

Supplementary Materials

Probing micro hydration induced effects on Carbonyl Compounds

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Figure S1: Outermost molecular orbitals of carbonyls – water clusters. Page 2

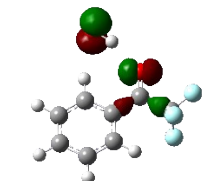
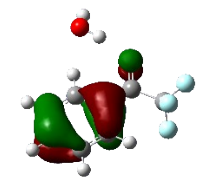
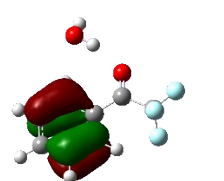
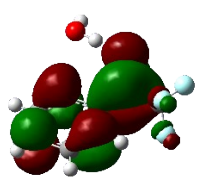
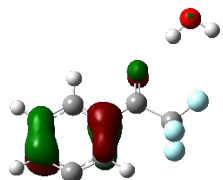
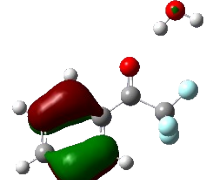
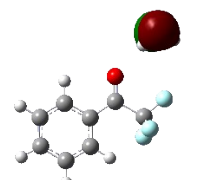
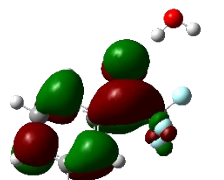
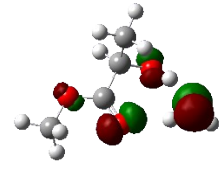
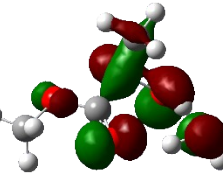
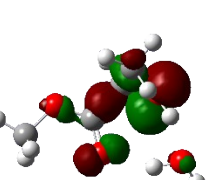
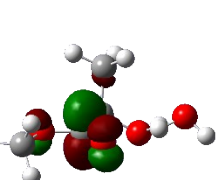
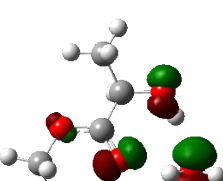
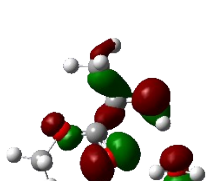
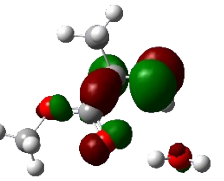
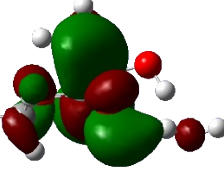
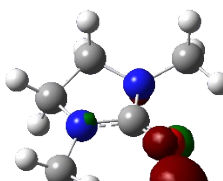
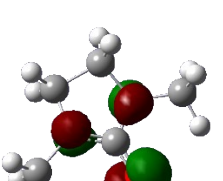
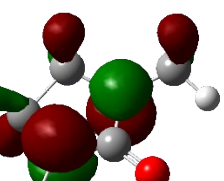
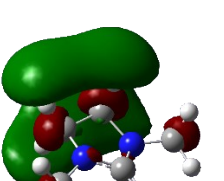
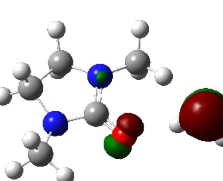
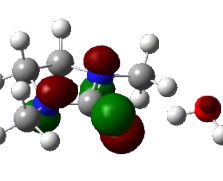
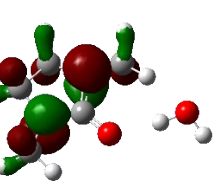
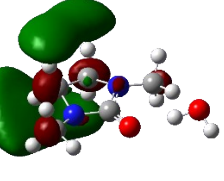
Table S1: Cartesian coordinates of the mono-hydrated complexes optimized at the PBE0/aug-cc-pVTZ with the GD3 correction. Energies are given in Hartree and include the ZPE correction. Page 4

Table S2 : Singlet excited states. Page 21

Table S3: Triplet excited states. Page 24

Table S4: Vibrational and Topological characterisation of the monohydrated complexes. Electron densities $\rho(r)$ at the intermolecular bond critical points are given in a.u. Scaled vibrational frequencies are given in cm⁻¹ (Scaling factor: 0.9604). Page 27

Figure S1: Outermost molecular orbitals of carbonyls – water clusters.

