

Supplementary Material

Complexes between 2,2'-azobis(2-methylpropionamide)
dihydrochloride (AAPH) and cucurbit[n]uril hosts modulate the yield
and fate of photolytically generated AAPH radicals

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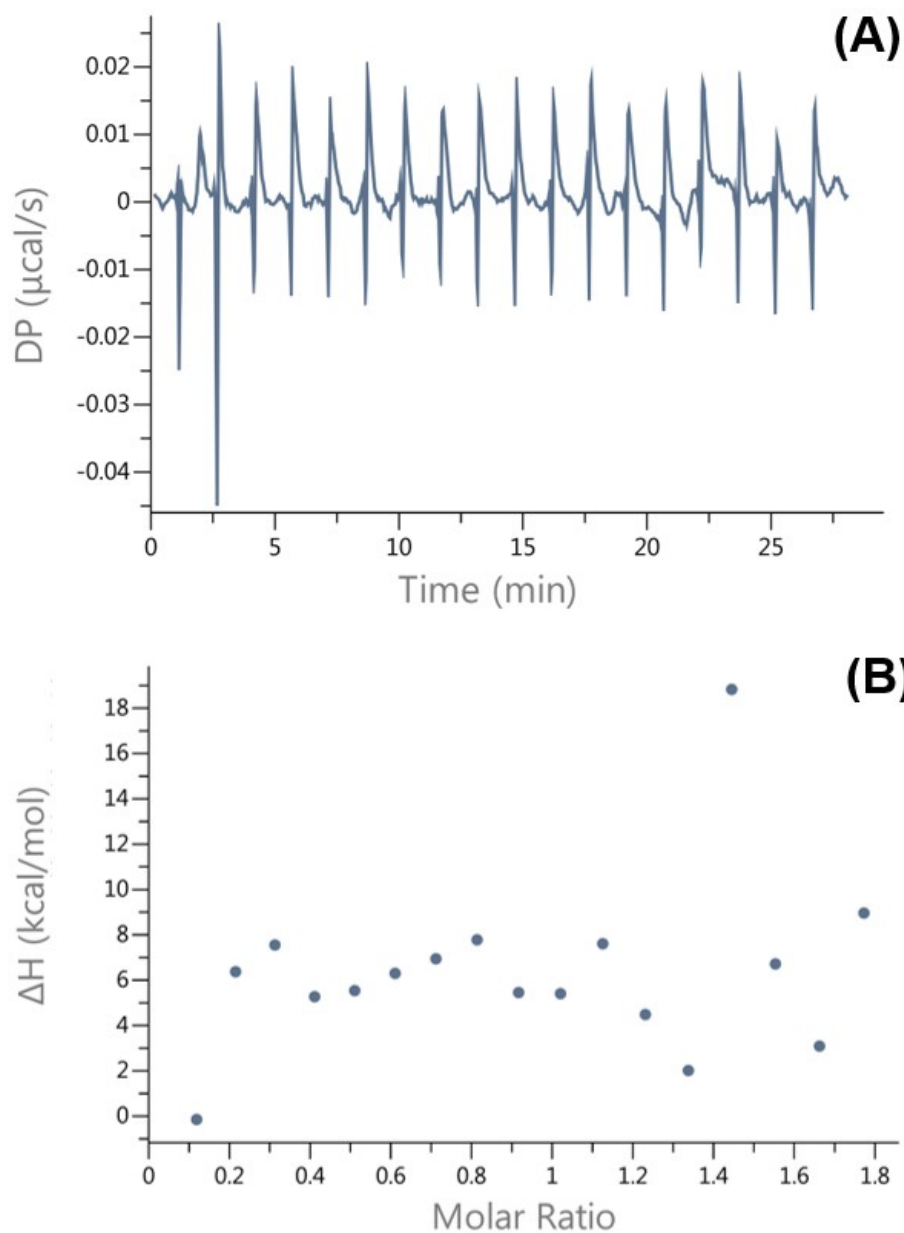


Figure S1. Representative enthalpogram for the interactions between AAPH and CB[6] in 10 mM phosphate buffer (pH 7.4) at 25 °C. Panel A: exothermic heat flows detected upon consecutive injections of 2 μL AAPH (1.4 mM) into a 150 μM CB[6] solution . Panel B: integrated heat values presented as a function of the molar ratios of the titrant and titrated species. Controls consisted of successive injections of buffer into a CB[6] solution giving heat flows accounting for dilution effects.

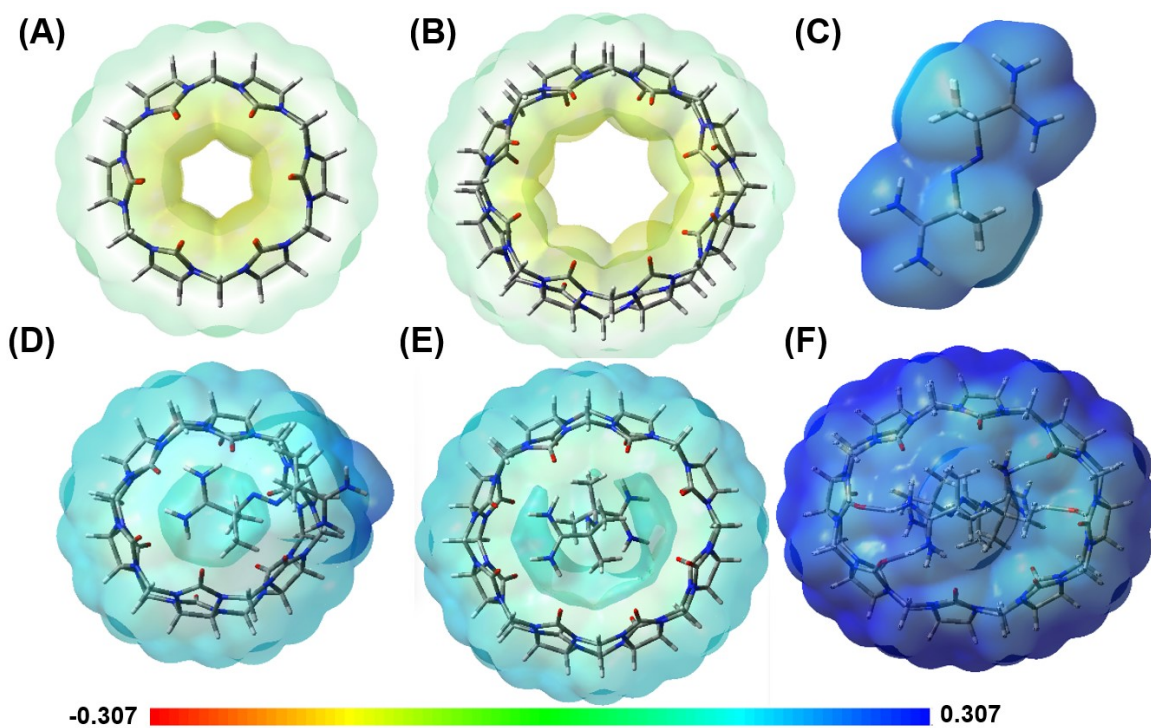


Figure S2. Molecular electrostatic potential (MEP) for CB[6], CB[8], AAPH, AAPH-CB[6], AAPH@CB[8] and 2AAPH@CB[8] complexes; panels A to F, respectively.

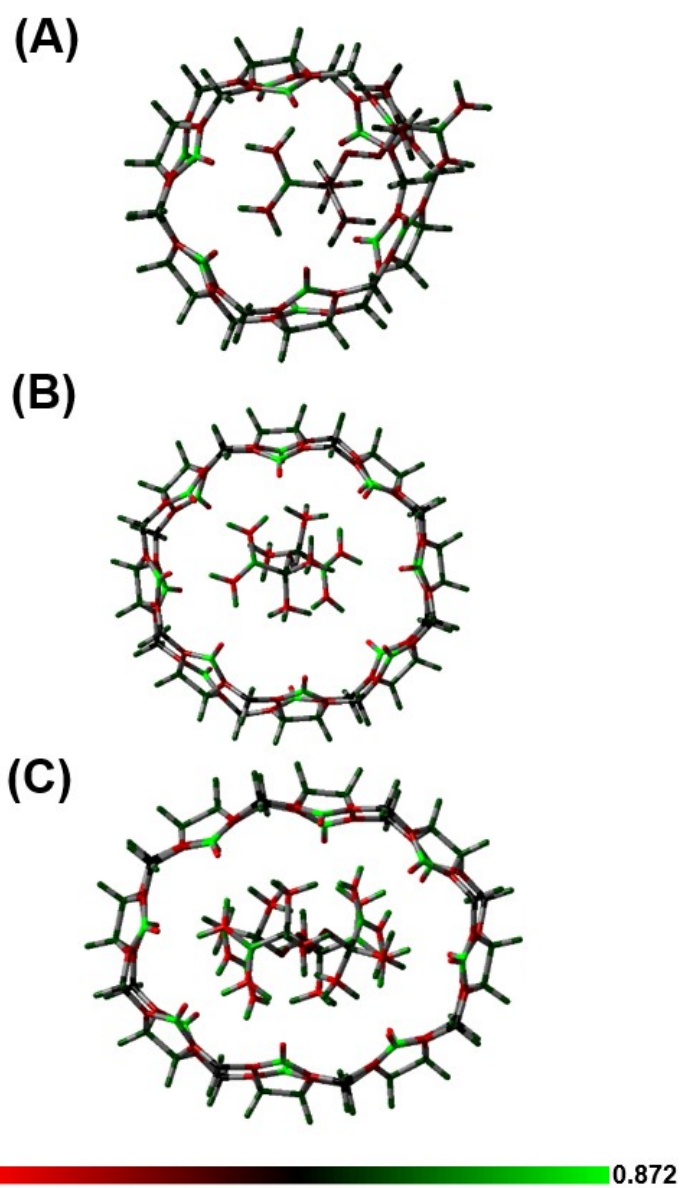


Figure S3. Atomic charges for AAPH-CB[6], AAPH@CB[8] and 2AAPH@CB[8] complexes, panels A, B and C, respectively.

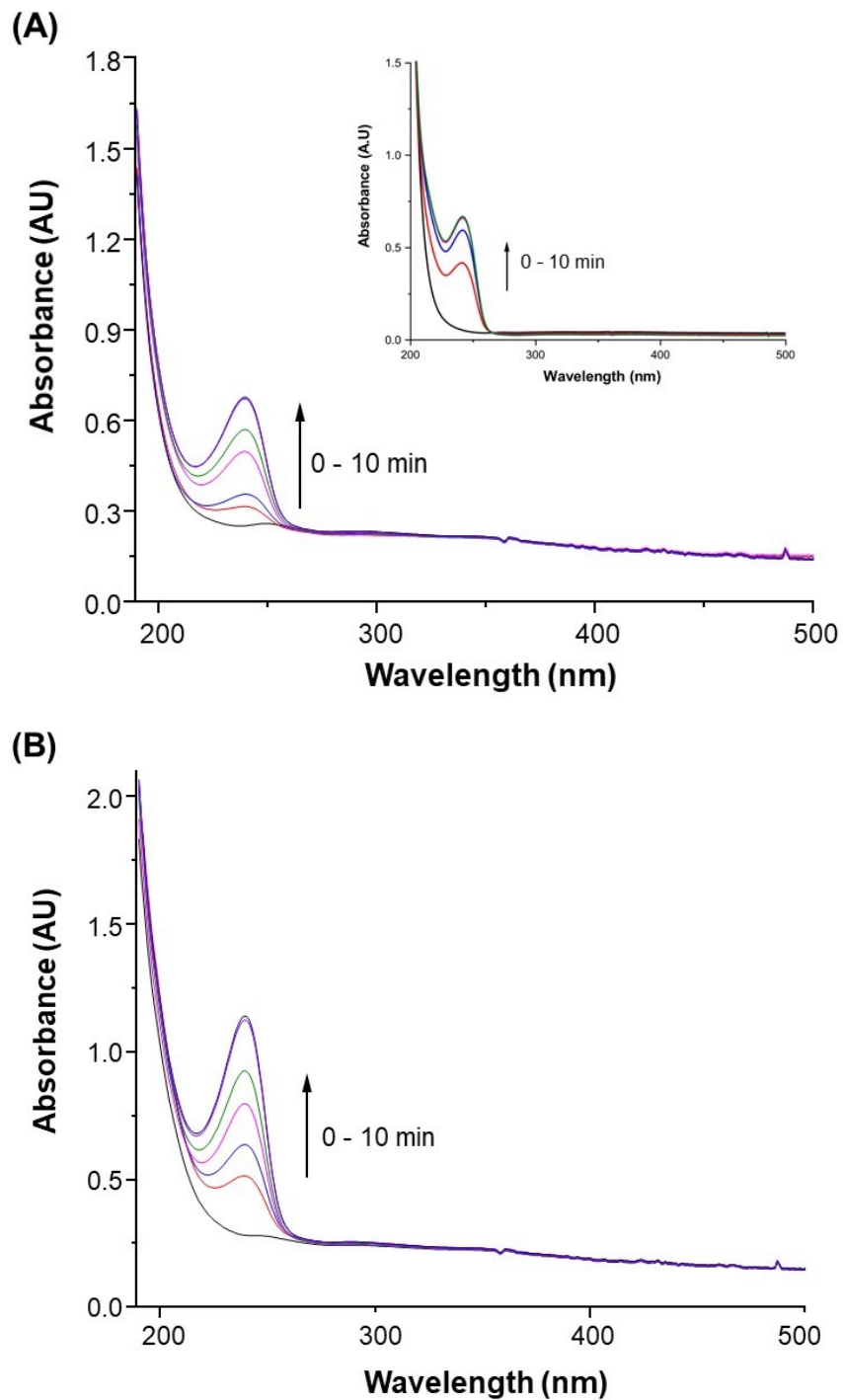


Figure S4. UV-vis spectra of 100 μM (panel A) and 200 μM (panel B) AAPH solutions irradiated at 365 nm in the absence of CB[8]. In both panels, color lines represent spectra registered at different times of irradiation (0-10 min). The insert in panel A shows the UV-vis spectra of AAPH 100 μM solutions irradiated at 365 nm in the presence of CB[8] for increasing periods of time. Solutions were prepared in 10 mM phosphate buffer (pH 7.4) with these then irradiated as described in the Materials and methods.

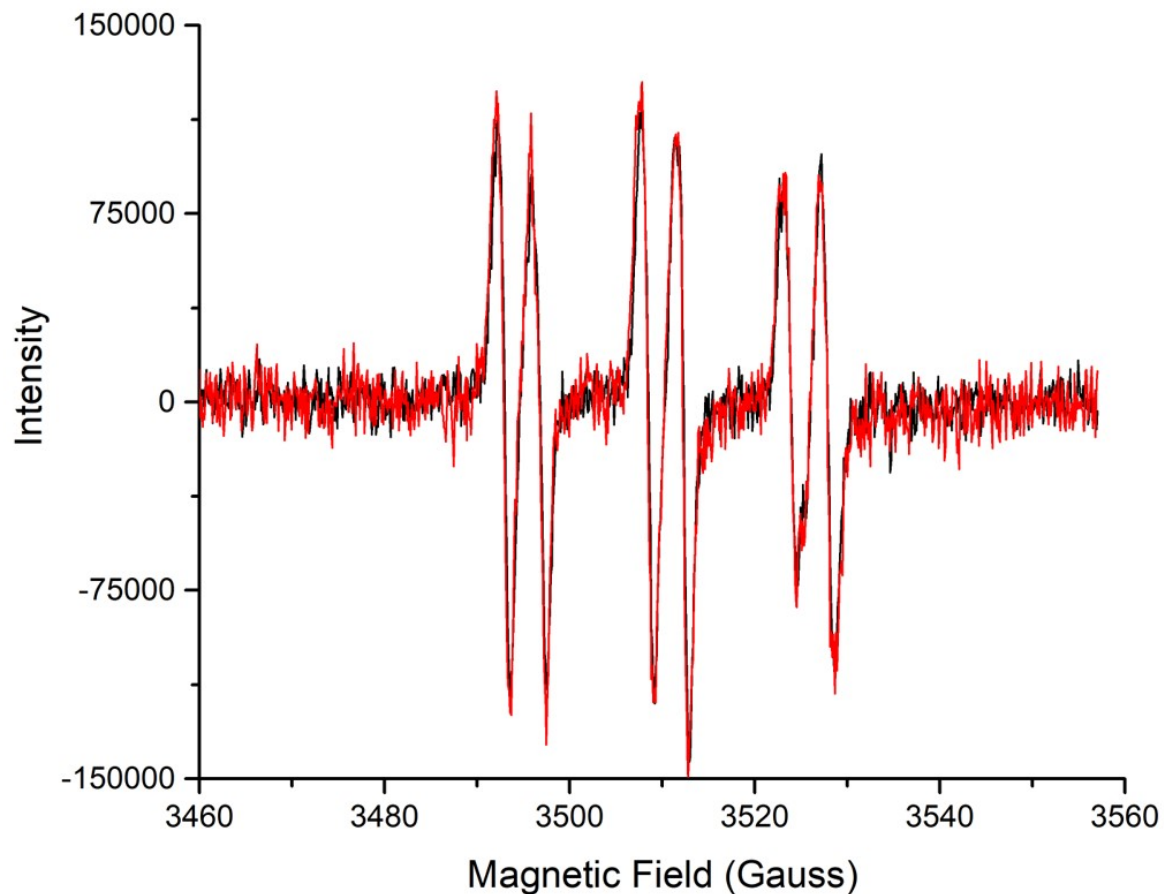


Figure S5. EPR spectra of the PBN-R• adduct arising from the photolysis of AAPH in the presence (red spectrum) or absence (black spectrum) of 100 μM CB[6]. Solutions containing 200 mM PBN and 100 μM of AAPH (prepared in 10 mM phosphate buffer, pH 7.4) were irradiated at 365 nm for 5 min. At defined times, aliquots were removed and immediately analyzed by EPR spectroscopy with a single recorded.

