIN-ENOL

C	-2.729334000	-1.488049000	0.399605000
C	-1.338959000	-1.413315000	0.376705000
C	-0.668865000	-0.219029000	0.066533000
C	-1.449008000	0.915577000	-0.246349000
C	-2.845558000	0.845187000	-0.225680000
C	-3.481378000	-0.349084000	0.100033000
H	-3.220583000	-2.422226000	0.655352000
H	-0.744849000	-2.288425000	0.627133000
H	-3.409469000	1.737892000	-0.477845000
H	-4.567246000	-0.390395000	0.115925000
C	0.818310000	-0.165737000	0.050199000
C	1.560664000	-1.133387000	-0.649301000
C	1.522999000	0.837886000	0.742316000
C	2.954019000	-1.101993000	-0.654776000
H	1.032719000	-1.905876000	-1.201610000
C	2.918781000	0.872574000	0.729870000
H	0.062253000	2.009088000	-0.679282000
H	0.972686000	1.572248000	1.325499000
C	3.639293000	-0.096310000	0.031264000
H	3.506961000	-1.859922000	-1.203550000
H	3.441465000	1.651740000	1.278421000
H	4.725459000	-0.070452000	0.022501000
O	-0.900648000	2.117552000	-0.598133000

S0-MIN-KETO

C	-1.387645000	-1.478392000	0.000001000
C	-2.749692000	-1.529477000	0.000002000
C	-3.521712000	-0.320532000	0.000000000
C	-2.909874000	0.892908000	-0.000001000
C	-1.456387000	1.027562000	-0.000002000
C	-0.659298000	-0.232736000	0.000000000
H	-0.843561000	-2.416068000	0.000003000
H	-3.258735000	-2.488967000	0.000003000
H	-4.607607000	-0.387195000	0.000000000
H	-3.468274000	1.824026000	-0.000003000
C	2.914273000	-1.347586000	-0.000002000
C	1.549496000	-1.383096000	-0.000002000
C	0.745367000	-0.190948000	0.000000000
C	1.493215000	1.123289000	0.000001000
C	2.982131000	1.056458000	0.000001000
C	3.655288000	-0.111068000	0.000000000
H	3.464923000	-2.285172000	-0.000003000
H	1.068808000	-2.353474000	-0.000003000
H	1.139047000	1.743470000	-0.839962000
H	3.512140000	2.006117000	0.000002000
H	4.741116000	-0.140456000	0.000000000
O	-0.933994000	2.159946000	-0.000003000
H	1.139047000	1.743468000	0.839966000

5. Cartesian Coordinates of All RI-ADC(2) Optimized Structures

C7H10 distance: 1.1

C	-1.355783000	-1.267178000	0.746064100
C	-2.767936200	-1.351759800	0.738585500
C	-3.544567200	-0.412365000	0.058358800
C	-2.911983100	0.624290400	-0.623347900
C	-1.488690600	0.755073100	-0.628917100
C	-0.705780100	-0.264926000	0.045464800
H	-0.763828800	-2.016933000	1.274093900
H	-3.252358900	-2.167025400	1.279654600
O	-0.928358700	1.750540000	-1.200559500
H	1.053863200	1.860440400	0.258556900
C	0.759846100	-0.179656500	-0.012537100
C	1.487240700	-0.968571800	-0.865957600
C	1.400790600	0.938579500	0.748507600
C	2.900292400	-0.881697300	-0.925707600
H	0.964228300	-1.711145500	-1.476028200
C	2.889489100	0.883843100	0.752642200
H	0.990036800	1.001596500	1.775442800
C	3.575935200	0.046814100	-0.086884500
H	3.464171700	-1.542677200	-1.588797700
H	3.433669900	1.581547800	1.395429700
H	4.668684800	0.071013000	-0.090560000
H	-3.471797100	1.387937100	-1.166044200

H	-4.632933600	-0.493472400	0.054711000

C7H10 distance: 1.2

C	-1.357089100	-1.269100600	0.723287100
C	-2.767265300	-1.378306200	0.674188500
C	-3.541001600	-0.424561000	0.014787400
C	-2.907105600	0.655295600	-0.599096000
C	-1.487696200	0.798770400	-0.578714200
C	-0.706824300	-0.236182300	0.070702300
H	-0.761232900	-2.031136800	1.228580900
H	-3.248180900	-2.232658200	1.154728400
O	-0.929501900	1.818228100	-1.118015800
H	1.060312100	1.936784900	0.171193300
C	0.760461900	-0.164592700	0.015804200
C	1.470015600	-0.979636500	-0.827107000
C	1.422794700	0.950813000	0.750497300
C	2.884286400	-0.914258800	-0.895157100
H	0.930836700	-1.728880600	-1.414536600
C	2.904159400	0.869961200	0.763347200
H	0.994418200	1.085903400	1.761434300
C	3.576734900	0.013370300	-0.073344900
H	3.434456800	-1.596111100	-1.548083700
H	3.459243600	1.555303500	1.410091400
H	4.669890100	0.010493400	-0.074097400
H	-3.470611700	1.431685900	-1.119752100
H	-4.626869400	-0.526918000	-0.028567200