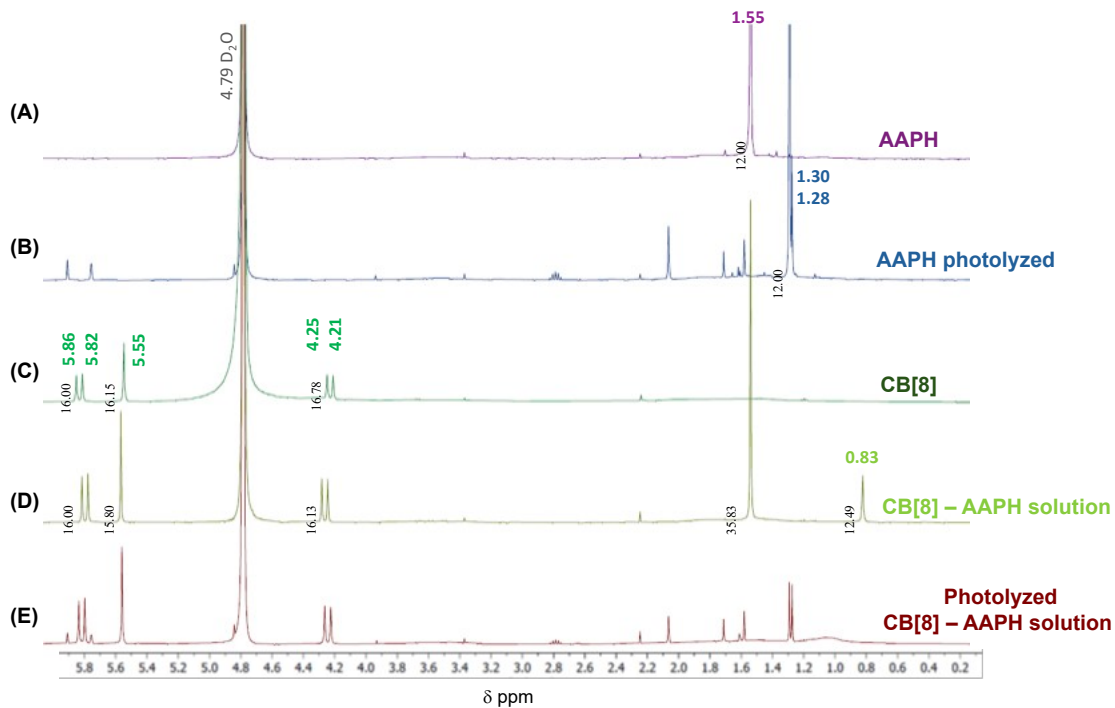


Figure S6. $^1\text{H-NMR}$ spectra of non-illuminated (panel A) and illuminated (panel B) solutions of AAPH and the respective mixture with CB[8] (2:1, AAPH:CB[8]), panels D and E. Panel C shows $^1\text{H-NMR}$ spectrum of a non-illuminated CB[8] solution. All solutions were prepared in D_2O . Illuminated solutions correspond to solutions exposed to light (365 nm) for 12 minutes

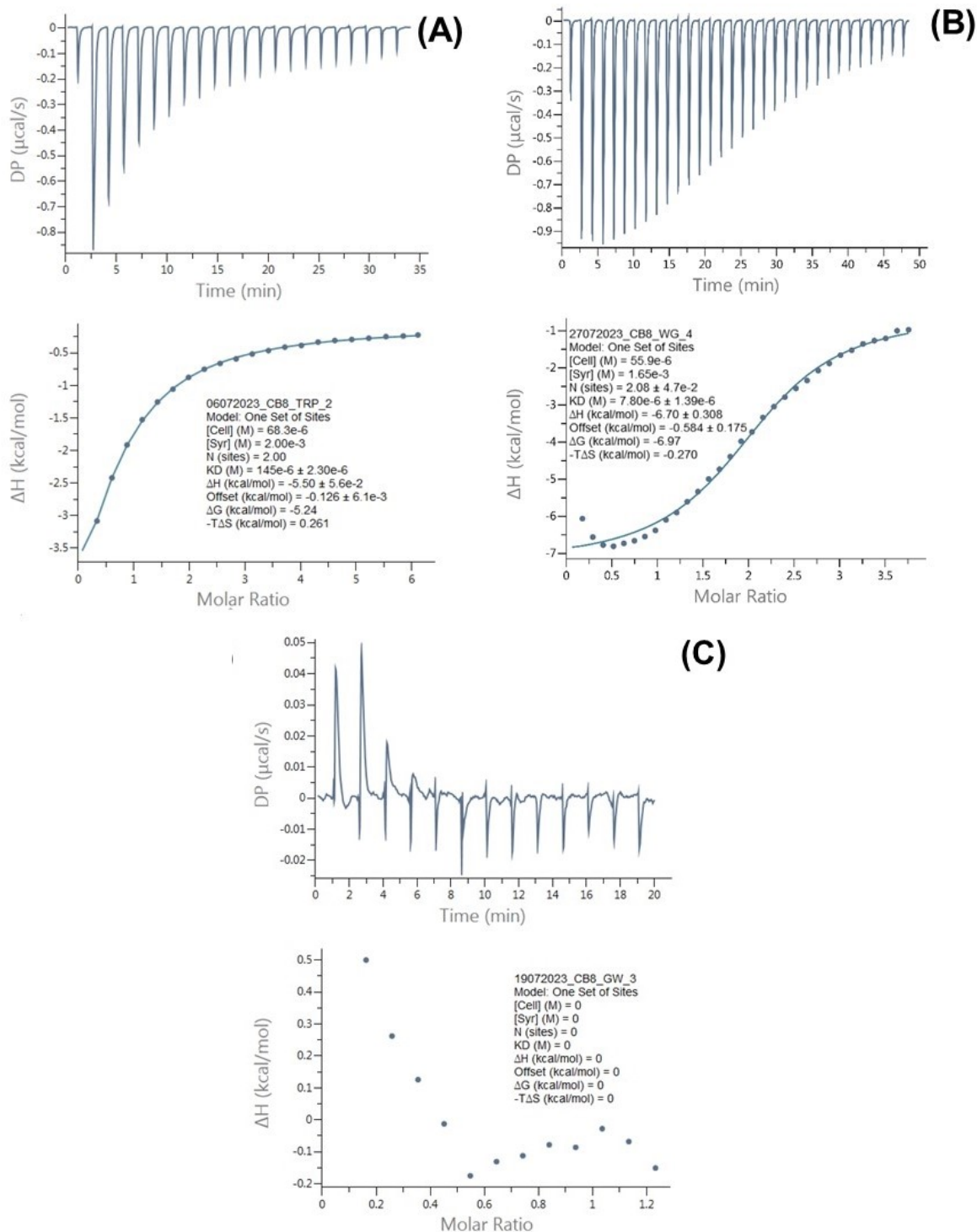


Figure S7. Representative results of isothermal titrating calorimetry (ITC) for the binding of free Trp, Trp-Gly, and Gly-Trp with CB[8] in 10 mM phosphate buffer (pH 7.4) at 25 °C. Each panel presents the exothermic heat flow detected from consecutive injections of aliquots (2 μL) of a peptide solution (~ 2 mM) into CB[8] (~ 60 -70 mM), and the corresponding integrated heat data plotted against the molar ratio of titrant and titrated species together with their thermodynamic data. Controls consisted of successive injections of a buffer solution into a CB[8] solution alone giving heat flows accounting for dilution effects. Panels, A, B, and C correspond to Trp, Trp-Gly, and Gly-Trp respectively.

Table S1: Geometries in cartesian coordinates of the stationary points and computed energies (hartree).

AAPH-CB[6] in the gas phase

Total Energy = -4256.99309822

Total and zero-point Energy= -4255.853354

Total and thermal Energy= -4255.784640

Total Energy and thermal Enthalpies= -4255.783696

Total and thermal Free Energy= -4255.951406

2 1

O	12.420072000000	9.312107000000	20.494264000000
O	9.966833000000	14.907990000000	20.717250000000
O	10.682493000000	9.430280000000	17.488011000000
O	7.290680000000	14.429330000000	18.534610000000
O	11.590289000000	10.708014000000	14.029713000000
O	8.483705000000	15.730730000000	15.692440000000
N	12.364694000000	11.167951000000	21.884327000000
N	10.482554000000	10.537111000000	20.857852000000
N	11.467544000000	13.468591000000	21.753017000000
N	9.427354000000	12.718992000000	21.199938000000
N	9.038381000000	10.194621000000	18.931376000000
N	8.862842000000	10.669896000000	16.750512000000
N	7.919512000000	12.347539000000	19.316665000000
N	7.359168000000	12.565822000000	17.169334000000
N	9.517237000000	11.582658000000	14.604026000000
N	10.763697000000	12.659623000000	13.089967000000
N	8.105870000000	13.540988000000	15.046325000000
N	9.726093000000	14.689455000000	14.029048000000
C	11.833435000000	10.230273000000	20.995875000000
C	10.259575000000	13.807643000000	21.162657000000
C	11.401676000000	12.120239000000	22.341160000000
H	11.418078000000	12.205465000000	23.433536000000
C	10.055632000000	11.554776000000	21.785725000000
H	9.406713000000	11.136038000000	22.563219000000
C	9.596929000000	9.643149000000	20.142795000000
H	10.200800000000	8.778858000000	19.864198000000
H	8.775113000000	9.325582000000	20.793200000000
C	8.067003000000	12.741044000000	20.697536000000
H	7.468195000000	12.085902000000	21.337280000000
H	7.691713000000	13.760178000000	20.775832000000
C	9.666900000000	10.034941000000	17.698804000000
C	7.513923000000	13.245999000000	18.355111000000
C	7.836662000000	10.966361000000	18.847787000000
H	7.006434000000	10.455836000000	19.347839000000
C	7.621451000000	11.143537000000	17.307771000000
H	6.770810000000	10.571535000000	16.920477000000
C	9.065155000000	10.425324000000	15.341944000000
H	9.849812000000	9.672307000000	15.253085000000
H	8.134388000000	10.044802000000	14.901321000000
C	7.004787000000	13.244982000000	15.943443000000
H	6.544382000000	14.190348000000	16.225094000000
H	6.278800000000	12.636841000000	15.398045000000
C	10.740038000000	11.549630000000	13.934289000000
C	8.754074000000	14.753406000000	15.006681000000
C	8.637932000000	12.599419000000	14.080242000000

H	7.815163000000	12.157603000000	13.506453000000
C	9.596719000000	13.473082000000	13.217100000000
H	9.188484000000	13.733166000000	12.234176000000
C	13.776846000000	11.213644000000	22.155144000000
H	13.944303000000	11.360735000000	23.226097000000
H	14.178507000000	10.248099000000	21.846960000000
C	12.361750000000	14.495573000000	22.270638000000
H	11.892365000000	15.465656000000	22.115877000000
H	12.489211000000	14.325044000000	23.347683000000
O	11.946886000000	17.381144000000	15.508605000000
O	14.475127000000	12.168734000000	13.247013000000
O	14.651886000000	17.922491000000	18.107351000000
O	16.144780000000	12.250870000000	16.203609000000
O	13.670450000000	16.824868000000	21.114313000000
O	15.141172000000	10.934456000000	19.626223000000
N	11.874839000000	15.824875000000	13.791532000000
N	13.862212000000	16.495235000000	14.558471000000
N	12.890539000000	13.806739000000	12.813666000000
N	14.846140000000	14.411209000000	13.708965000000
N	15.475461000000	16.596262000000	16.389456000000
N	16.204223000000	16.248368000000	18.470848000000
N	16.407154000000	14.464975000000	15.567289000000
N	16.595255000000	13.938417000000	17.732272000000
N	15.475735000000	15.440678000000	20.676831000000
N	13.662894000000	14.552655000000	21.629966000000
N	15.842704000000	13.135005000000	19.881527000000
N	14.498446000000	12.238518000000	21.432592000000
C	12.498659000000	16.636138000000	14.715340000000
C	14.109560000000	13.310695000000	13.271089000000
C	12.817090000000	15.237242000000	12.843911000000
H	12.619388000000	15.639000000000	11.843009000000
C	14.209995000000	15.663793000000	13.416608000000
H	14.806858000000	16.251138000000	12.708310000000
C	14.811697000000	17.289833000000	15.302096000000
H	14.262841000000	18.118291000000	15.746148000000
H	15.563210000000	17.676829000000	14.604195000000
C	16.210529000000	14.261709000000	14.150172000000
H	16.861062000000	14.953622000000	13.605173000000
H	16.494644000000	13.233253000000	13.924827000000
C	15.353002000000	17.011019000000	17.697686000000
C	16.339884000000	13.404563000000	16.468731000000
C	16.638536000000	15.719951000000	16.207218000000
H	17.436927000000	16.275816000000	15.702722000000
C	16.989642000000	15.320322000000	17.675696000000
H	18.052627000000	15.440563000000	17.916239000000
C	16.275113000000	16.373538000000	19.911886000000
H	15.930429000000	17.374557000000	20.159384000000
H	17.319203000000	16.262386000000	20.216085000000
C	16.856517000000	13.071245000000	18.853506000000
H	16.859987000000	12.047870000000	18.474337000000
H	17.838401000000	13.309784000000	19.283863000000
C	14.199063000000	15.721534000000	21.128292000000
C	15.144956000000	11.972294000000	20.226951000000
C	15.873594000000	14.078191000000	20.973026000000
H	16.853683000000	14.082100000000	21.465536000000
C	14.725791000000	13.567713000000	21.889865000000

H	14.978677000000	13.578768000000	22.956261000000
C	10.444394000000	15.861724000000	13.575116000000
H	10.257184000000	16.003594000000	12.504042000000
H	10.052876000000	16.716467000000	14.122183000000
C	11.896136000000	12.932831000000	12.237250000000
H	12.394910000000	11.981989000000	12.047647000000
H	11.533885000000	13.356304000000	11.295417000000
N	11.462915000000	19.030823000000	18.442965000000
N	12.358873000000	19.402482000000	19.189010000000
C	10.821951000000	17.781420000000	18.956867000000
C	13.034019000000	20.666547000000	18.820299000000
C	11.793643000000	16.609341000000	18.685782000000
H	12.737555000000	16.841406000000	19.160590000000
H	11.381916000000	15.696601000000	19.108097000000
H	11.946902000000	16.498608000000	17.614314000000
C	10.454416000000	17.961233000000	20.436147000000
H	9.829543000000	18.847942000000	20.565532000000
H	9.930662000000	17.093789000000	20.822150000000
H	11.369812000000	18.077021000000	21.010560000000
C	12.085302000000	21.814468000000	19.229021000000
H	11.795219000000	21.731255000000	20.277701000000
H	12.540126000000	22.792470000000	19.065520000000
H	11.189320000000	21.742721000000	18.612268000000
C	13.423826000000	20.739646000000	17.339104000000
H	13.819197000000	21.723080000000	17.077256000000
H	14.155204000000	19.968076000000	17.110247000000
H	12.528515000000	20.563954000000	16.744670000000
C	9.616076000000	17.490849000000	18.089294000000
C	14.270253000000	20.698934000000	19.719927000000
N	8.774053000000	16.578917000000	18.502838000000
N	9.482986000000	18.084384000000	16.918448000000
N	14.479466000000	19.728773000000	20.572966000000
N	15.083753000000	21.741352000000	19.631078000000
H	10.272229000000	18.622537000000	16.590608000000
H	8.909105000000	17.615537000000	16.223889000000
H	8.961873000000	16.040847000000	19.343032000000
H	8.088416000000	16.160256000000	17.882192000000
H	15.905633000000	21.840313000000	20.209147000000
H	14.883951000000	22.490842000000	18.988081000000
H	15.272692000000	19.732087000000	21.198255000000
H	13.888312000000	18.893291000000	20.540426000000

AAPH-CB[6] in PCM model

Total Energy= -4257.23849981

Total and zero-point Energy= -4256.096461

Total and thermal Energy= -4256.028133

Total Energy and thermal Enthalpies= -4256.027189

Total and thermal Free Energy= -4256.193309

2 1

O	12.452987000000	9.349490000000	20.304683000000
O	9.930556000000	14.896157000000	20.777968000000
O	10.589475000000	9.389287000000	17.356027000000
O	7.239734000000	14.423263000000	18.553344000000
O	11.483897000000	10.631903000000	14.065074000000
O	8.481769000000	15.731558000000	15.702912000000
N	12.392599000000	11.163842000000	21.744700000000

N	10.498341000000	10.497200000000	20.785946000000
N	11.453285000000	13.440425000000	21.757527000000
N	9.438304000000	12.673386000000	21.145586000000
N	9.040065000000	10.221265000000	18.863713000000
N	8.741423000000	10.618830000000	16.690210000000
N	7.872038000000	12.333169000000	19.311885000000
N	7.338118000000	12.579518000000	17.162319000000
N	9.408669000000	11.540696000000	14.553169000000
N	10.760524000000	12.641092000000	13.165126000000
N	8.088613000000	13.548136000000	15.048987000000
N	9.713218000000	14.689585000000	14.031810000000
C	11.852359000000	10.244331000000	20.866632000000
C	10.246569000000	13.782345000000	21.173810000000
C	11.413545000000	12.073515000000	22.281540000000
H	11.461975000000	12.094127000000	23.372893000000
C	10.068389000000	11.511635000000	21.728256000000
H	9.424823000000	11.077030000000	22.496938000000
C	9.605018000000	9.628354000000	20.054511000000
H	10.192679000000	8.764778000000	19.749272000000
H	8.787808000000	9.304083000000	20.703161000000
C	8.060863000000	12.709966000000	20.694242000000
H	7.474430000000	12.055413000000	21.342461000000
H	7.700129000000	13.731649000000	20.792877000000
C	9.580263000000	10.018042000000	17.609524000000
C	7.474202000000	13.241095000000	18.359265000000
C	7.805106000000	10.963398000000	18.825350000000
H	7.013088000000	10.418005000000	19.343865000000
C	7.539195000000	11.149633000000	17.296920000000
H	6.658601000000	10.611269000000	16.938150000000
C	8.892608000000	10.398664000000	15.270845000000
H	9.609339000000	9.590133000000	15.139700000000
H	7.927078000000	10.105887000000	14.847725000000
C	6.979883000000	13.266366000000	15.939872000000
H	6.535371000000	14.216973000000	16.226500000000
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C	10.652349000000	11.511271000000	13.952644000000
C	8.745451000000	14.756697000000	15.009896000000
C	8.580914000000	12.621337000000	14.053373000000
H	7.750425000000	12.229247000000	13.461453000000
C	9.588624000000	13.475155000000	13.229816000000
H	9.235444000000	13.724324000000	12.226164000000
C	13.801700000000	11.202112000000	22.045472000000
H	13.938855000000	11.319381000000	23.122490000000
H	14.217444000000	10.249833000000	21.722836000000
C	12.350108000000	14.451743000000	22.305547000000
H	11.875297000000	15.423820000000	22.189326000000
H	12.490392000000	14.241971000000	23.371103000000
O	11.944839000000	17.362444000000	15.513962000000
O	14.449288000000	12.112994000000	13.414116000000
O	14.573237000000	17.925911000000	18.087759000000
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N	11.882961000000	15.777958000000	13.825986000000
N	13.868892000000	16.479798000000	14.574528000000
N	12.904168000000	13.754003000000	12.879336000000

N	14.839285000000	14.365489000000	13.795111000000
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N	16.139373000000	16.275977000000	18.501462000000
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N	15.428191000000	15.479538000000	20.702275000000
N	13.638716000000	14.530590000000	21.644696000000
N	15.957169000000	13.193714000000	19.938127000000
N	14.531749000000	12.252936000000	21.373308000000
C	12.506103000000	16.612885000000	14.733029000000
C	14.098220000000	13.276391000000	13.381901000000
C	12.827448000000	15.194617000000	12.885318000000
H	12.633853000000	15.571875000000	11.877811000000
C	14.214814000000	15.626470000000	13.456465000000
H	14.829974000000	16.176906000000	12.739652000000
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H	14.275242000000	18.139250000000	15.715862000000
H	15.569689000000	17.668298000000	14.587386000000
C	16.205549000000	14.231971000000	14.244632000000
H	16.846189000000	14.917488000000	13.684644000000
H	16.503120000000	13.205105000000	14.041649000000
C	15.307086000000	17.032848000000	17.703577000000
C	16.448461000000	13.444246000000	16.576449000000
C	16.642343000000	15.762748000000	16.246882000000
H	17.435155000000	16.285550000000	15.705928000000
C	17.014503000000	15.421076000000	17.725034000000
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C	16.198229000000	16.443697000000	19.940943000000
H	15.797492000000	17.427905000000	20.164400000000
H	17.240137000000	16.398443000000	20.261846000000
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H	17.139300000000	12.163104000000	18.616648000000
H	17.953092000000	13.526103000000	19.428563000000
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C	15.262360000000	12.030979000000	20.222089000000
C	15.881035000000	14.147113000000	21.031838000000
H	16.836121000000	14.195134000000	21.561936000000
C	14.720354000000	13.577453000000	21.895870000000
H	14.947474000000	13.540833000000	22.964823000000
C	10.456915000000	15.851269000000	13.584067000000
H	10.285100000000	15.995787000000	12.512860000000
H	10.076434000000	16.712470000000	14.128052000000
C	11.903833000000	12.881398000000	12.313804000000
H	12.385897000000	11.921927000000	12.137605000000
H	11.553817000000	13.296452000000	11.366246000000
N	11.481842000000	19.022655000000	18.443098000000
N	12.362670000000	19.422694000000	19.192763000000
C	10.835066000000	17.785772000000	18.975650000000
C	13.049122000000	20.670361000000	18.790904000000
C	11.797807000000	16.602428000000	18.718928000000
H	12.756264000000	16.852784000000	19.152104000000
H	11.401603000000	15.706043000000	19.189049000000
H	11.916316000000	16.449008000000	17.647818000000
C	10.462837000000	17.976812000000	20.451088000000
H	9.839854000000	18.866477000000	20.568208000000
H	9.938441000000	17.110508000000	20.840456000000

H	11.377605000000	18.098319000000	21.024694000000
C	12.152039000000	21.826358000000	19.287928000000
H	11.922564000000	21.710785000000	20.348102000000
H	12.636065000000	22.790398000000	19.133313000000
H	11.222053000000	21.800176000000	18.719366000000
C	13.327133000000	20.766988000000	17.288459000000
H	13.722929000000	21.747442000000	17.020736000000
H	14.028830000000	19.992097000000	16.988785000000
H	12.389016000000	20.625633000000	16.754629000000
C	9.633337000000	17.487283000000	18.106658000000
C	14.341187000000	20.679533000000	19.609373000000
N	8.818424000000	16.538717000000	18.501093000000
N	9.477159000000	18.109342000000	16.955976000000
N	14.524614000000	19.775354000000	20.540487000000
N	15.215501000000	21.640803000000	19.384994000000
H	10.237848000000	18.702003000000	16.653513000000
H	8.903916000000	17.663289000000	16.247458000000
H	9.029189000000	15.988628000000	19.328506000000
H	8.148344000000	16.116955000000	17.866879000000
H	16.077605000000	21.716000000000	19.906091000000
H	15.045456000000	22.341149000000	18.680786000000
H	15.352302000000	19.773221000000	21.120048000000
H	13.883706000000	18.985802000000	20.594817000000

AAPH@CB[8] in the gas phase

Total Energy= -5460.98676976

Total and zero-point Energy= -5459.568690

Total and thermal Energy= -5459.482413

Total Energy and thermal Enthalpies= -5459.481469

Total and thermal Free Energy= -5459.688870

2 1

O	13.173714000000	22.987695000000	19.346346000000
O	15.762050000000	22.486940000000	21.399060000000
O	16.597156000000	24.095028000000	24.866119000000
O	15.308459000000	26.470960000000	27.598304000000
O	16.042738000000	27.632830000000	16.982054000000
O	19.167297000000	26.810937000000	19.026633000000
O	19.907930000000	28.082873000000	21.980068000000
O	17.881986000000	30.641313000000	24.220689000000
N	13.115581000000	24.523934000000	17.609686000000
N	14.972681000000	23.320054000000	17.920133000000
N	16.870289000000	22.881499000000	19.400395000000
N	17.916530000000	23.346111000000	21.322998000000
N	18.462942000000	24.283962000000	23.496516000000
N	18.368097000000	25.502539000000	25.371941000000
N	17.427570000000	27.133289000000	26.929298000000
N	16.002607000000	28.682511000000	27.675986000000
N	14.284400000000	26.262221000000	16.364617000000
N	16.149325000000	25.323722000000	17.150513000000
N	18.081095000000	24.824196000000	18.534098000000
N	19.497187000000	24.873015000000	20.249375000000
N	20.044661000000	25.816252000000	22.438502000000
N	19.542022000000	27.212584000000	24.094928000000
N	18.476106000000	28.837396000000	25.545399000000
N	17.152030000000	30.413715000000	26.409052000000
C	13.698473000000	23.548819000000	18.418996000000

C	15.857808000000	22.348958000000	18.519039000000
H	16.349156000000	21.779647000000	17.724608000000
H	15.231761000000	21.686109000000	19.116120000000
C	16.722009000000	22.870328000000	20.782007000000
C	18.214608000000	23.095161000000	22.713525000000
C	17.670842000000	24.577248000000	24.603694000000
C	17.981294000000	25.814609000000	26.728162000000
C	16.142590000000	27.323427000000	27.412938000000
C	14.911615000000	29.170432000000	28.483507000000
C	13.942799000000	24.862676000000	16.470583000000
H	13.498806000000	24.504252000000	15.535212000000
C	15.303691000000	24.183997000000	16.821683000000
H	15.740438000000	23.615374000000	15.993655000000
C	18.124912000000	23.437788000000	18.983688000000
H	18.600928000000	22.807609000000	18.224627000000
C	18.935354000000	23.543438000000	20.312138000000
H	19.732479000000	22.797302000000	20.402612000000
C	19.753743000000	24.935091000000	23.547873000000
C	19.596596000000	25.915337000000	24.751413000000
C	18.197519000000	28.349379000000	26.880264000000
C	17.222682000000	29.424273000000	27.459004000000
C	15.540896000000	26.529327000000	16.855731000000
C	17.588576000000	25.226778000000	17.240704000000
H	17.940894000000	24.515842000000	16.482345000000
H	18.001882000000	26.212941000000	17.031685000000
C	18.931425000000	25.637514000000	19.252833000000
C	20.506848000000	25.393301000000	21.137216000000
H	21.277641000000	24.629879000000	21.274702000000
H	20.938680000000	26.267900000000	20.652481000000
C	19.829699000000	27.139528000000	22.748850000000
C	19.656958000000	28.458033000000	24.810399000000
C	17.828639000000	30.031797000000	25.271195000000
C	16.689305000000	31.766038000000	26.609405000000
O	15.198385000000	33.457182000000	24.881987000000
O	12.609942000000	33.958223000000	22.829397000000
O	11.774773000000	32.350272000000	19.362392000000
O	13.063666000000	29.974192000000	16.630356000000
O	12.329397000000	28.812270000000	27.246717000000
O	9.205041000000	29.634096000000	25.201889000000
O	8.464361000000	28.362171000000	22.248600000000
O	10.490305000000	25.803737000000	20.007903000000
N	15.256567000000	31.921091000000	26.618779000000
N	13.399461000000	33.124956000000	26.308289000000
N	11.501807000000	33.563638000000	24.828114000000
N	10.455476000000	33.099024000000	22.905561000000
N	9.909036000000	32.161186000000	20.732041000000
N	10.003983000000	30.942536000000	18.856670000000
N	10.944554000000	29.311812000000	17.299312000000
N	12.369568000000	27.762625000000	16.552651000000
N	14.087771000000	30.182907000000	27.864002000000
N	12.222829000000	31.121367000000	27.078104000000
N	10.291099000000	31.620897000000	25.694460000000
N	8.874931000000	31.572047000000	23.979244000000
N	8.327465000000	30.628774000000	21.790123000000
N	8.830166000000	29.232441000000	20.133716000000
N	9.896118000000	27.607662000000	18.683237000000

N	11.220166000000	26.031358000000	17.819507000000
C	14.673650000000	32.896143000000	25.809404000000
C	12.514361000000	34.096105000000	25.709429000000
C	11.650020000000	33.574818000000	23.446494000000
C	10.157311000000	33.349986000000	21.515051000000
C	10.701151000000	31.867940000000	19.624862000000
C	10.390789000000	30.630475000000	17.500447000000
C	12.229552000000	29.121707000000	16.815703000000
C	13.460578000000	27.274734000000	15.745139000000
H	14.097496000000	28.132391000000	15.530113000000
H	13.069070000000	26.862326000000	14.807496000000
C	14.429375000000	31.582438000000	27.757928000000
C	13.068483000000	32.261105000000	27.406820000000
C	10.247220000000	33.007306000000	25.244885000000
C	9.436713000000	32.901648000000	23.916474000000
C	8.618295000000	31.509936000000	20.680726000000
C	8.775510000000	30.529674000000	19.477206000000
C	10.174647000000	28.095698000000	17.348365000000
H	9.244105000000	28.197112000000	16.778140000000
C	11.149501000000	27.020837000000	16.769593000000
H	10.798716000000	26.563635000000	15.837333000000
C	12.831252000000	29.915776000000	27.372952000000
C	10.783588000000	31.218330000000	26.987877000000
C	9.440800000000	30.807547000000	24.975725000000
C	7.865281000000	31.051711000000	23.091417000000
C	8.542513000000	29.305505000000	21.479797000000
C	8.715270000000	27.986972000000	19.418268000000
H	7.872749000000	28.051608000000	18.716308000000
H	8.511540000000	27.210030000000	20.153778000000
C	10.543602000000	26.413258000000	18.957401000000
C	11.682848000000	24.679029000000	17.619085000000
H	11.310181000000	24.073749000000	18.445378000000
H	11.261506000000	24.311535000000	16.673766000000
H	19.085713000000	22.429703000000	22.786735000000
H	17.340386000000	22.603670000000	23.141722000000
H	20.559482000000	24.203750000000	23.673494000000
H	20.428635000000	25.879310000000	25.463286000000
H	19.128040000000	28.247935000000	27.450517000000
H	17.573478000000	29.881504000000	28.391244000000
H	14.873399000000	31.940924000000	28.693260000000
H	12.631771000000	32.829804000000	28.234814000000
H	9.771224000000	33.637465000000	26.003976000000
H	8.639556000000	33.647756000000	23.826054000000
H	7.812487000000	32.241200000000	20.555097000000
H	7.943467000000	30.565632000000	18.765334000000
H	19.860754000000	29.234975000000	24.074907000000
H	20.499450000000	28.393345000000	25.512389000000
H	17.061970000000	32.371284000000	25.783086000000
H	17.110620000000	32.133591000000	27.554713000000
H	13.140414000000	34.758925000000	25.112320000000
H	12.023083000000	34.665437000000	26.503889000000
H	11.031474000000	33.841554000000	21.086821000000
H	9.286151000000	34.015377000000	21.441904000000
H	11.166444000000	31.339829000000	17.211603000000
H	9.514873000000	30.755582000000	16.852741000000
H	18.857206000000	25.689468000000	27.375867000000

H	17.205614000000	25.105284000000	27.017005000000
H	15.303150000000	29.582881000000	29.421120000000
H	14.274706000000	28.312782000000	28.698586000000
H	7.094451000000	31.815097000000	22.953943000000
H	7.433497000000	30.177094000000	23.576161000000
H	10.370271000000	30.232175000000	27.196907000000
H	10.431256000000	31.929287000000	27.746211000000
N	14.666727000000	28.602076000000	22.148760000000
N	13.705531000000	27.842960000000	22.080080000000
C	14.994112000000	29.311642000000	20.852945000000
C	13.378088000000	27.133397000000	23.375875000000
C	14.154838000000	28.854974000000	19.664233000000
H	13.104926000000	29.053559000000	19.875324000000
H	14.419292000000	29.410758000000	18.764128000000
H	14.253860000000	27.784481000000	19.479486000000
C	14.775582000000	30.812257000000	21.138923000000
H	15.285259000000	31.139097000000	22.045910000000
H	15.134249000000	31.408619000000	20.299059000000
H	13.708605000000	31.007334000000	21.250967000000
C	14.217295000000	27.590076000000	24.564628000000
H	14.118286000000	28.660574000000	24.749356000000
H	13.952785000000	27.034309000000	25.464725000000
H	15.267213000000	27.391466000000	24.353595000000
C	13.596641000000	25.632781000000	23.089929000000
H	13.237913000000	25.036429000000	23.929774000000
H	13.087029000000	25.305933000000	22.182908000000
H	14.663624000000	25.437701000000	22.977966000000
C	16.491828000000	29.028424000000	20.674131000000
C	11.880355000000	27.416630000000	23.554575000000
N	16.939729000000	28.508955000000	19.552903000000
N	17.311005000000	29.290639000000	21.671222000000
N	11.061245000000	27.154463000000	22.557416000000
N	11.432397000000	27.936070000000	24.675794000000
H	16.991921000000	29.713966000000	22.533812000000
H	18.307090000000	29.069939000000	21.624538000000
H	16.352152000000	28.336932000000	18.740595000000
H	17.914017000000	28.225449000000	19.440806000000
H	10.458124000000	28.219638000000	24.787874000000
H	12.019952000000	28.108020000000	25.488131000000
H	10.065156000000	27.375164000000	22.604041000000
H	11.380396000000	26.731161000000	21.694840000000

AAPH@CB[8] in PCM model

Total Energy= -5461.23366832

Total and zero-point Energy= -5459.812743

Total and thermal Energy= -5459.727122

Total Energy and thermal Enthalpies= -5459.726178

Total and thermal Free Energy= -5459.931114

2 1

O	12.732787000000	23.006889000000	19.052524000000
O	15.475785000000	22.680642000000	21.573531000000
O	16.515486000000	24.078190000000	25.064419000000
O	15.359380000000	26.561068000000	27.758564000000
O	16.056165000000	27.714075000000	17.154506000000
O	19.265738000000	26.689349000000	19.104740000000
O	20.202224000000	27.912124000000	22.151213000000

O	18.200277000000	30.546019000000	24.262364000000
N	12.887183000000	24.504959000000	17.291614000000
N	14.751854000000	23.553162000000	18.053548000000
N	16.578962000000	23.017783000000	19.564301000000
N	17.698048000000	23.339930000000	21.467510000000
N	18.342433000000	24.208085000000	23.639666000000
N	18.337754000000	25.440410000000	25.500820000000
N	17.473796000000	27.142508000000	27.008416000000
N	16.149428000000	28.738697000000	27.822004000000
N	14.220914000000	26.426620000000	16.583415000000
N	16.101279000000	25.398450000000	17.199219000000
N	17.956607000000	24.826655000000	18.662511000000
N	19.365937000000	24.764512000000	20.383560000000
N	20.005604000000	25.643955000000	22.564159000000
N	19.652233000000	27.065809000000	24.237448000000
N	18.691044000000	28.772569000000	25.669954000000
N	17.278626000000	30.345478000000	26.376628000000
C	13.384347000000	23.628261000000	18.234531000000
C	15.542842000000	22.525292000000	18.689497000000
H	16.006310000000	21.895984000000	17.924309000000
H	14.859697000000	21.928383000000	19.290084000000
C	16.466647000000	22.990509000000	20.939406000000
C	18.016470000000	23.045035000000	22.846269000000
C	17.602976000000	24.533050000000	24.763146000000
C	17.985951000000	25.799283000000	26.853889000000
C	16.228249000000	27.387619000000	27.547384000000
C	15.072952000000	29.301806000000	28.600745000000
C	13.908371000000	25.017292000000	16.409464000000
H	13.658828000000	24.810764000000	15.365737000000
C	15.202313000000	24.301819000000	16.900065000000
H	15.648526000000	23.637691000000	16.155708000000
C	17.881508000000	23.442886000000	19.124321000000
H	18.278059000000	22.766142000000	18.363889000000
C	18.714720000000	23.475552000000	20.437224000000
H	19.454315000000	22.675217000000	20.512581000000
C	19.676896000000	24.779794000000	23.676121000000
C	19.599525000000	25.759859000000	24.881812000000
C	18.317740000000	28.319798000000	26.994084000000
C	17.372012000000	29.444474000000	27.511026000000
C	15.512457000000	26.625296000000	17.006508000000
C	17.528901000000	25.236819000000	17.342052000000
H	17.869468000000	24.500884000000	16.606948000000
H	17.997179000000	26.197010000000	17.137018000000
C	18.892673000000	25.550351000000	19.363617000000
C	20.431357000000	25.183975000000	21.262652000000
H	21.125275000000	24.351630000000	21.394569000000
H	20.942069000000	26.013217000000	20.778612000000
C	19.967582000000	26.972031000000	22.902826000000
C	19.860838000000	28.291420000000	24.973699000000
C	18.062693000000	29.946547000000	25.320901000000
C	16.789377000000	31.700593000000	26.486216000000
O	15.251364000000	33.089793000000	24.511643000000
O	12.255040000000	33.853402000000	22.455203000000
O	11.167370000000	32.645016000000	19.169219000000
O	12.869749000000	30.090005000000	16.979847000000
O	12.412970000000	28.778955000000	27.603953000000