C7H10 distance: 1.3

C	-1.354019700	-1.329581100	0.653774900
C	-2.765695800	-1.419319200	0.614512800
C	-3.535185900	-0.409828600	0.042310400
C	-2.892723300	0.704367600	-0.503897800
C	-1.475542900	0.818459100	-0.504539600
C	-0.699483100	-0.259693000	0.068189100
H	-0.763672400	-2.129408600	1.105531600
H	-3.250795700	-2.298149300	1.042867200
O	-0.914640900	1.861667100	-1.018233500
H	0.974483800	1.948783000	-0.024697300
C	0.768240400	-0.192333400	0.021691700
C	1.492968200	-1.035410400	-0.780213700
C	1.409313700	0.962829300	0.695104700
C	2.907708400	-0.953731200	-0.838293800
H	0.971578800	-1.817927100	-1.340524900
C	2.882096700	0.917205300	0.723088300
H	0.951717000	1.196643100	1.673249900
C	3.575612500	0.025946200	-0.064285400
H	3.471848300	-1.665385900	-1.445783100
H	3.420254700	1.641300500	1.340990300
H	4.668700800	0.044002200	-0.058268100
H	-3.454360100	1.518058200	-0.965608700
H	-4.624171500	-0.484228000	0.025205300

C7H10 distance: 1.4

C	-1.353915300	-1.384663400	0.554888400

C	-2.765635200	-1.457230900	0.524074600
C	-3.529780000	-0.390310400	0.062017100
C	-2.881269400	0.765623000	-0.381608400
C	-1.467147000	0.843920100	-0.425612800
C	-0.692344200	-0.268625700	0.066311700
H	-0.765780000	-2.220283000	0.940026700
H	-3.256827800	-2.367792600	0.873915300
O	-0.916383300	1.905280800	-0.939460500
H	0.916384000	1.954744700	-0.227768500
C	0.774533900	-0.204136400	0.031863400
C	1.512201000	-1.089966200	-0.713945400
C	1.406378200	0.977821100	0.646260100
C	2.924313300	-0.997584500	-0.770594900
H	0.998924000	-1.898365800	-1.243934900
C	2.867387300	0.943696000	0.701085400
H	0.910301700	1.321762500	1.569789400
C	3.575971900	0.021151500	-0.039794200
H	3.499130400	-1.728261700	-1.342778400
H	3.394631900	1.694217700	1.294347500
H	4.668821900	0.044361100	-0.015049500
H	-3.437117500	1.626961500	-0.755254900
H	-4.618547800	-0.448052800	0.053393400

C7H10 distance: 1.5

C	-1.358144400	-1.408695900	0.502594900
C	-2.770540800	-1.475297200	0.497464300
C	-3.538422100	-0.392141600	0.079748600
C	-2.887172900	0.774385400	-0.334891700
C	-1.472553900	0.845114800	-0.395945600
C	-0.691244000	-0.276208900	0.055561500
H	-0.778110200	-2.263647000	0.853807300
H	-3.259743000	-2.393000700	0.834333700
O	-0.937610500	1.921295200	-0.906614800
H	0.920290300	2.015988500	-0.334763000
C	0.779315200	-0.197072900	0.027473000
C	1.524803500	-1.103182400	-0.694464500
C	1.418731900	0.979425500	0.627177200
C	2.935363600	-1.018291000	-0.737527000
H	1.006538600	-1.923137600	-1.203316300
C	2.871789900	0.948477400	0.698428800
H	0.902898200	1.398370900	1.504507500
C	3.586435000	0.007349000	-0.018285100
H	3.509026900	-1.752468000	-1.304675600
H	3.389539500	1.720348700	1.275590100
H	4.679551900	0.029707700	0.013450800
H	-3.438804400	1.652968600	-0.673959700
H	-4.627706300	-0.446022000	0.096476000

C7H10 distance: 1.6

C	-1.412439400	-1.545439900	0.199495000
C	-2.809018900	-1.481351900	0.219200900
C	-3.513334000	-0.261308200	0.063061300
C	-2.791417800	0.913147900	-0.102932600
C	-1.376875900	0.860907600	-0.186509000
C	-0.634191600	-0.374656900	0.082296500