O	9.309197000000	29.371893000000	25.332575000000
O	8.699162000000	28.040640000000	22.077707000000
O	9.905460000000	25.355849000000	19.391064000000
N	15.351695000000	31.819366000000	26.449850000000
N	13.451563000000	32.874300000000	25.955576000000
N	11.497366000000	33.229756000000	24.554561000000
N	10.130320000000	32.997837000000	22.806489000000
N	9.429842000000	32.173178000000	20.629054000000
N	9.666613000000	30.917195000000	18.805433000000
N	10.698180000000	29.335529000000	17.269848000000
N	12.268834000000	27.868931000000	16.668723000000
N	14.206784000000	30.212600000000	27.882900000000
N	12.297208000000	31.033643000000	27.075190000000
N	10.324963000000	31.422477000000	25.706906000000
N	8.943390000000	31.208808000000	23.978404000000
N	8.364603000000	30.313532000000	21.793635000000
N	8.657083000000	29.041530000000	19.989387000000
N	9.661193000000	27.460436000000	18.443301000000
N	10.937165000000	25.953802000000	17.404133000000
C	14.736728000000	32.637163000000	25.517151000000
C	12.574231000000	33.822340000000	25.313210000000
C	11.395942000000	33.398536000000	23.187077000000
C	9.600050000000	33.311712000000	21.497618000000
C	10.205388000000	31.979380000000	19.504545000000
C	10.061462000000	30.618313000000	17.448658000000
C	12.040332000000	29.198817000000	16.984761000000
C	13.463323000000	27.485659000000	15.952993000000
H	14.104133000000	28.363147000000	15.902350000000
H	13.196429000000	27.166877000000	14.939104000000
C	14.520780000000	31.599301000000	27.620525000000
C	13.152783000000	32.207210000000	27.198061000000
C	10.267109000000	32.764664000000	25.151788000000
C	9.308147000000	32.611365000000	23.932303000000
C	8.306143000000	31.266250000000	20.702353000000
C	8.485244000000	30.373485000000	19.436758000000
C	9.981520000000	28.089150000000	17.169807000000
H	9.081393000000	28.209003000000	16.560936000000
C	11.026074000000	27.116441000000	16.558701000000
H	10.827016000000	26.852889000000	15.516753000000
C	12.921742000000	29.891336000000	27.526158000000
C	10.852616000000	31.128230000000	27.017821000000
C	9.514467000000	30.543269000000	25.030606000000
C	7.934511000000	30.606977000000	23.141853000000
C	8.592339000000	29.030916000000	21.360953000000
C	8.496469000000	27.834985000000	19.211123000000
H	7.640386000000	27.968046000000	18.540116000000
H	8.294464000000	27.020183000000	19.902877000000
C	10.151978000000	26.166068000000	18.517409000000
C	11.470794000000	24.658921000000	17.058181000000
H	10.964055000000	23.920351000000	17.675652000000
H	11.258955000000	24.466664000000	16.002631000000
H	18.854899000000	22.340717000000	22.879733000000
H	17.135394000000	22.586680000000	23.290877000000
H	20.430988000000	23.997331000000	23.787969000000
H	20.421097000000	25.652136000000	25.593980000000
H	19.205806000000	28.170330000000	27.612429000000

H	17.750520000000	29.971897000000	28.389583000000
H	14.959469000000	32.069562000000	28.503594000000
H	12.737395000000	32.907487000000	27.926225000000
H	9.910358000000	33.469705000000	25.906521000000
H	8.415194000000	33.238197000000	23.989984000000
H	7.362707000000	31.816132000000	20.727624000000
H	7.632024000000	30.396794000000	18.754816000000
H	20.161899000000	29.050355000000	24.254914000000
H	20.662040000000	28.143643000000	25.704918000000
H	17.180198000000	32.261224000000	25.639982000000
H	17.166630000000	32.132261000000	27.419374000000
H	13.176328000000	34.401918000000	24.616726000000
H	12.153649000000	34.482931000000	26.076515000000
H	10.307591000000	33.981129000000	21.012696000000
H	8.637083000000	33.815941000000	21.618602000000
H	10.776122000000	31.382187000000	17.149700000000
H	9.181244000000	30.662519000000	16.800829000000
H	18.868774000000	25.674550000000	27.488003000000
H	17.199993000000	25.122070000000	27.181260000000
H	15.491600000000	29.832453000000	29.459933000000
H	14.459204000000	28.472159000000	28.944458000000
H	7.069264000000	31.272866000000	23.091551000000
H	7.649038000000	29.668296000000	23.611399000000
H	10.449458000000	30.165637000000	27.324913000000
H	10.521142000000	31.903426000000	27.716300000000
N	15.107623000000	29.030502000000	22.332059000000
N	14.087455000000	28.352982000000	22.341322000000
C	15.445530000000	29.633669000000	20.994404000000
C	13.766129000000	27.739974000000	23.668687000000
C	14.476866000000	29.268316000000	19.875933000000
H	13.482430000000	29.632444000000	20.130711000000
H	14.768430000000	29.745296000000	18.940545000000
H	14.408958000000	28.191020000000	19.724335000000
C	15.465438000000	31.155621000000	21.238519000000
H	16.061046000000	31.414597000000	22.113636000000
H	15.870362000000	31.666614000000	20.363979000000
H	14.444368000000	31.501916000000	21.405699000000
C	14.492190000000	28.386073000000	24.842670000000
H	14.251403000000	29.444773000000	24.935032000000
H	14.250201000000	27.870707000000	25.770510000000
H	15.565012000000	28.297758000000	24.687420000000
C	14.151966000000	26.249774000000	23.532666000000
H	13.874852000000	25.709494000000	24.437753000000
H	13.661295000000	25.789359000000	22.674830000000
H	15.232402000000	26.179377000000	23.403725000000
C	16.870677000000	29.126435000000	20.750684000000
C	12.242356000000	27.845160000000	23.777714000000
N	17.177714000000	28.528298000000	19.623702000000
N	17.764275000000	29.291674000000	21.701692000000
N	11.538789000000	27.826674000000	22.664513000000
N	11.666632000000	27.907005000000	24.955575000000
H	17.533608000000	29.727192000000	22.589624000000
H	18.704758000000	28.897493000000	21.637528000000
H	16.515514000000	28.387541000000	18.864504000000
H	18.089851000000	28.088156000000	19.484055000000
H	10.674431000000	28.139118000000	25.037206000000

H	12.195242000000	28.003660000000	25.818299000000
H	10.516876000000	27.843935000000	22.642275000000
H	12.043517000000	27.850204000000	21.789132000000

2AAPH@CB[8] in the gas phase

Total Energy= -6106.00003063

Total and zero-point Energy= -6104.274040

Total and thermal Energy= -6104.171161

Total Energy and thermal Enthalpies= -6104.170217

Total and thermal Free Energy= -6104.404589

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O	-1.157631000000	4.214259000000	3.045383000000
O	-4.365985000000	2.380390000000	2.965893000000
O	-5.702243000000	-1.131658000000	3.222781000000
O	-3.063000000000	-3.792787000000	3.068174000000
O	-1.008608000000	4.014333000000	-2.915570000000
O	-4.500664000000	2.200425000000	-2.792149000000
O	-5.253399000000	-0.740387000000	-2.835085000000
O	-2.817357000000	-3.354355000000	-2.883289000000
N	-0.129652000000	5.230940000000	1.232534000000
N	-2.365453000000	5.051291000000	1.257879000000
N	-4.574841000000	3.986951000000	1.308639000000
N	-5.910397000000	2.182533000000	1.241344000000
N	-6.604987000000	-0.157902000000	1.321435000000
N	-6.141319000000	-2.347754000000	1.297868000000
N	-4.413063000000	-4.087150000000	1.200226000000
N	-2.345668000000	-4.969471000000	1.206998000000
N	-0.082362000000	5.275641000000	-1.204474000000
N	-2.277636000000	4.823721000000	-1.149580000000
N	-4.460533000000	3.778770000000	-1.105755000000
N	-6.157333000000	2.332982000000	-1.182414000000
N	-6.646435000000	-0.057180000000	-1.119514000000
N	-5.906602000000	-2.158150000000	-1.132377000000
N	-4.316681000000	-3.982670000000	-1.233839000000
N	-2.276482000000	-4.876287000000	-1.220394000000
C	-1.209203000000	4.771007000000	1.973256000000
C	-3.683308000000	4.977561000000	1.871618000000
H	-4.161512000000	5.959093000000	1.802941000000
H	-3.529973000000	4.718236000000	2.918666000000
C	-4.890159000000	2.796588000000	1.961303000000
C	-6.760605000000	1.169528000000	1.866068000000
C	-6.105959000000	-1.205020000000	2.091061000000
C	-5.669826000000	-3.627293000000	1.784660000000
C	-3.257450000000	-4.227766000000	1.959073000000
C	-1.195966000000	-5.578934000000	1.834678000000
C	-0.537082000000	5.908555000000	0.019624000000
H	-0.240906000000	6.962225000000	0.037960000000
C	-2.081726000000	5.694609000000	-0.000883000000
H	-2.652014000000	6.621700000000	-0.114068000000
C	-5.275391000000	4.130859000000	0.064547000000
H	-5.707506000000	5.128227000000	-0.051094000000
C	-6.333179000000	2.981898000000	0.105605000000
H	-7.362480000000	3.330200000000	0.220577000000
C	-7.213711000000	-0.616439000000	0.093428000000
C	-6.787605000000	-2.122096000000	0.029018000000
C	-4.338171000000	-4.814916000000	-0.048422000000

C	-2.906702000000	-5.439099000000	-0.038127000000
C	-1.098850000000	4.636493000000	-1.875776000000
C	-3.575594000000	4.714619000000	-1.778191000000
H	-4.053053000000	5.700827000000	-1.805141000000
H	-3.426845000000	4.363714000000	-2.797231000000
C	-5.005384000000	2.718004000000	-1.800814000000
C	-6.970902000000	1.235109000000	-1.671245000000
H	-8.016529000000	1.464406000000	-1.457504000000
H	-6.826869000000	1.183512000000	-2.748930000000
C	-5.866395000000	-0.958203000000	-1.803462000000
C	-5.497815000000	-3.376989000000	-1.794052000000
C	-3.106462000000	-3.997163000000	-1.887216000000
C	-1.141839000000	-5.485276000000	-1.875183000000
O	1.158852000000	-4.211489000000	-3.042512000000
O	4.368855000000	-2.381820000000	-2.965247000000
O	5.703370000000	1.129309000000	-3.222442000000
O	3.061663000000	3.790576000000	-3.068197000000
O	1.006650000000	-4.016021000000	2.916894000000
O	4.498065000000	-2.197565000000	2.792678000000
O	5.255398000000	0.744794000000	2.837457000000
O	2.819938000000	3.354428000000	2.882771000000
N	0.130301000000	-5.230896000000	-1.231464000000
N	2.366201000000	-5.051855000000	-1.256352000000
N	4.575492000000	-3.987096000000	-1.306485000000
N	5.911461000000	-2.182948000000	-1.239207000000
N	6.607111000000	0.157195000000	-1.320772000000
N	6.140449000000	2.346392000000	-1.297686000000
N	4.412578000000	4.086008000000	-1.200945000000
N	2.345652000000	4.969236000000	-1.207917000000
N	0.082088000000	-5.277918000000	1.205418000000
N	2.276811000000	-4.823500000000	1.150860000000
N	4.459216000000	-3.777492000000	1.107624000000
N	6.156425000000	-2.332189000000	1.184880000000
N	6.644853000000	0.057911000000	1.120298000000
N	5.908856000000	2.160200000000	1.133061000000
N	4.318508000000	3.984464000000	1.233374000000
N	2.276873000000	4.875045000000	1.219353000000
C	1.210104000000	-4.770155000000	-1.971323000000
C	3.684242000000	-4.977833000000	-1.869666000000
C	4.891836000000	-2.797317000000	-1.959765000000
C	6.762603000000	-1.170714000000	-1.864096000000
C	6.106791000000	1.203439000000	-2.090656000000
C	5.669036000000	3.625552000000	-1.785531000000
C	3.256776000000	4.226457000000	-1.959546000000
C	1.194986000000	5.577283000000	-1.835042000000
H	1.154001000000	5.205778000000	-2.858283000000
H	1.316432000000	6.666901000000	-1.848305000000
C	0.537498000000	-5.909571000000	-0.019009000000
C	2.082050000000	-5.694964000000	0.002339000000
C	5.275022000000	-4.130449000000	-0.061785000000
C	6.333138000000	-2.981809000000	-0.102679000000
C	7.213985000000	0.616392000000	-0.092218000000
C	6.788281000000	2.122268000000	-0.029262000000
C	4.338491000000	4.815249000000	0.046994000000
H	5.141115000000	5.556064000000	0.113485000000
C	2.906685000000	5.438679000000	0.037197000000

H	2.907031000000	6.532529000000	0.087602000000
C	1.097701000000	-4.637789000000	1.876955000000
C	3.574341000000	-4.713398000000	1.780123000000
C	5.003687000000	-2.716292000000	1.802320000000
C	6.969416000000	-1.233727000000	1.673407000000
C	5.867268000000	0.960751000000	1.804813000000
C	5.500282000000	3.379740000000	1.793403000000
H	6.320990000000	4.102782000000	1.749161000000
H	5.289318000000	3.138484000000	2.833729000000
C	3.108207000000	3.997330000000	1.886567000000
C	1.143103000000	5.484691000000	1.875186000000
H	1.081092000000	5.080199000000	2.884246000000
H	1.308466000000	6.568050000000	1.929180000000
H	-7.803460000000	1.492669000000	1.780532000000
H	-6.485518000000	1.110713000000	2.919420000000
H	-8.297968000000	-0.469085000000	0.105810000000
H	-7.628885000000	-2.807011000000	-0.114684000000
H	-5.141106000000	-5.555249000000	-0.116589000000
H	-2.907576000000	-6.532970000000	-0.088081000000
H	0.241722000000	-6.963326000000	-0.038456000000
H	2.652705000000	-6.621748000000	0.116133000000
H	5.706787000000	-5.127855000000	0.054851000000
H	7.362439000000	-3.330436000000	-0.216647000000
H	8.298232000000	0.468766000000	-0.102872000000
H	7.629943000000	2.807155000000	0.112364000000
H	-5.285975000000	-3.134524000000	-2.833910000000
H	-6.318810000000	-4.099837000000	-1.751406000000
H	-1.079289000000	-5.080696000000	-2.884174000000
H	-1.306563000000	-6.568715000000	-1.929310000000
H	3.531278000000	-4.718493000000	-2.916764000000
H	4.162456000000	-5.959344000000	-1.800824000000
H	6.488390000000	-1.112727000000	-2.917720000000
H	7.805256000000	-1.494160000000	-1.777391000000
H	5.505719000000	3.512451000000	-2.857372000000
H	6.435299000000	4.387029000000	-1.611231000000
H	-6.435941000000	-4.388659000000	1.609325000000
H	-5.506951000000	-3.515171000000	2.856668000000
H	-1.318290000000	-6.668460000000	1.847120000000
H	-1.155491000000	-5.208142000000	2.858200000000
H	8.015234000000	-1.463066000000	1.460578000000
H	6.824602000000	-1.181254000000	2.750947000000
H	3.424771000000	-4.362114000000	2.798906000000
H	4.052368000000	-5.699319000000	1.807911000000
N	-1.018499000000	0.332894000000	2.227897000000
N	-0.342990000000	-0.429167000000	2.910939000000
C	-1.848232000000	-0.352837000000	1.192472000000
C	0.290337000000	0.208678000000	4.118497000000
C	-1.179767000000	-1.552537000000	0.518894000000
H	-0.728621000000	-2.168584000000	1.294719000000
H	-1.912246000000	-2.172358000000	0.000602000000
H	-0.414471000000	-1.255427000000	-0.196120000000
C	-3.126131000000	-0.771667000000	1.943845000000
H	-3.574577000000	0.071212000000	2.467234000000
H	-3.835661000000	-1.179033000000	1.226816000000
H	-2.878115000000	-1.547123000000	2.666758000000
C	-0.408004000000	-0.480200000000	5.313986000000

H	-0.409331000000	-1.565818000000	5.220693000000
H	0.091666000000	-0.203456000000	6.243454000000
H	-1.442204000000	-0.137820000000	5.359457000000
C	0.129712000000	1.718000000000	4.198285000000
H	0.581954000000	2.093953000000	5.117726000000
H	0.570221000000	2.241154000000	3.351334000000
H	-0.925308000000	1.978339000000	4.224540000000
C	-2.277941000000	0.725831000000	0.209196000000
C	1.749613000000	-0.241962000000	4.049654000000
N	-2.182014000000	1.982676000000	0.571604000000
N	-2.795166000000	0.365886000000	-0.951722000000
N	2.010875000000	-1.531082000000	3.993419000000
N	2.711998000000	0.654517000000	4.022245000000
H	-2.866405000000	-0.608768000000	-1.201554000000
H	-3.213807000000	1.026983000000	-1.601177000000
H	-1.832129000000	2.174733000000	1.507095000000
H	-2.532187000000	2.750507000000	0.007248000000
H	3.693947000000	0.406445000000	3.904778000000
H	2.514801000000	1.648919000000	3.981298000000
H	2.961910000000	-1.873518000000	3.876374000000
H	1.273367000000	-2.217893000000	3.881630000000
N	1.018118000000	-0.332776000000	-2.230949000000
N	0.341689000000	0.429447000000	-2.912919000000
C	1.847504000000	0.352531000000	-1.195031000000
C	-0.290836000000	-0.207459000000	-4.121345000000
C	3.126249000000	0.770184000000	-1.945788000000
H	2.879334000000	1.545301000000	-2.669445000000
H	3.835389000000	1.177669000000	-1.228425000000
H	3.574714000000	-0.073301000000	-2.468192000000
C	1.179535000000	1.552832000000	-0.522065000000
H	0.413461000000	1.256399000000	0.192411000000
H	1.912100000000	2.172198000000	-0.003332000000
H	0.729332000000	2.169125000000	-1.298232000000
C	-0.128193000000	-1.716502000000	-4.203417000000
H	-0.568371000000	-2.241480000000	-3.357385000000
H	-0.579538000000	-2.091507000000	-5.123692000000
H	0.927162000000	-1.975489000000	-4.229562000000
C	0.406503000000	0.484250000000	-5.315777000000
H	-0.092836000000	0.208337000000	-6.245671000000
H	0.406379000000	1.569715000000	-5.220691000000
H	1.441162000000	0.143336000000	-5.361863000000
C	2.276211000000	-0.726206000000	-0.211462000000
C	-1.750818000000	0.240923000000	-4.052021000000
N	2.180932000000	-1.983048000000	-0.574014000000
N	2.792224000000	-0.366289000000	0.950037000000
N	-2.014204000000	1.529535000000	-3.993602000000
N	-2.711593000000	-0.657316000000	-4.026839000000
H	2.862661000000	0.608348000000	1.200140000000
H	3.210311000000	-1.027389000000	1.599837000000
H	1.832031000000	-2.175439000000	-1.509847000000
H	2.530875000000	-2.750651000000	-0.009215000000
H	-3.694004000000	-0.411571000000	-3.908662000000
H	-2.512225000000	-1.651249000000	-3.986284000000
H	-2.965820000000	1.870466000000	-3.877030000000
H	-1.277809000000	2.217406000000	-3.880724000000

2AAPH@CB[8] in PCM model

Total Energy= -6106.63289656

Total and zero-point Energy= -6104.900562

Total and thermal Energy= -6104.799545

Total Energy and thermal Enthalpies= -6104.798601

Total and thermal Free Energy= -6105.025663

4 1

O	-0.924001000000	-4.559038000000	-3.112311000000
O	-4.343627000000	-2.627384000000	-3.028481000000
O	-5.787446000000	0.863009000000	-3.290954000000
O	-3.305687000000	3.672816000000	-3.213754000000
O	-0.808282000000	-3.921111000000	3.007428000000
O	-4.546263000000	-2.292144000000	2.881000000000
O	-5.521214000000	0.633639000000	2.895791000000
O	-3.094938000000	3.489934000000	2.931176000000
N	0.125745000000	-5.241749000000	-1.157614000000
N	-2.107996000000	-5.081090000000	-1.192318000000
N	-4.342650000000	-4.103070000000	-1.242001000000
N	-5.823190000000	-2.423395000000	-1.251116000000
N	-6.609775000000	-0.120867000000	-1.358946000000
N	-6.248720000000	2.080403000000	-1.373003000000
N	-4.620981000000	3.897611000000	-1.315754000000
N	-2.568191000000	4.790135000000	-1.321966000000
N	0.157230000000	-5.133412000000	1.288352000000
N	-2.048154000000	-4.725806000000	1.212059000000
N	-4.296264000000	-3.839772000000	1.176904000000
N	-6.089576000000	-2.517134000000	1.180509000000
N	-6.720017000000	-0.169965000000	1.090204000000
N	-6.056836000000	1.955443000000	1.074999000000
N	-4.513173000000	3.818646000000	1.128561000000
N	-2.518217000000	4.816160000000	1.119350000000
C	-0.961009000000	-4.920247000000	-1.952810000000
C	-3.432415000000	-5.084748000000	-1.789682000000
H	-3.876748000000	-6.076901000000	-1.674806000000
H	-3.303574000000	-4.860710000000	-2.846266000000
C	-4.784237000000	-3.003034000000	-1.959375000000
C	-6.720577000000	-1.464505000000	-1.878695000000
C	-6.171198000000	0.931721000000	-2.139869000000
C	-5.858473000000	3.379010000000	-1.876155000000
C	-3.480897000000	4.070503000000	-2.077683000000
C	-1.421783000000	5.412508000000	-1.944292000000
C	-0.281210000000	-5.840106000000	0.100223000000
H	0.025068000000	-6.887891000000	0.147558000000
C	-1.821576000000	-5.647264000000	0.104288000000
H	-2.375533000000	-6.575274000000	0.261901000000
C	-5.055020000000	-4.270460000000	-0.001729000000
H	-5.408832000000	-5.294975000000	0.122301000000
C	-6.195043000000	-3.212409000000	-0.086582000000
H	-7.190827000000	-3.641941000000	-0.204611000000
C	-7.266755000000	0.337886000000	-0.148731000000
C	-6.905175000000	1.855402000000	-0.105467000000
C	-4.559737000000	4.632984000000	-0.069076000000
C	-3.152539000000	5.295552000000	-0.095423000000
C	-0.881163000000	-4.526845000000	1.952208000000
C	-3.345379000000	-4.693651000000	1.862087000000
H	-3.748546000000	-5.709334000000	1.919267000000

H	-3.209080000000	-4.304515000000	2.867627000000
C	-4.946449000000	-2.831542000000	1.851414000000
C	-6.990318000000	-1.477658000000	1.635575000000
H	-8.010395000000	-1.768085000000	1.383366000000
H	-6.887755000000	-1.412124000000	2.716112000000
C	-6.036159000000	0.786809000000	1.796476000000
C	-5.690072000000	3.208596000000	1.697477000000
C	-3.347857000000	3.981313000000	1.840257000000
C	-1.419489000000	5.514551000000	1.750262000000
O	0.923956000000	4.559176000000	3.112462000000
O	4.343570000000	2.627403000000	3.028577000000
O	5.787371000000	-0.862947000000	3.291079000000
O	3.305638000000	-3.672776000000	3.213908000000
O	0.808221000000	3.921181000000	-3.007320000000
O	4.546200000000	2.292148000000	-2.880880000000
O	5.521152000000	-0.633654000000	-2.895640000000
O	3.094917000000	-3.489797000000	-2.930989000000
N	-0.125790000000	5.241826000000	1.157745000000
N	2.107949000000	5.081119000000	1.192437000000
N	4.342597000000	4.103094000000	1.242102000000
N	5.823140000000	2.423422000000	1.251218000000
N	6.609758000000	0.120907000000	1.359086000000
N	6.248675000000	-2.080357000000	1.373146000000
N	4.620931000000	-3.897563000000	1.315907000000
N	2.568149000000	-4.790101000000	1.322122000000
N	-0.157278000000	5.133461000000	-1.288225000000
N	2.048106000000	4.725844000000	-1.211945000000
N	4.296216000000	3.839805000000	-1.176804000000
N	6.089524000000	2.517163000000	-1.180405000000
N	6.719955000000	0.169993000000	-1.090064000000
N	6.056844000000	-1.955435000000	-1.074859000000
N	4.513165000000	-3.818623000000	-1.128408000000
N	2.518167000000	-4.816054000000	-1.119192000000
C	0.960963000000	4.920331000000	1.952947000000
C	3.432370000000	5.084774000000	1.789794000000
C	4.784182000000	3.003057000000	1.959473000000
C	6.720539000000	1.464553000000	1.878814000000
C	6.171150000000	-0.931671000000	2.140003000000
C	5.858422000000	-3.378959000000	1.876309000000
C	3.480849000000	-4.070463000000	2.077838000000
C	1.421729000000	-5.412465000000	1.944434000000
H	1.358714000000	-5.028778000000	2.960043000000
H	1.562732000000	-6.498096000000	1.971197000000
C	0.281172000000	5.840159000000	-0.100101000000
C	1.821536000000	5.647297000000	-0.104169000000
C	5.054970000000	4.270489000000	0.001834000000
C	6.194993000000	3.212438000000	0.086686000000
C	7.266722000000	-0.337848000000	0.148866000000
C	6.905158000000	-1.855370000000	0.105619000000
C	4.559696000000	-4.632949000000	0.069235000000
H	5.381081000000	-5.350720000000	0.008163000000
C	3.152487000000	-5.295494000000	0.095566000000
H	3.187925000000	-6.387719000000	0.101768000000
C	0.881110000000	4.526899000000	-1.952092000000
C	3.345328000000	4.693687000000	-1.861982000000
C	4.946395000000	2.831567000000	-1.851305000000

C	6.990258000000	1.477674000000	-1.635459000000
C	6.036118000000	-0.786801000000	-1.796331000000
C	5.690075000000	-3.208593000000	-1.697319000000
H	6.527432000000	-3.907737000000	-1.619594000000
H	5.483638000000	-3.005739000000	-2.745863000000
C	3.347831000000	-3.981219000000	-1.840088000000
C	1.419449000000	-5.514436000000	-1.750134000000
H	1.373128000000	-5.194488000000	-2.788529000000
H	1.616984000000	-6.591128000000	-1.707356000000
H	-7.747821000000	-1.821578000000	-1.768182000000
H	-6.463967000000	-1.417239000000	-2.935174000000
H	-8.340699000000	0.143896000000	-0.195055000000
H	-7.774144000000	2.508647000000	0.000245000000
H	-5.381132000000	5.350742000000	-0.007983000000
H	-3.187993000000	6.387777000000	-0.101657000000
H	-0.025092000000	6.887948000000	-0.147448000000
H	2.375502000000	6.575302000000	-0.261779000000
H	5.408781000000	5.295005000000	-0.122194000000
H	7.190777000000	3.641970000000	0.204714000000
H	8.340665000000	-0.143846000000	0.195168000000
H	7.774134000000	-2.508610000000	-0.000064000000
H	-5.483620000000	3.005727000000	2.746016000000
H	-6.527438000000	3.907733000000	1.619774000000
H	-1.373167000000	5.194638000000	2.788667000000
H	-1.617011000000	6.591244000000	1.707448000000
H	3.303535000000	4.860735000000	2.846378000000
H	3.876707000000	6.076926000000	1.674917000000
H	6.463926000000	1.417299000000	2.935292000000
H	7.747778000000	1.821639000000	1.768297000000
H	5.709879000000	-3.275551000000	2.949113000000
H	6.660878000000	-4.094869000000	1.682404000000
H	-6.660929000000	4.094916000000	-1.682239000000
H	-5.709935000000	3.275613000000	-2.948961000000
H	-1.562794000000	6.498138000000	-1.971054000000
H	-1.358777000000	5.028822000000	-2.959903000000
H	8.010338000000	1.768102000000	-1.383261000000
H	6.887690000000	1.412123000000	-2.715995000000
H	3.209021000000	4.304555000000	-2.867521000000
H	3.748498000000	5.709369000000	-1.919162000000
N	-0.945272000000	-0.426189000000	-2.213545000000
N	-0.300012000000	0.314226000000	-2.944761000000
C	-1.844789000000	0.277131000000	-1.256323000000
C	0.457507000000	-0.402846000000	-4.025292000000
C	-1.225181000000	1.515013000000	-0.605103000000
H	-0.760623000000	2.116130000000	-1.383838000000
H	-1.984367000000	2.129222000000	-0.122796000000
H	-0.476648000000	1.252714000000	0.137444000000
C	-3.102971000000	0.633492000000	-2.064040000000
H	-3.517322000000	-0.244050000000	-2.557389000000
H	-3.845970000000	1.055239000000	-1.392436000000
H	-2.841951000000	1.381940000000	-2.809306000000
C	-0.164325000000	0.113538000000	-5.341122000000
H	-0.198931000000	1.201881000000	-5.370800000000
H	0.419229000000	-0.247502000000	-6.188871000000
H	-1.180921000000	-0.272645000000	-5.420908000000
C	0.375341000000	-1.917977000000	-3.949196000000

H	0.899255000000	-2.363867000000	-4.795469000000
H	0.796656000000	-2.317070000000	-3.028670000000
H	-0.663364000000	-2.232231000000	-4.000369000000
C	-2.258488000000	-0.777455000000	-0.238241000000
C	1.882190000000	0.133476000000	-3.908227000000
N	-2.027405000000	-2.036202000000	-0.508805000000
N	-2.887781000000	-0.393746000000	0.853754000000
N	2.058855000000	1.437238000000	-3.871389000000
N	2.894236000000	-0.704181000000	-3.854285000000
H	-3.024195000000	0.585455000000	1.044873000000
H	-3.246984000000	-1.053445000000	1.532263000000
H	-1.547891000000	-2.238247000000	-1.378497000000
H	-2.287052000000	-2.799785000000	0.107639000000
H	3.859031000000	-0.397205000000	-3.720848000000
H	2.754960000000	-1.707897000000	-3.772651000000
H	2.986091000000	1.841268000000	-3.735724000000
H	1.275735000000	2.071721000000	-3.751718000000
N	0.945268000000	0.426240000000	2.213676000000
N	0.299945000000	-0.314159000000	2.944854000000
C	1.844821000000	-0.277088000000	1.256497000000
C	-0.457576000000	0.402940000000	4.025363000000
C	3.102958000000	-0.633459000000	2.064283000000
H	2.841885000000	-1.381896000000	2.809544000000
H	3.845987000000	-1.055225000000	1.392724000000
H	3.517293000000	0.244080000000	2.557649000000
C	1.225240000000	-1.514962000000	0.605240000000
H	0.476756000000	-1.252654000000	-0.137354000000
H	1.984449000000	-2.129179000000	0.122977000000
H	0.760627000000	-2.116077000000	1.383943000000
C	-0.375388000000	1.918069000000	3.949239000000
H	-0.796694000000	2.317144000000	3.028700000000
H	-0.899302000000	2.363986000000	4.795496000000
H	0.663320000000	2.232312000000	4.000417000000
C	0.164244000000	-0.113427000000	5.341206000000
H	-0.419311000000	0.247635000000	6.188945000000
H	0.198837000000	-1.201770000000	5.370904000000
H	1.180843000000	0.272747000000	5.420991000000
C	2.258579000000	0.777501000000	0.238442000000
C	-1.882268000000	-0.133358000000	3.908313000000
N	2.027478000000	2.036248000000	0.508997000000
N	2.887940000000	0.393796000000	-0.853514000000
N	-2.058956000000	-1.437117000000	3.871480000000
N	-2.894295000000	0.704322000000	3.854389000000
H	3.024339000000	-0.585404000000	-1.044653000000
H	3.247197000000	1.053500000000	-1.531990000000
H	1.547917000000	2.238285000000	1.378663000000
H	2.287145000000	2.799838000000	-0.107429000000
H	-3.859105000000	0.397381000000	3.720974000000
H	-2.754994000000	1.708036000000	3.772765000000
H	-2.986204000000	-1.841140000000	3.735880000000
H	-1.275849000000	-2.071618000000	3.751811000000

2R* from AAPH@CB[8] in the gas phase

Total Energy = -5460.99857304

Total and zero-point Energy= -5459.591303

Total and thermal Energy= -5459.499433

Total Energy and thermal Enthalpies= -5459.498489

Total and thermal Free Energy= -5459.725162

2 3

O	12.914938000000	23.122459000000	19.551585000000
O	15.709917000000	22.613517000000	21.738096000000
O	16.768249000000	24.023362000000	25.100714000000
O	15.426628000000	26.393800000000	27.475219000000
O	15.953438000000	27.710257000000	17.159224000000
O	19.132099000000	26.803671000000	19.223812000000
O	20.075710000000	28.005260000000	22.151719000000
O	18.253876000000	30.652653000000	24.338722000000
N	12.921280000000	24.584081000000	17.750357000000
N	14.797765000000	23.478012000000	18.246809000000
N	16.709858000000	22.985870000000	19.680358000000
N	17.913012000000	23.310818000000	21.533219000000
N	18.601374000000	24.186576000000	23.689519000000
N	18.564741000000	25.417084000000	25.551724000000
N	17.593058000000	27.091570000000	27.035284000000
N	16.057366000000	28.623973000000	27.566034000000
N	14.164937000000	26.346078000000	16.612239000000
N	16.031840000000	25.403270000000	17.386283000000
N	17.971438000000	24.857576000000	18.742870000000
N	19.449868000000	24.840682000000	20.405659000000
N	20.132410000000	25.731481000000	22.575238000000
N	19.752074000000	27.123042000000	24.268256000000
N	18.679751000000	28.797756000000	25.664948000000
N	17.312001000000	30.382556000000	26.435861000000
C	13.483161000000	23.670734000000	18.639091000000
C	15.636789000000	22.478629000000	18.861141000000
H	16.065344000000	21.842642000000	18.078928000000
H	14.991308000000	21.884603000000	19.508085000000
C	16.655648000000	22.943672000000	21.065886000000
C	18.294848000000	23.022629000000	22.895306000000
C	17.839110000000	24.497034000000	24.809042000000
C	18.180922000000	25.782240000000	26.892977000000
C	16.256747000000	27.261863000000	27.356981000000
C	14.908333000000	29.072900000000	28.314577000000
C	13.827058000000	24.944386000000	16.680819000000
H	13.446451000000	24.595757000000	15.713767000000
C	15.168514000000	24.269690000000	17.105511000000
H	15.612431000000	23.641890000000	16.324413000000
C	17.968518000000	23.470843000000	19.187218000000
H	18.357892000000	22.817641000000	18.398671000000
C	18.865369000000	23.520311000000	20.464099000000
H	19.650945000000	22.757139000000	20.482425000000
C	19.889852000000	24.842719000000	23.688900000000
C	19.784925000000	25.816025000000	24.906272000000
C	18.326743000000	28.327620000000	26.992928000000
C	17.285262000000	29.383851000000	27.478151000000
C	15.434469000000	26.613163000000	17.076671000000
C	17.467541000000	25.283604000000	17.460518000000
H	17.802644000000	24.575396000000	16.691090000000
H	17.893187000000	26.265474000000	17.257373000000
C	18.869762000000	25.634534000000	19.442003000000
C	20.519764000000	25.315433000000	21.249693000000
H	21.271567000000	24.525793000000	21.336230000000