H	-0.911851500	-2.500027100	0.366361800
H	-3.375435300	-2.403433700	0.363902500
O	-0.743006300	1.931533000	-0.581909600
H	0.344221500	1.769774500	-0.340426100
C	0.791629400	-0.295469000	0.154463000
C	1.626816400	-1.320795100	-0.355066900
C	1.387829200	0.984909800	0.583921500
C	2.992608900	-1.127114800	-0.500843500
H	1.176419600	-2.257549400	-0.697781300
C	2.807257300	1.126970300	0.424749800
H	0.944247400	1.460021500	1.476399700
C	3.577039600	0.128457900	-0.132221900
H	3.619629800	-1.919462500	-0.913867600
H	3.285851600	2.045904400	0.774341700
H	4.652239600	0.276574800	-0.257314400
H	-3.270642500	1.880117000	-0.268114300
H	-4.603345300	-0.247443400	0.090963900

C7H10 distance: 1.7

C	-1.402258400	-1.548145000	0.159770200
C	-2.801789000	-1.484355700	0.204117000
C	-3.513492200	-0.263476900	0.096497400
C	-2.794346100	0.921144900	-0.063953900
C	-1.386612600	0.865040200	-0.172254500
C	-0.627603400	-0.368228500	0.071031200
H	-0.896983900	-2.503681400	0.304842500
H	-3.362275800	-2.413482800	0.327875400
O	-0.753624500	1.942661600	-0.578890200
H	0.275511900	1.776443800	-0.415459400
C	0.790911700	-0.280369100	0.133937000
C	1.633048000	-1.319644000	-0.357407100
C	1.406137900	0.976534100	0.570256200
C	2.999077800	-1.140385400	-0.472662100
H	1.178445400	-2.253152900	-0.699912300
C	2.813887300	1.116625300	0.434893100
H	0.914217200	1.539822600	1.376220400
C	3.592306600	0.110524000	-0.108844700
H	3.623127200	-1.948688700	-0.859134100
H	3.290372900	2.034433800	0.790995900
H	4.669226500	0.249492400	-0.220685900
H	-3.280971400	1.887312600	-0.208601000
H	-4.602081200	-0.252158100	0.149539200

C7H10 distance: 1.8

C	-1.399895900	-1.549158100	0.146741100
C	-2.805872900	-1.483417500	0.205941000
C	-3.524826600	-0.267949700	0.109276500
C	-2.799949700	0.922318000	-0.057010100
C	-1.394426200	0.864050800	-0.147730100
C	-0.622623600	-0.363294300	0.094235500
H	-0.899295700	-2.510297100	0.269265700
H	-3.361526600	-2.416273000	0.322721800
O	-0.764658300	1.949810600	-0.561474100
H	0.234413100	1.777067400	-0.461175700
C	0.794682900	-0.271241500	0.143544600

C	1.637508200	-1.317447300	-0.348572900
C	1.434412300	0.953348100	0.597800000
C	3.001481800	-1.136087100	-0.471880500
H	1.182276500	-2.250716300	-0.689359700
C	2.827193300	1.105134200	0.452752300
H	0.910140200	1.596658800	1.313949900
C	3.607907500	0.100690600	-0.106997100
H	3.618411100	-1.944390600	-0.870871500
H	3.301636300	2.020346300	0.817855700
H	4.683757300	0.238799200	-0.226575400
H	-3.283058400	1.885842700	-0.228400700
H	-4.613454700	-0.259527300	0.158133800

C7H10 distance: 1.9

C	-1.383005600	-1.538855100	0.129977900
C	-2.793474800	-1.491030300	0.208833900
C	-3.531925600	-0.287755300	0.128040500
C	-2.820265400	0.916258000	-0.039053900
C	-1.414930800	0.875502500	-0.137911700
C	-0.620270300	-0.338357600	0.087462800
H	-0.871983500	-2.494680300	0.248138500
H	-3.334000400	-2.433322900	0.323626700
O	-0.810068200	1.982490400	-0.548176400
H	0.176573600	1.816515300	-0.520940200
C	0.798306400	-0.239894200	0.114454400
C	1.630676700	-1.302083800	-0.364920500
C	1.460241100	0.957183100	0.585290900
C	3.001121800	-1.147919100	-0.462308200
H	1.163305700	-2.223910700	-0.718421900
C	2.850751000	1.087714100	0.467551300
H	0.918626500	1.663679300	1.222135700
C	3.628340500	0.064494000	-0.074581400
H	3.606210000	-1.968477900	-0.855203600
H	3.333044800	1.990837100	0.850770900
H	4.710557800	0.176494000	-0.160155400
H	-3.313866900	1.874188800	-0.208999800
H	-4.619732500	-0.294802900	0.186559800