H	20.953984000000	26.183936000000	20.756119000000
C	19.981163000000	27.058365000000	22.911827000000
C	19.878425000000	28.366628000000	24.985172000000
C	18.086873000000	30.010906000000	25.358667000000
C	16.770490000000	31.711482000000	26.575825000000
O	15.332313000000	33.251322000000	24.654172000000
O	12.541258000000	33.772844000000	22.485624000000
O	11.446467000000	32.370971000000	19.087009000000
O	12.797729000000	30.013112000000	16.769810000000
O	12.323427000000	28.685442000000	27.089879000000
O	9.157025000000	29.563228000000	25.006173000000
O	8.214582000000	28.358426000000	22.089668000000
O	10.018988000000	25.711165000000	19.876660000000
N	15.333829000000	31.798573000000	26.462941000000
N	13.461357000000	32.920735000000	25.982721000000
N	11.545306000000	33.399338000000	24.545447000000
N	10.342831000000	33.059696000000	22.693603000000
N	9.650823000000	32.169731000000	20.543188000000
N	9.650409000000	30.969384000000	18.659007000000
N	10.632900000000	29.292127000000	17.180661000000
N	12.196902000000	27.773969000000	16.686260000000
N	14.098161000000	30.062662000000	27.650491000000
N	12.237272000000	30.990605000000	26.846153000000
N	10.297357000000	31.521477000000	25.486502000000
N	8.814400000000	31.525555000000	23.827268000000
N	8.115202000000	30.631237000000	21.662256000000
N	8.524104000000	29.243397000000	19.971519000000
N	9.582136000000	27.572718000000	18.563149000000
N	10.935979000000	25.988783000000	17.769073000000
C	14.769446000000	32.713747000000	25.576417000000
C	12.616733000000	33.913523000000	25.362913000000
C	11.598175000000	33.436751000000	23.158685000000
C	9.957584000000	33.339555000000	21.331156000000
C	10.387494000000	31.884242000000	19.398477000000
C	10.026908000000	30.594725000000	17.317932000000
C	11.976520000000	29.135991000000	16.881516000000
C	13.359812000000	27.340773000000	15.948466000000
H	13.983539000000	28.221224000000	15.796419000000
H	13.048137000000	26.937581000000	14.975938000000
C	14.438944000000	31.461003000000	27.550884000000
C	13.094754000000	32.129595000000	27.125899000000
C	10.289721000000	32.907063000000	25.040210000000
C	9.392230000000	32.848599000000	23.764144000000
C	8.357300000000	31.520427000000	20.549160000000
C	8.452602000000	30.548800000000	19.330956000000
C	9.918309000000	28.045583000000	17.231033000000
H	9.018558000000	28.087319000000	16.606698000000
C	10.971989000000	27.003315000000	16.743701000000
H	10.739498000000	26.566866000000	15.765508000000
C	12.836029000000	29.785266000000	27.172299000000
C	10.800581000000	31.103174000000	26.770942000000
C	9.406138000000	30.734889000000	24.787363000000
C	7.740089000000	31.045662000000	22.992294000000
C	8.291387000000	29.306389000000	21.329285000000
C	8.390250000000	27.998818000000	19.256624000000
H	7.572387000000	28.089104000000	18.529330000000

H	8.140029000000	27.231760000000	19.988511000000
C	10.175482000000	26.356489000000	18.857522000000
C	11.486187000000	24.664893000000	17.621685000000
H	11.062620000000	24.042798000000	18.409664000000
H	11.182992000000	24.274911000000	16.641340000000
H	19.161286000000	22.348375000000	22.893130000000
H	17.444817000000	22.528663000000	23.366866000000
H	20.701731000000	24.112397000000	23.775669000000
H	20.631910000000	25.750895000000	25.598065000000
H	19.221927000000	28.270494000000	27.622720000000
H	17.534343000000	29.835000000000	28.445597000000
H	14.830612000000	31.828509000000	28.506325000000
H	12.648457000000	32.756558000000	27.906141000000
H	9.896394000000	33.559173000000	25.827748000000
H	8.602651000000	33.607668000000	23.743921000000
H	7.548717000000	32.254876000000	20.466492000000
H	7.589007000000	30.596848000000	18.658603000000
H	20.140497000000	29.132558000000	24.256293000000
H	20.686344000000	28.274242000000	25.722978000000
H	17.188267000000	32.322699000000	25.776313000000
H	17.086926000000	32.110753000000	27.548435000000
H	13.259338000000	34.507734000000	24.713317000000
H	12.186523000000	34.550491000000	26.143188000000
H	10.805074000000	33.832805000000	20.854252000000
H	9.089717000000	34.012449000000	21.331978000000
H	10.766171000000	31.319702000000	16.977480000000
H	9.138409000000	30.642209000000	16.679236000000
H	19.062792000000	25.714818000000	27.539661000000
H	17.427345000000	25.065691000000	27.219747000000
H	15.236356000000	29.487473000000	29.276507000000
H	14.282449000000	28.197798000000	28.487338000000
H	6.983646000000	31.831434000000	22.912069000000
H	7.314106000000	30.175102000000	23.489408000000
H	10.380046000000	30.119729000000	26.977450000000
H	10.461410000000	31.812854000000	27.537320000000
N	16.772434000000	26.547289000000	22.304379000000
N	16.194685000000	26.288343000000	21.410404000000
C	15.744861000000	30.515077000000	20.642581000000
C	12.614420000000	25.911797000000	23.533616000000
C	14.764727000000	30.451691000000	19.517405000000
H	13.943384000000	31.152317000000	19.658774000000
H	15.226266000000	30.680411000000	18.549893000000
H	14.337010000000	29.445888000000	19.409996000000
C	15.503757000000	31.382343000000	21.834336000000
H	15.385112000000	30.786679000000	22.749609000000
H	16.339889000000	32.062537000000	22.032055000000
H	14.610012000000	31.992434000000	21.714064000000
C	13.645522000000	26.038879000000	24.607334000000
H	14.158391000000	27.010267000000	24.548800000000
H	13.227071000000	25.980982000000	25.616589000000
H	14.404972000000	25.262152000000	24.525802000000
C	12.874197000000	25.065110000000	22.330713000000
H	12.006070000000	24.475368000000	22.022993000000
H	13.143435000000	25.684212000000	21.462438000000
H	13.697443000000	24.372259000000	22.500914000000
C	16.933101000000	29.693031000000	20.593250000000

C	11.404555000000	26.702079000000	23.605923000000
N	17.160283000000	28.893546000000	19.549864000000
N	17.809955000000	29.708075000000	21.598428000000
N	10.506169000000	26.657897000000	22.620665000000
N	11.176640000000	27.500639000000	24.650377000000
H	17.698112000000	30.296264000000	22.415056000000
H	18.652593000000	29.135728000000	21.588873000000
H	16.529266000000	28.828261000000	18.760866000000
H	17.986443000000	28.300393000000	19.495553000000
H	10.336692000000	28.072765000000	24.716885000000
H	11.809863000000	27.569609000000	25.436784000000
H	9.654066000000	27.215242000000	22.643170000000
H	10.620720000000	26.076914000000	21.799696000000

2R[•] from AAPH@CB[8] in PCM model

Total Energy= -5461.23208585

Total and zero-point Energy= -5459.822500

Total and thermal Energy= -5459.731702

Total Energy and thermal Enthalpies= -5459.730757

Total and thermal Free Energy= -5459.951348

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O	12.961417000000	23.095591000000	19.605124000000
O	15.904503000000	22.514050000000	21.745767000000
O	17.006994000000	23.891358000000	25.043224000000
O	15.546529000000	26.394444000000	27.360543000000
O	15.970588000000	27.681942000000	17.071623000000
O	19.214635000000	26.775982000000	19.057194000000
O	20.159641000000	28.027635000000	21.973160000000
O	18.323916000000	30.723571000000	24.195912000000
N	12.934697000000	24.545432000000	17.795989000000
N	14.832271000000	23.487169000000	18.293824000000
N	16.785641000000	22.985481000000	19.655418000000
N	18.084046000000	23.246245000000	21.447609000000
N	18.786040000000	24.162771000000	23.580670000000
N	18.699473000000	25.430279000000	25.411105000000
N	17.684445000000	27.121104000000	26.835020000000
N	16.159350000000	28.628021000000	27.443163000000
N	14.149539000000	26.318288000000	16.646203000000
N	16.048003000000	25.378975000000	17.343486000000
N	18.023588000000	24.833464000000	18.644777000000
N	19.528861000000	24.839221000000	20.282097000000
N	20.234049000000	25.759869000000	22.424313000000
N	19.804932000000	27.166487000000	24.094635000000
N	18.764306000000	28.853787000000	25.497479000000
N	17.359433000000	30.399039000000	26.273402000000
C	13.518510000000	23.654100000000	18.678178000000
C	15.686966000000	22.476351000000	18.870211000000
H	16.089932000000	21.852018000000	18.068081000000
H	15.067227000000	21.872905000000	19.530040000000
C	16.817186000000	22.886751000000	21.031302000000
C	18.535340000000	22.978159000000	22.792976000000
C	18.039521000000	24.442325000000	24.709336000000
C	18.311903000000	25.823236000000	26.743314000000
C	16.369057000000	27.280083000000	27.216830000000
C	15.008011000000	29.086166000000	28.183089000000

C	13.824027000000	24.910510000000	16.710447000000
H	13.430969000000	24.562919000000	15.751648000000
C	15.170639000000	24.243843000000	17.112750000000
H	15.586458000000	23.591872000000	16.340669000000
C	18.033575000000	23.450257000000	19.102713000000
H	18.378917000000	22.787021000000	18.306325000000
C	18.983143000000	23.500531000000	20.337571000000
H	19.785895000000	22.760159000000	20.310734000000
C	20.046388000000	24.881988000000	23.558124000000
C	19.903650000000	25.869669000000	24.753277000000
C	18.417199000000	28.364882000000	26.821666000000
C	17.376874000000	29.406063000000	27.325620000000
C	15.441671000000	26.578490000000	17.035688000000
C	17.486833000000	25.244451000000	17.368816000000
H	17.786777000000	24.521450000000	16.602963000000
H	17.915009000000	26.217281000000	17.137104000000
C	18.942225000000	25.608436000000	19.310575000000
C	20.614950000000	25.322460000000	21.101615000000
H	21.361125000000	24.531781000000	21.196511000000
H	21.049869000000	26.178016000000	20.590026000000
C	20.063225000000	27.081867000000	22.746355000000
C	19.953845000000	28.417132000000	24.803279000000
C	18.158633000000	30.057053000000	25.209664000000
C	16.829423000000	31.730761000000	26.444339000000
O	15.371429000000	33.258395000000	24.508335000000
O	12.423535000000	33.880117000000	22.352835000000
O	11.345598000000	32.458950000000	19.068287000000
O	12.797940000000	29.988362000000	16.721994000000
O	12.393907000000	28.648398000000	27.045919000000
O	9.120511000000	29.555704000000	24.978549000000
O	8.110542000000	28.349884000000	22.072039000000
O	9.986424000000	25.698134000000	19.916908000000
N	15.393366000000	31.821431000000	26.327110000000
N	13.489875000000	32.854938000000	25.801117000000
N	11.545515000000	33.371035000000	24.435411000000
N	10.253853000000	33.112339000000	22.638726000000
N	9.540042000000	32.215396000000	20.501636000000
N	9.636496000000	30.945258000000	18.672900000000
N	10.658018000000	29.262578000000	17.241800000000
N	12.190378000000	27.752550000000	16.660328000000
N	14.187194000000	30.043400000000	27.480017000000
N	12.289185000000	30.946944000000	26.739300000000
N	10.331054000000	31.484617000000	25.406651000000
N	8.803601000000	31.512097000000	23.787674000000
N	8.073026000000	30.622760000000	21.640691000000
N	8.475512000000	29.224032000000	19.959101000000
N	9.556652000000	27.543986000000	18.579656000000
N	10.990302000000	25.998316000000	17.853129000000
C	14.809667000000	32.700525000000	25.432785000000
C	12.640296000000	33.872629000000	25.228523000000
C	11.515340000000	33.485641000000	23.060472000000
C	9.799876000000	33.392902000000	21.296698000000
C	10.299234000000	31.923366000000	19.385350000000
C	10.031534000000	30.560145000000	17.339262000000
C	11.976555000000	29.102414000000	16.870576000000
C	13.347284000000	27.286339000000	15.935341000000

H	13.972864000000	28.153812000000	15.737373000000
H	13.027446000000	26.839987000000	14.987914000000
C	14.496167000000	31.453816000000	27.405523000000
C	13.145897000000	32.097370000000	26.979764000000
C	10.305652000000	32.879707000000	24.979833000000
C	9.354674000000	32.848184000000	23.747053000000
C	8.273665000000	31.507500000000	20.513397000000
C	8.412847000000	30.526485000000	19.310544000000
C	9.925821000000	28.018353000000	17.257254000000
H	9.043505000000	28.079890000000	16.615616000000
C	10.975379000000	26.972595000000	16.782052000000
H	10.722680000000	26.494087000000	15.832615000000
C	12.905544000000	29.760385000000	27.074582000000
C	10.849390000000	31.062487000000	26.688141000000
C	9.398655000000	30.724972000000	24.739344000000
C	7.706061000000	31.050042000000	22.970178000000
C	8.220348000000	29.300704000000	21.307107000000
C	8.347826000000	27.976575000000	19.243212000000
H	7.552293000000	28.071861000000	18.496570000000
H	8.076222000000	27.213680000000	19.969632000000
C	10.168022000000	26.350346000000	18.896841000000
C	11.499102000000	24.655740000000	17.695144000000
H	11.073766000000	24.044531000000	18.487957000000
H	11.171929000000	24.274316000000	16.721929000000
H	19.446036000000	22.372352000000	22.753474000000
H	17.746002000000	22.420308000000	23.292875000000
H	20.888539000000	24.192219000000	23.650226000000
H	20.751453000000	25.856493000000	25.442142000000
H	19.309707000000	28.296043000000	27.448165000000
H	17.639104000000	29.865154000000	28.281832000000
H	14.872998000000	31.816033000000	28.365438000000
H	12.707942000000	32.745199000000	27.742939000000
H	9.953949000000	33.519734000000	25.792274000000
H	8.555134000000	33.591731000000	23.784132000000
H	7.438193000000	32.205332000000	20.422600000000
H	7.576050000000	30.563899000000	18.609357000000
H	20.208315000000	29.178611000000	24.069342000000
H	20.769457000000	28.321022000000	25.528325000000
H	17.255144000000	32.359080000000	25.665216000000
H	17.138484000000	32.103164000000	27.426556000000
H	13.263633000000	34.479634000000	24.575423000000
H	12.235961000000	34.492202000000	26.033860000000
H	10.591362000000	33.950338000000	20.799738000000
H	8.892255000000	34.002931000000	21.341595000000
H	10.756934000000	31.291879000000	16.990034000000
H	9.148771000000	30.578042000000	16.694376000000
H	19.197580000000	25.812097000000	27.384327000000
H	17.589910000000	25.092254000000	27.100926000000
H	15.337351000000	29.539536000000	29.123542000000
H	14.393261000000	28.213813000000	28.393074000000
H	6.968922000000	31.850825000000	22.891023000000
H	7.264821000000	30.193334000000	23.474394000000
H	10.430177000000	30.081493000000	26.900453000000
H	10.524578000000	31.770760000000	27.458022000000
N	15.423048000000	28.857585000000	24.169885000000
N	14.403836000000	29.232842000000	24.308128000000

C	15.635508000000	30.220505000000	20.659031000000
C	12.642311000000	26.103762000000	23.395857000000
C	14.583432000000	29.970581000000	19.627679000000
H	13.773200000000	30.693139000000	19.718118000000
H	14.967787000000	30.032785000000	18.605078000000
H	14.152128000000	28.966952000000	19.736118000000
C	15.369167000000	31.257617000000	21.694545000000
H	16.112925000000	31.334430000000	22.484716000000
H	15.291839000000	32.242285000000	21.216496000000
H	14.396084000000	31.078846000000	22.163195000000
C	13.600194000000	25.941699000000	24.525147000000
H	13.434628000000	26.597451000000	25.377359000000
H	13.562012000000	24.907849000000	24.892753000000
H	14.625245000000	26.094956000000	24.174830000000
C	12.933727000000	25.391708000000	22.115014000000
H	12.099581000000	24.770407000000	21.774880000000
H	13.140594000000	26.102406000000	21.304523000000
H	13.803272000000	24.744347000000	22.221052000000
C	16.865700000000	29.466493000000	20.616736000000
C	11.442890000000	26.898631000000	23.510438000000
N	17.089127000000	28.617288000000	19.612842000000
N	17.795093000000	29.598477000000	21.563429000000
N	10.563454000000	26.922375000000	22.507966000000
N	11.186447000000	27.615023000000	24.605016000000
H	17.672274000000	30.173720000000	22.387298000000
H	18.650180000000	29.041921000000	21.550294000000
H	16.458875000000	28.518707000000	18.825403000000
H	17.950708000000	28.075967000000	19.546281000000
H	10.358069000000	28.207712000000	24.668294000000
H	11.840903000000	27.710930000000	25.371469000000
H	9.700274000000	27.462124000000	22.561613000000
H	10.655816000000	26.343583000000	21.681092000000

4R[•] from 2AAPH@CB[8] in the gas phase

Total energy = -6106.00529581

Total and zero-point Energy= -6104.301862

Total and thermal Energy= -6104.188016

Total energy and thermal Enthalpies= -6104.187071

Total and thermal Free Energy= -6104.462075

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O	1.125251000000	-3.161865000000	3.217511000000
O	3.754066000000	-0.384360000000	3.870663000000
O	3.868634000000	2.946775000000	3.931371000000
O	1.004573000000	5.001213000000	3.298753000000
O	3.897476000000	-4.133119000000	-2.070490000000
O	5.939763000000	-1.597297000000	-1.381758000000
O	4.900059000000	1.660088000000	-1.711033000000
O	1.455453000000	3.700082000000	-2.409780000000
N	1.266157000000	-4.839857000000	1.626963000000
N	3.138513000000	-3.773541000000	2.233793000000
N	4.823831000000	-2.099362000000	2.737746000000
N	5.873469000000	-0.142116000000	2.966005000000
N	5.540954000000	2.229827000000	2.490176000000
N	4.470992000000	4.146638000000	2.044814000000
N	2.494826000000	5.515412000000	1.598488000000
N	0.295844000000	5.693380000000	1.197637000000

N	2.289435000000	-4.916797000000	-0.587660000000
N	4.321107000000	-4.407941000000	0.189823000000
N	5.983655000000	-2.672511000000	0.664704000000
N	6.379481000000	-0.474468000000	0.603094000000
N	6.222509000000	1.921464000000	0.165473000000
N	4.705623000000	3.488458000000	-0.288972000000
N	2.641348000000	4.733703000000	-0.704450000000
N	0.591494000000	5.478148000000	-1.209304000000
C	1.764387000000	-3.834649000000	2.443289000000
C	3.989214000000	-3.171489000000	3.234071000000
H	4.627286000000	-3.943279000000	3.682854000000
H	3.340100000000	-2.745371000000	3.998850000000
C	4.711237000000	-0.826061000000	3.269702000000
C	6.085606000000	1.228608000000	3.382797000000
C	4.537039000000	3.089431000000	2.939484000000
C	3.719370000000	5.348962000000	2.343882000000
C	1.242195000000	5.354701000000	2.172603000000
C	-1.048049000000	6.060084000000	1.618337000000
C	2.280759000000	-5.412422000000	0.784696000000
H	2.232292000000	-6.506561000000	0.803016000000
C	3.604819000000	-4.838477000000	1.364345000000
H	4.193835000000	-5.570786000000	1.926879000000
C	6.093314000000	-2.299773000000	2.060844000000
H	6.731948000000	-3.004913000000	2.599693000000
C	6.657833000000	-0.850981000000	1.995792000000
H	7.727267000000	-0.777725000000	2.209160000000
C	6.248879000000	2.764170000000	1.345786000000
C	5.357240000000	3.975697000000	0.929757000000
C	2.430195000000	5.859549000000	0.209494000000
C	0.925227000000	6.208426000000	-0.008429000000
C	3.539234000000	-4.441773000000	-0.950886000000
C	5.707366000000	-4.014043000000	0.181641000000
H	6.281850000000	-4.714079000000	0.792873000000
H	6.057103000000	-4.071490000000	-0.846947000000
C	6.079464000000	-1.588338000000	-0.169087000000
C	6.979960000000	0.706071000000	-0.000600000000
H	7.975368000000	0.864717000000	0.423521000000
H	7.077385000000	0.511468000000	-1.066256000000
C	5.239871000000	2.297270000000	-0.718208000000
C	3.961621000000	4.360226000000	-1.175297000000
C	1.546216000000	4.550360000000	-1.539119000000
C	-0.565540000000	5.729291000000	-2.035418000000
O	-2.351691000000	3.969264000000	-3.418806000000
O	-4.804313000000	1.928194000000	-4.202480000000
O	-3.589222000000	-1.242567000000	-3.847479000000
O	-0.178977000000	-3.484216000000	-3.093732000000
O	-2.729829000000	3.785071000000	2.398406000000
O	-5.313865000000	0.768285000000	1.601531000000
O	-5.419205000000	-2.676226000000	1.536300000000
O	-2.702231000000	-4.503471000000	2.287969000000
N	-1.811372000000	5.199711000000	-1.523119000000
N	-3.957634000000	4.689618000000	-1.908307000000
N	-5.680690000000	3.018824000000	-2.355869000000
N	-6.125885000000	0.846269000000	-2.632322000000
N	-5.672933000000	-1.531797000000	-2.879672000000
N	-4.080554000000	-3.062732000000	-2.488119000000

N	-2.050752000000	-4.331392000000	-2.003517000000
N	-0.012242000000	-5.043650000000	-1.387608000000
N	-2.118451000000	5.431992000000	0.877003000000
N	-3.958005000000	4.218281000000	0.474394000000
N	-5.566866000000	2.445298000000	0.018094000000
N	-6.650574000000	0.505552000000	-0.265161000000
N	-6.168644000000	-1.876463000000	-0.512191000000
N	-5.141802000000	-3.850361000000	-0.434571000000
N	-3.096858000000	-5.074757000000	0.077660000000
N	-1.004738000000	-5.144530000000	0.840468000000
C	-2.670999000000	4.545751000000	-2.407281000000
C	-5.137941000000	4.323994000000	-2.658158000000
C	-5.455077000000	1.930229000000	-3.190819000000
C	-6.310362000000	-0.354204000000	-3.420629000000
C	-4.355931000000	-1.862444000000	-3.149862000000
C	-3.023128000000	-3.917103000000	-2.996888000000
C	-0.686689000000	-4.199968000000	-2.261009000000
C	1.368225000000	-5.421222000000	-1.591753000000
H	1.690176000000	-5.015113000000	-2.549365000000
H	1.424804000000	-6.516657000000	-1.625511000000
C	-2.538388000000	5.844351000000	-0.438729000000
C	-3.958150000000	5.229794000000	-0.579502000000
C	-6.408677000000	2.664583000000	-1.175734000000
C	-6.932711000000	1.229362000000	-1.491981000000
C	-6.250556000000	-2.383882000000	-1.886660000000
C	-5.278240000000	-3.593918000000	-1.847542000000
C	-2.319362000000	-5.426797000000	-1.083763000000
H	-2.770290000000	-6.276587000000	-1.606966000000
C	-0.913304000000	-5.725083000000	-0.493934000000
H	-0.676772000000	-6.793164000000	-0.439472000000
C	-2.904552000000	4.409031000000	1.377026000000
C	-5.163082000000	3.547602000000	0.894679000000
C	-5.809207000000	1.192198000000	0.563567000000
C	-7.059128000000	-0.857941000000	0.003237000000
C	-5.552160000000	-2.783238000000	0.326604000000
C	-4.537054000000	-5.035754000000	0.123512000000
H	-4.930846000000	-5.903587000000	-0.411767000000
H	-4.833952000000	-5.096730000000	1.168359000000
C	-2.311571000000	-4.858684000000	1.191600000000
C	-0.021877000000	-5.434864000000	1.864172000000
H	-0.411358000000	-5.039454000000	2.800737000000
H	0.105908000000	-6.521471000000	1.953548000000
H	7.160931000000	1.382098000000	3.509209000000
H	5.585154000000	1.359159000000	4.341745000000
H	7.277737000000	3.035912000000	1.598435000000
H	5.921696000000	4.889386000000	0.721446000000
H	3.111132000000	6.681554000000	-0.032738000000
H	0.733908000000	7.278220000000	-0.136932000000
H	-2.518329000000	6.934622000000	-0.533869000000
H	-4.770907000000	5.948891000000	-0.439988000000
H	-7.200519000000	3.384221000000	-0.950878000000
H	-8.001913000000	1.188918000000	-1.718460000000
H	-7.281829000000	-2.648304000000	-2.136411000000
H	-5.652475000000	-4.479257000000	-2.369941000000
H	3.838214000000	3.834320000000	-2.120676000000
H	4.548034000000	5.272548000000	-1.343978000000

H	-0.394560000000	5.254939000000	-3.000929000000
H	-0.650944000000	6.814221000000	-2.171469000000
H	-4.867023000000	4.308653000000	-3.713283000000
H	-5.906069000000	5.081920000000	-2.487177000000
H	-5.867578000000	-0.151314000000	-4.395444000000
H	-7.375985000000	-0.568629000000	-3.542367000000
H	-2.486599000000	-3.352141000000	-3.758618000000
H	-3.470450000000	-4.809058000000	-3.456329000000
H	4.362644000000	6.216354000000	2.168492000000
H	3.445421000000	5.302657000000	3.397643000000
H	-1.174298000000	7.146173000000	1.543511000000
H	-1.137899000000	5.756548000000	2.660976000000
H	-8.058610000000	-0.994677000000	-0.418968000000
H	-7.111381000000	-0.986982000000	1.082338000000
H	-4.971749000000	3.128616000000	1.881826000000
H	-5.991800000000	4.264014000000	0.955677000000
N	-1.556722000000	-1.510028000000	2.945465000000
N	-1.471311000000	-1.819159000000	3.991650000000
C	0.900743000000	1.767324000000	1.232159000000
C	-4.718674000000	-1.718514000000	6.185661000000
C	-0.216238000000	2.442610000000	0.524857000000
H	-1.160870000000	2.189314000000	1.006955000000
H	-0.122237000000	3.529378000000	0.624675000000
H	-0.281585000000	2.215929000000	-0.537561000000
C	0.868782000000	1.670719000000	2.720619000000
H	1.720205000000	2.179594000000	3.189270000000
H	-0.037224000000	2.129749000000	3.111982000000
H	0.907211000000	0.626620000000	3.059688000000
C	-5.319060000000	-0.443506000000	6.670669000000
H	-4.549933000000	0.336074000000	6.770548000000
H	-6.109262000000	-0.059575000000	6.022679000000
H	-5.744642000000	-0.581945000000	7.666514000000
C	-4.140504000000	-2.670029000000	7.178195000000
H	-4.865581000000	-3.455173000000	7.437900000000
H	-3.231359000000	-3.159206000000	6.818427000000
H	-3.898170000000	-2.153916000000	8.107468000000
C	2.024862000000	1.251308000000	0.503643000000
C	-4.697797000000	-2.035979000000	4.780865000000
N	2.982600000000	0.590638000000	1.162640000000
N	2.128736000000	1.387611000000	-0.823457000000
N	-5.031896000000	-1.124545000000	3.863558000000
N	-4.321749000000	-3.247698000000	4.368338000000
H	1.573379000000	2.072109000000	-1.328007000000
H	3.018324000000	1.190164000000	-1.275485000000
H	2.935382000000	0.439716000000	2.165537000000
H	3.787556000000	0.220737000000	0.679498000000
H	-4.189913000000	-3.473452000000	3.387195000000
H	-4.085343000000	-3.960915000000	5.037117000000
H	-5.165899000000	-1.389151000000	2.890781000000
H	-5.267715000000	-0.184034000000	4.128952000000
N	2.772177000000	-1.403528000000	-1.879177000000
N	2.621745000000	-1.382789000000	-2.963623000000
C	-1.236737000000	-0.367944000000	-1.393464000000
C	5.686469000000	-1.409328000000	-6.150071000000
C	-0.821334000000	-0.028800000000	-2.781304000000
H	-0.496335000000	1.017251000000	-2.869222000000

H	-0.014181000000	-0.675805000000	-3.113056000000
H	-1.657103000000	-0.166356000000	-3.477875000000
C	-0.536387000000	-1.411332000000	-0.588369000000
H	-0.114024000000	-0.999745000000	0.336963000000
H	-1.220934000000	-2.215320000000	-0.293111000000
H	0.269019000000	-1.862095000000	-1.157582000000
C	5.713157000000	-0.081388000000	-6.828124000000
H	5.089742000000	0.668873000000	-6.335631000000
H	6.739718000000	0.309874000000	-6.878074000000
H	5.369332000000	-0.174486000000	-7.859177000000
C	5.808681000000	-2.645105000000	-6.975718000000
H	6.339755000000	-3.453435000000	-6.468062000000
H	4.816513000000	-3.020681000000	-7.266000000000
H	6.340357000000	-2.430678000000	-7.903820000000
C	-2.340127000000	0.332210000000	-0.791889000000
C	5.555167000000	-1.496637000000	-4.718792000000
N	-2.953176000000	1.320009000000	-1.446556000000
N	-2.725151000000	0.022469000000	0.450892000000
N	5.390313000000	-2.679365000000	-4.124276000000
N	5.586689000000	-0.394077000000	-3.962606000000
H	-2.234121000000	-0.684591000000	0.975299000000
H	-3.521741000000	0.451135000000	0.917969000000
H	-2.737549000000	1.531735000000	-2.412540000000
H	-3.684028000000	1.865396000000	-1.003940000000
H	5.573981000000	-0.455172000000	-2.949603000000
H	5.773628000000	0.502758000000	-4.376498000000
H	5.242572000000	-2.767466000000	-3.124276000000
H	5.233815000000	-3.505139000000	-4.677280000000

2R• and 2,2,3,3-tetramethylbutane-1,4-bisamidine (the compound generated by self-reaction of two R•) from 2AAPH@CB[8] in the gas phase

Total Energy= -6106.06208141

Total and zero-point Energy= -6104.350364

Total and thermal Energy= -6104.239219

Total Energy and thermal Enthalpies= -6104.238275

Total and thermal Free Energy= -6104.505656

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O	-0.481402000000	-4.862878000000	2.781976000000
O	2.347760000000	-2.882479000000	3.367638000000
O	3.349835000000	0.794648000000	3.495360000000
O	2.193827000000	4.134842000000	3.471448000000
O	1.261560000000	-3.600055000000	-2.751761000000
O	5.105227000000	-2.792040000000	-1.891277000000
O	6.103086000000	0.306093000000	-1.523261000000
O	3.697298000000	2.850377000000	-1.975687000000
N	-0.965633000000	-5.568749000000	0.631289000000
N	1.164273000000	-5.469418000000	1.265095000000
N	3.263334000000	-4.490208000000	1.975344000000
N	4.434500000000	-2.640778000000	2.378544000000
N	5.170975000000	-0.348825000000	2.629728000000
N	5.229794000000	1.876668000000	2.673071000000
N	4.030284000000	3.904989000000	2.066593000000
N	2.455156000000	5.409417000000	1.553143000000
N	-0.274133000000	-4.906305000000	-1.597471000000
N	1.891238000000	-4.994150000000	-1.010646000000

N	4.068652000000	-4.138523000000	-0.307906000000
N	5.754629000000	-2.821419000000	0.331909000000
N	6.516662000000	-0.504449000000	0.602944000000
N	5.966001000000	1.648667000000	0.367108000000
N	4.879528000000	3.761923000000	-0.208494000000
N	2.889179000000	4.626994000000	-0.716845000000
C	-0.129823000000	-5.253606000000	1.687025000000
C	2.267053000000	-5.506685000000	2.191828000000
H	2.756876000000	-6.483986000000	2.141518000000
H	1.847717000000	-5.361307000000	3.186486000000
C	3.238640000000	-3.288770000000	2.652492000000
C	4.915163000000	-1.618483000000	3.271215000000
C	4.459122000000	0.777579000000	2.995249000000
C	4.856022000000	3.222730000000	3.038451000000
C	2.804940000000	4.443341000000	2.481678000000
C	1.337294000000	6.304507000000	1.766923000000
C	-0.238228000000	-5.923988000000	-0.566986000000
H	-0.575718000000	-6.890386000000	-0.956164000000
C	1.253585000000	-5.924348000000	-0.105951000000
H	1.732406000000	-6.907435000000	-0.158826000000
C	4.364932000000	-4.572139000000	1.058024000000
H	4.809553000000	-5.571730000000	1.064354000000
C	5.318948000000	-3.450099000000	1.554201000000
H	6.173963000000	-3.816210000000	2.130958000000
C	6.419065000000	-0.021422000000	1.964993000000
C	6.303437000000	1.520843000000	1.788500000000
C	4.573791000000	4.614321000000	0.923564000000
C	3.342813000000	5.427944000000	0.428671000000
C	0.990456000000	-4.401928000000	-1.889290000000
C	3.316855000000	-4.950921000000	-1.248538000000
H	3.703191000000	-5.977213000000	-1.236534000000
H	3.476795000000	-4.514953000000	-2.233824000000
C	4.980900000000	-3.197835000000	-0.751917000000
C	6.836035000000	-1.872800000000	0.232881000000
H	7.659749000000	-2.210404000000	0.865709000000
H	7.168092000000	-1.856928000000	-0.802992000000
C	6.180805000000	0.457903000000	-0.316029000000
C	6.049126000000	2.923699000000	-0.325531000000
C	3.811068000000	3.671977000000	-1.067936000000
C	1.900872000000	5.111605000000	-1.663487000000
O	-0.248558000000	3.596647000000	-2.804168000000
O	-4.090771000000	2.871818000000	-3.937907000000
O	-5.260382000000	-0.058755000000	-4.219408000000
O	-2.767865000000	-2.599334000000	-3.632699000000
O	-1.095037000000	5.093077000000	2.787010000000
O	-4.310455000000	2.775084000000	2.025310000000
O	-5.490366000000	-0.735507000000	1.649716000000
O	-3.976571000000	-3.682774000000	1.909204000000
N	0.535888000000	5.068846000000	-1.188473000000
N	-1.635251000000	5.118297000000	-1.737953000000
N	-3.853280000000	4.149874000000	-2.014188000000
N	-5.744111000000	2.980214000000	-2.312929000000
N	-6.614187000000	0.705745000000	-2.499161000000
N	-5.990980000000	-1.449933000000	-2.509913000000
N	-4.623406000000	-3.468071000000	-2.545770000000
N	-2.592913000000	-4.302302000000	-2.061039000000

N	0.139091000000	5.984187000000	1.034964000000
N	-1.977412000000	5.364173000000	0.655071000000
N	-4.201629000000	4.408065000000	0.382306000000
N	-5.624012000000	2.713870000000	0.117682000000
N	-6.506902000000	0.459193000000	-0.060267000000
N	-6.519546000000	-1.757838000000	-0.148551000000
N	-5.034192000000	-3.691254000000	-0.153795000000
N	-3.286641000000	-5.030353000000	0.150042000000
C	-0.442511000000	4.492613000000	-2.003184000000
C	-2.810660000000	4.985303000000	-2.568323000000
C	-4.511888000000	3.269724000000	-2.885648000000
C	-6.688705000000	2.083481000000	-2.940829000000
C	-5.868864000000	-0.235624000000	-3.201610000000
C	-5.637541000000	-2.674887000000	-3.201807000000
C	-3.273761000000	-3.353780000000	-2.842210000000
C	-1.344672000000	-4.843542000000	-2.571431000000
H	-1.015198000000	-4.189116000000	-3.378124000000
H	-1.522948000000	-5.850977000000	-2.972065000000
C	-0.020415000000	6.154688000000	-0.378597000000
C	-1.550563000000	5.985095000000	-0.589648000000
C	-4.730926000000	4.601976000000	-0.949564000000
C	-5.905161000000	3.584581000000	-1.024472000000
C	-7.214378000000	0.165567000000	-1.318582000000
C	-6.992364000000	-1.370987000000	-1.467641000000
C	-4.872440000000	-4.354454000000	-1.450516000000
H	-5.723752000000	-5.011302000000	-1.649986000000
C	-3.519116000000	-5.102163000000	-1.276484000000
H	-3.543494000000	-6.142584000000	-1.614064000000
C	-0.983896000000	5.432984000000	1.635336000000
C	-3.365812000000	5.356736000000	1.074280000000
C	-4.662781000000	3.249346000000	0.958500000000
C	-6.573930000000	1.747149000000	0.602513000000
C	-6.115623000000	-0.677155000000	0.581802000000
C	-6.291406000000	-3.116308000000	0.276926000000
H	-7.114512000000	-3.728504000000	-0.101789000000
H	-6.308639000000	-3.137025000000	1.364369000000
C	-4.083353000000	-4.097138000000	0.757756000000
C	-2.355055000000	-5.875373000000	0.855994000000
H	-2.543351000000	-5.762030000000	1.922356000000
H	-2.550118000000	-6.912410000000	0.561840000000
H	5.836637000000	-1.957830000000	3.760683000000
H	4.143624000000	-1.457774000000	4.023466000000
H	7.283125000000	-0.341594000000	2.553219000000
H	7.218881000000	2.069590000000	2.023746000000
H	5.437498000000	5.228706000000	1.192612000000
H	3.577398000000	6.448830000000	0.114852000000
H	0.366897000000	7.122656000000	-0.712107000000
H	-2.078833000000	6.926352000000	-0.770839000000
H	-5.041455000000	5.642095000000	-1.093296000000
H	-6.894639000000	4.040335000000	-0.919895000000
H	-8.264294000000	0.457028000000	-1.227699000000
H	-7.898863000000	-1.927063000000	-1.723334000000
H	6.205924000000	2.706478000000	-1.379549000000
H	6.905277000000	3.491202000000	0.050601000000
H	1.964177000000	4.487661000000	-2.553524000000
H	2.156737000000	6.145001000000	-1.932680000000

H	-2.511792000000	4.524867000000	-3.509476000000
H	-3.194103000000	5.994385000000	-2.764181000000
H	-6.469069000000	2.083583000000	-4.008138000000
H	-7.701049000000	2.458256000000	-2.774330000000
H	-5.244684000000	-2.376246000000	-4.173861000000
H	-6.524580000000	-3.301079000000	-3.342093000000
H	5.774309000000	3.788986000000	3.223621000000
H	4.273318000000	3.168236000000	3.957446000000
H	1.652563000000	7.319660000000	1.509969000000
H	1.085877000000	6.256099000000	2.825953000000
H	-7.589023000000	2.141324000000	0.479780000000
H	-6.383814000000	1.592028000000	1.662607000000
H	-3.371292000000	5.103193000000	2.133225000000
H	-3.799723000000	6.354788000000	0.938329000000
N	0.115166000000	-1.295686000000	4.844629000000
N	0.985266000000	-1.096784000000	5.479200000000
C	-2.902395000000	-0.188434000000	5.695759000000
C	-2.270470000000	1.128745000000	5.982904000000
H	-2.080015000000	1.740861000000	5.100440000000
H	-2.902921000000	1.712227000000	6.666943000000
H	-1.320120000000	0.982834000000	6.501618000000
C	-2.820307000000	-1.276195000000	6.714530000000
H	-3.809289000000	-1.666907000000	6.979453000000
H	-2.219393000000	-2.120797000000	6.351513000000
H	-2.352427000000	-0.917218000000	7.629679000000
C	-3.631021000000	-0.414871000000	4.477369000000
N	-3.824772000000	0.562301000000	3.589216000000
N	-4.104943000000	-1.634184000000	4.185880000000
H	-4.681712000000	-1.793017000000	3.367285000000
H	-3.982085000000	-2.401305000000	4.825579000000
H	-4.441602000000	0.413626000000	2.794760000000
H	-3.612734000000	1.525995000000	3.794166000000
N	2.941226000000	-0.729430000000	-2.246994000000
N	2.940102000000	-0.914072000000	-3.326082000000
C	6.006848000000	-0.169924000000	-6.308559000000
C	5.618838000000	1.022350000000	-7.115767000000
H	4.758608000000	1.559923000000	-6.709612000000
H	6.457245000000	1.729851000000	-7.193083000000
H	5.372641000000	0.725608000000	-8.136244000000
C	6.577957000000	-1.358363000000	-7.005016000000
H	7.324898000000	-1.890540000000	-6.411612000000
H	5.784745000000	-2.071886000000	-7.272256000000
H	7.050792000000	-1.058840000000	-7.941323000000
C	5.838844000000	-0.171511000000	-4.878928000000
N	6.054068000000	-1.282223000000	-4.171863000000
N	5.454486000000	0.936910000000	-4.235280000000
H	5.432205000000	0.961612000000	-3.220407000000
H	5.362332000000	1.803738000000	-4.736203000000
H	5.868711000000	-1.341063000000	-3.175078000000
H	6.216337000000	-2.153869000000	-4.647805000000
C	-0.173948000000	0.763990000000	0.646738000000
C	-1.308470000000	1.690372000000	0.151837000000
H	-1.525465000000	1.607761000000	-0.913541000000
H	-2.222916000000	1.496044000000	0.709699000000
H	-1.047627000000	2.729575000000	0.355176000000
C	-0.110158000000	0.908835000000	2.181423000000

H	0.635672000000	0.271277000000	2.654964000000
H	0.097290000000	1.942868000000	2.465068000000
H	-1.079017000000	0.645631000000	2.605894000000
C	1.142472000000	1.241530000000	0.020291000000
N	2.251740000000	1.234867000000	0.740978000000
N	1.184318000000	1.635834000000	-1.233566000000
H	0.349039000000	1.834957000000	-1.771924000000
H	2.056149000000	1.978637000000	-1.648874000000
H	2.264201000000	1.009445000000	1.731780000000
H	3.131426000000	1.527975000000	0.337039000000
C	-0.363042000000	-0.786293000000	0.226760000000
C	-0.639190000000	-0.982882000000	-1.283843000000
H	0.247709000000	-0.741715000000	-1.863190000000
H	-0.872157000000	-2.028243000000	-1.482315000000
H	-1.462510000000	-0.385616000000	-1.675726000000
C	0.891420000000	-1.612476000000	0.573042000000
H	1.205943000000	-1.525758000000	1.613216000000
H	0.714460000000	-2.666565000000	0.359419000000
H	1.724309000000	-1.306076000000	-0.054830000000
C	-1.570145000000	-1.364586000000	0.976720000000
N	-1.427246000000	-2.199399000000	1.981188000000
N	-2.790327000000	-1.047248000000	0.573255000000
H	-2.921304000000	-0.478505000000	-0.245971000000
H	-3.626936000000	-1.347503000000	1.067613000000
H	-0.522047000000	-2.491538000000	2.324087000000
H	-2.229551000000	-2.724138000000	2.333291000000

2R[•] and 2,2,3,3-tetramethylbutane-1,4-bisamidine (the compound generated by self-reaction of two R[•]) from 2AAPH@CB[8] in PCM model

Total Energy= -6106.69527173

Total and zero-point Energy= -6104.976443

Total and thermal Energy= -6104.868114

Total Energy and thermal Enthalpies= -6104.867170

Total and thermal Free Energy= -6105.119854

4 3

O	1.209782000000	-4.852711000000	-2.771177000000
O	-2.287417000000	-3.202459000000	-3.496453000000
O	-3.961014000000	0.180223000000	-3.582823000000
O	-3.281615000000	3.665326000000	-3.461665000000
O	-0.760591000000	-4.323931000000	3.000932000000
O	-4.595996000000	-3.780554000000	2.049330000000
O	-5.999799000000	-0.812369000000	1.832911000000
O	-4.079060000000	2.684452000000	2.350852000000
N	1.708117000000	-5.538454000000	-0.620151000000
N	-0.422010000000	-5.548771000000	-1.271897000000
N	-2.660632000000	-4.870559000000	-1.935757000000
N	-4.276983000000	-3.387424000000	-2.327641000000
N	-5.407396000000	-1.233246000000	-2.449901000000
N	-5.743578000000	0.971035000000	-2.339826000000
N	-5.047071000000	3.284611000000	-2.011920000000
N	-3.492204000000	4.773909000000	-1.434936000000
N	0.919862000000	-5.192703000000	1.668130000000
N	-1.206471000000	-5.481158000000	1.041342000000
N	-3.466215000000	-4.906283000000	0.368952000000
N	-5.314611000000	-3.774931000000	-0.147952000000

N	-6.461951000000	-1.627808000000	-0.282670000000
N	-6.267771000000	0.571661000000	-0.006733000000
N	-5.262888000000	2.754083000000	0.350909000000
N	-3.997695000000	4.506494000000	0.942369000000
C	0.867237000000	-5.263936000000	-1.670532000000
C	-1.498510000000	-5.678326000000	-2.231511000000
H	-1.814448000000	-6.723780000000	-2.290547000000
H	-1.107318000000	-5.363886000000	-3.196493000000
C	-3.001182000000	-3.762874000000	-2.671741000000
C	-5.034211000000	-2.454895000000	-3.133390000000
C	-4.940440000000	-0.012670000000	-2.874179000000
C	-5.759050000000	2.335388000000	-2.833486000000
C	-3.867693000000	3.880754000000	-2.419301000000
C	-2.499291000000	5.793720000000	-1.705377000000
C	1.013832000000	-6.084123000000	0.522470000000
H	1.454190000000	-7.039557000000	0.818073000000
C	-0.456946000000	-6.193394000000	0.031822000000
H	-0.813777000000	-7.221952000000	-0.057880000000
C	-3.710606000000	-5.262500000000	-1.021808000000
H	-3.930574000000	-6.327388000000	-1.119005000000
C	-4.898738000000	-4.334592000000	-1.411663000000
H	-5.726136000000	-4.853271000000	-1.898838000000
C	-6.601804000000	-1.105212000000	-1.621133000000
C	-6.691571000000	0.432359000000	-1.395772000000
C	-5.483116000000	3.738536000000	-0.717579000000
C	-4.478931000000	4.878769000000	-0.375931000000
C	-0.390609000000	-4.924681000000	2.002472000000
C	-2.621020000000	-5.686419000000	1.247705000000
H	-2.841096000000	-6.750456000000	1.116931000000
H	-2.860114000000	-5.392365000000	2.267124000000
C	-4.466326000000	-4.108698000000	0.878141000000
C	-6.534073000000	-3.028849000000	0.067014000000
H	-7.337559000000	-3.490406000000	-0.508634000000
H	-6.763889000000	-3.087031000000	1.128307000000
C	-6.209052000000	-0.643969000000	0.640215000000
C	-6.319556000000	1.813327000000	0.722718000000
C	-4.421203000000	3.273106000000	1.329854000000
C	-3.208833000000	5.363097000000	1.811129000000
O	-1.039616000000	4.450905000000	3.474641000000
O	2.779571000000	3.575575000000	4.385027000000
O	4.613302000000	0.406923000000	4.767357000000
O	2.846014000000	-2.777089000000	4.065234000000
O	0.142255000000	4.871532000000	-2.439028000000
O	3.776145000000	3.580513000000	-1.648338000000
O	5.416111000000	0.283699000000	-1.269416000000
O	4.392207000000	-3.121957000000	-1.700357000000
N	-1.801624000000	5.404946000000	1.500328000000
N	0.364977000000	5.580783000000	2.017343000000
N	2.651441000000	4.874783000000	2.468499000000
N	4.491713000000	3.657189000000	2.825255000000
N	5.689363000000	1.544453000000	3.059982000000
N	5.731137000000	-0.684468000000	3.055387000000
N	4.775457000000	-2.906543000000	2.787172000000
N	3.077267000000	-4.277836000000	2.311416000000
N	-1.331114000000	5.726365000000	-0.867210000000
N	0.841098000000	5.659705000000	-0.372302000000

N	3.123269000000	4.981538000000	0.074015000000
N	4.847430000000	3.615465000000	0.403859000000
N	5.985044000000	1.489686000000	0.626219000000
N	6.197530000000	-0.722064000000	0.655162000000
N	5.334176000000	-2.975304000000	0.412177000000
N	3.844348000000	-4.574852000000	0.019003000000
C	-0.841734000000	5.068719000000	2.445023000000
C	1.516919000000	5.671570000000	2.886090000000
C	3.253379000000	3.984343000000	3.341728000000
C	5.466239000000	2.882181000000	3.564405000000
C	5.266405000000	0.420469000000	3.741722000000
C	5.598834000000	-2.023197000000	3.584302000000
C	3.490586000000	-3.255316000000	3.151612000000
C	1.965086000000	-5.123237000000	2.671893000000
H	1.522942000000	-4.713148000000	3.576896000000
H	2.329514000000	-6.137475000000	2.870036000000
C	-1.273288000000	6.275402000000	0.465664000000
C	0.248515000000	6.316350000000	0.776941000000
C	3.555150000000	5.303359000000	1.416697000000
C	4.805261000000	4.398257000000	1.624513000000
C	6.547813000000	1.225594000000	1.941514000000
C	6.635215000000	-0.330169000000	1.980971000000
C	5.269213000000	-3.687700000000	1.678635000000
H	6.238111000000	-4.131926000000	1.916028000000
C	4.138586000000	-4.726826000000	1.428513000000
H	4.424690000000	-5.757054000000	1.651983000000
C	-0.091963000000	5.356120000000	-1.345907000000
C	2.239294000000	5.813673000000	-0.702489000000
C	3.893698000000	4.003784000000	-0.509370000000
C	5.974761000000	2.804077000000	0.024942000000
C	5.811354000000	0.347059000000	-0.106997000000
C	6.384026000000	-2.038137000000	0.094112000000
H	7.335997000000	-2.435818000000	0.454446000000
H	6.421726000000	-1.942409000000	-0.988269000000
C	4.510344000000	-3.514131000000	-0.542014000000
C	3.144605000000	-5.562867000000	-0.766474000000
H	3.365174000000	-5.372610000000	-1.814271000000
H	3.512509000000	-6.553533000000	-0.485998000000
H	-5.942649000000	-2.948520000000	-3.490192000000
H	-4.411568000000	-2.178774000000	-3.981646000000
H	-7.471245000000	-1.535274000000	-2.120591000000
H	-7.687469000000	0.849436000000	-1.550470000000
H	-6.525714000000	4.059875000000	-0.730107000000
H	-4.927218000000	5.873098000000	-0.350866000000
H	-1.757616000000	7.254505000000	0.502917000000
H	0.644570000000	7.328526000000	0.890960000000
H	3.768090000000	6.371850000000	1.503163000000
H	5.736487000000	4.956065000000	1.750685000000
H	7.514579000000	1.723745000000	2.041831000000
H	7.640048000000	-0.711522000000	2.175631000000
H	-6.203792000000	1.572358000000	1.776834000000
H	-7.286089000000	2.301119000000	0.566374000000
H	-3.309871000000	4.982436000000	2.824834000000
H	-3.630506000000	6.369858000000	1.752798000000
H	1.217058000000	5.313046000000	3.868307000000
H	1.819572000000	6.721822000000	2.954429000000

H	5.095947000000	2.781010000000	4.582394000000
H	6.415762000000	3.423778000000	3.567501000000
H	5.134009000000	-1.929932000000	4.563562000000
H	6.588931000000	-2.475626000000	3.687471000000
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H	-2.958420000000	6.779914000000	-1.592075000000
H	-2.175396000000	5.655368000000	-2.734617000000
H	6.898919000000	3.319927000000	0.301438000000
H	5.944529000000	2.679744000000	-1.055099000000
H	2.359758000000	5.535494000000	-1.747071000000
H	2.527619000000	6.861317000000	-0.565598000000
N	-1.176588000000	-0.883894000000	-5.602602000000
N	-2.154045000000	-1.202270000000	-5.979009000000
C	2.512288000000	0.304687000000	-5.067593000000
C	1.751196000000	1.549233000000	-5.370798000000
H	1.592376000000	2.198912000000	-4.510006000000
H	2.277187000000	2.133765000000	-6.138038000000
H	0.774071000000	1.294624000000	-5.786359000000
C	2.363882000000	-0.868808000000	-5.975712000000
H	3.320352000000	-1.348302000000	-6.201479000000
H	1.709549000000	-1.628744000000	-5.529039000000
H	1.905907000000	-0.565746000000	-6.916547000000
C	3.400340000000	0.231454000000	-3.937123000000
N	3.609682000000	1.286559000000	-3.156744000000
N	4.020624000000	-0.912632000000	-3.629328000000
H	4.622980000000	-0.972469000000	-2.815122000000
H	3.864126000000	-1.753206000000	-4.158529000000
H	4.250782000000	1.221719000000	-2.367823000000
H	3.218665000000	2.193609000000	-3.347292000000
N	2.245178000000	0.913038000000	3.044529000000
N	2.750088000000	1.100645000000	2.090492000000
C	-1.348683000000	-0.269204000000	4.050860000000
C	-1.233424000000	1.185183000000	4.350887000000
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H	-1.327941000000	1.346990000000	5.433515000000
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C	-0.243926000000	-1.172372000000	4.489940000000
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N	-3.591158000000	-0.074437000000	3.161499000000
H	-4.427482000000	-0.461817000000	2.723978000000
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H	-1.822749000000	-2.769293000000	3.372910000000
C	-0.453145000000	0.682101000000	-1.148279000000
C	0.803149000000	1.519068000000	-0.841249000000
H	1.059101000000	1.579228000000	0.214701000000
H	1.666104000000	1.100298000000	-1.355273000000
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C	-0.689868000000	0.759127000000	-2.668949000000
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H	-0.618083000000	1.873245000000	1.208028000000
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C	-0.330255000000	-0.848898000000	-0.648770000000
C	0.170467000000	-0.963683000000	0.802409000000
H	-0.568798000000	-0.552830000000	1.484491000000
H	0.310126000000	-2.013356000000	1.062464000000
H	1.105319000000	-0.443228000000	0.986020000000
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H	-2.199046000000	-1.455340000000	-1.659104000000
H	-1.552884000000	-2.635760000000	-0.510945000000
H	-2.352817000000	-1.190161000000	0.069535000000
C	0.662753000000	-1.589089000000	-1.555093000000
N	0.249459000000	-2.225670000000	-2.627072000000
N	1.944678000000	-1.603798000000	-1.239045000000
H	2.271086000000	-1.171938000000	-0.391137000000
H	2.642007000000	-2.135275000000	-1.759009000000
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