Complex	HOMO-2	HOMO-1	HOMO	LUMO
TPH_1				
TPH_2				
MLA_1				
MLA_2				
DMI_1				
DMI_2				

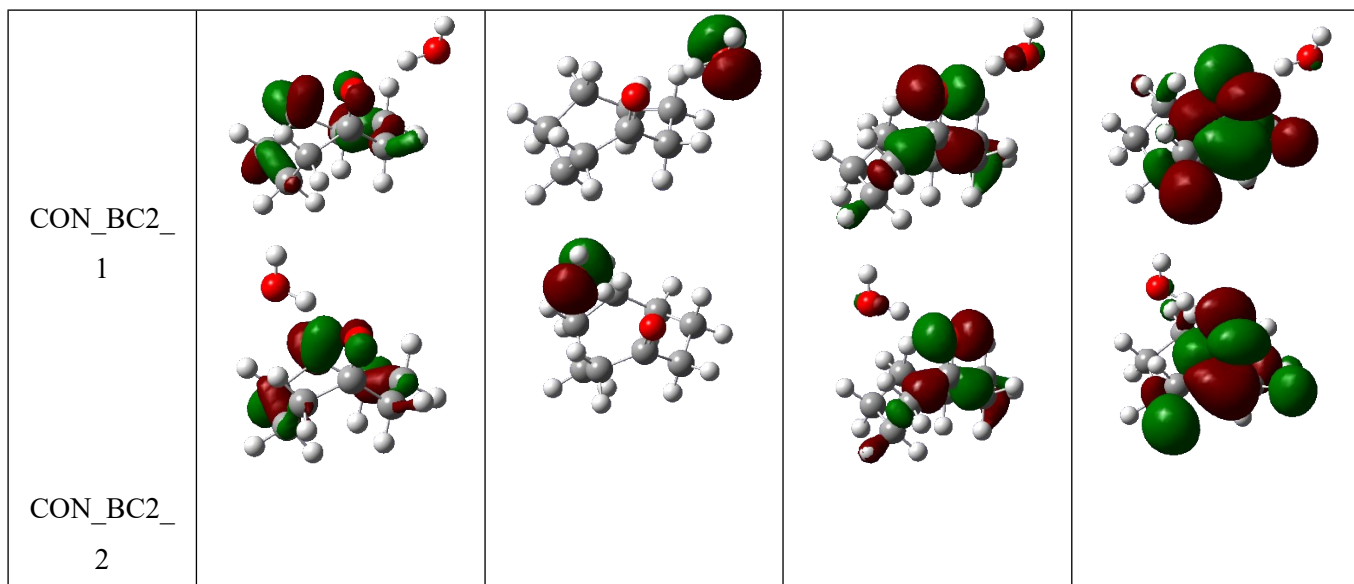


Table S1: Cartesian coordinates of the mono-hydrated complexes optimized at the PBE0/aug-cc-pVTZ with the GD3 correction. Energies are given in Hartree and include the ZPE correction.

1. TPH

a. TPH ; $E_{\text{ZPE}} = -682.037459$

C	-2.325010000	-1.428412000	0.000344000
C	-3.326789000	-0.468992000	0.000077000
C	-0.994088000	-1.044984000	0.000294000
H	-4.366352000	-0.773978000	0.000111000
H	-0.225162000	-1.804569000	0.000517000
C	-3.000287000	0.882159000	-0.000222000
C	-0.660284000	0.309941000	-0.000014000
H	-3.782985000	1.630441000	-0.000425000
C	-1.674763000	1.269889000	-0.000256000
H	-2.580304000	-2.480616000	0.000593000
H	-1.396767000	2.316163000	-0.000475000
C	0.731697000	0.806022000	-0.000041000
C	1.886226000	-0.235853000	-0.000065000
F	3.064562000	0.359070000	0.000529000
F	1.816285000	-1.023812000	1.082725000
F	1.817018000	-1.023062000	-1.083430000
O	1.031322000	1.970522000	0.000070000

b. TPH_1 ; $E_{\text{ZPE}} = -758.402739$

C	3.000014000	0.068401000	0.042161000
C	3.154868000	-1.311815000	0.002550000
C	2.040884000	-2.138258000	-0.035031000
C	0.770374000	-1.590248000	-0.033200000
C	0.607760000	-0.202508000	0.004438000
C	1.735404000	0.624389000	0.042737000
H	3.868866000	0.713754000	0.071969000
H	4.148079000	-1.744781000	0.001180000
H	2.161570000	-3.213746000	-0.065940000
H	-0.086220000	-2.248288000	-0.063166000
H	1.615029000	1.699671000	0.075257000
C	-0.715320000	0.441636000	0.004388000
O	-0.901755000	1.633856000	0.004580000
C	-1.982548000	-0.461583000	0.006183000
F	-2.017907000	-1.232510000	-1.089188000
F	-1.992419000	-1.266744000	1.077141000
F	-3.083335000	0.267001000	0.030779000
O	0.873884000	3.905316000	-0.088177000
H	0.555251000	4.705282000	0.331193000
H	0.134728000	3.284926000	-0.055674000

c. TPH_2 ; $E_{\text{ZPE}} = -758.401043$

C	-3.110892000	-0.830811000	0.064064000
C	-3.750435000	0.399972000	0.033523000
C	-3.008025000	1.574089000	-0.021206000
C	-1.628991000	1.515126000	-0.045126000
C	-0.977260000	0.279170000	-0.015026000

C	-1.728330000	-0.896604000	0.039791000
H	-3.691199000	-1.743838000	0.106991000
H	-4.832722000	0.445505000	0.052525000
H	-3.508833000	2.533768000	-0.044895000
H	-1.030616000	2.416351000	-0.087119000
H	-1.244468000	-1.862861000	0.064285000
C	0.494167000	0.296908000	-0.042376000
O	1.152606000	1.305936000	-0.083431000
C	1.255505000	-1.058379000	-0.018207000
F	0.966439000	-1.746261000	1.093393000
F	0.917545000	-1.812841000	-1.070873000
F	2.563857000	-0.866980000	-0.053891000
O	4.022855000	2.100433000	0.100967000
H	3.095911000	1.843889000	0.041363000
H	4.503241000	1.274150000	0.036277000

d. TPH_3 ; E_{ZPE} = -758.400056

C	-3.291920000	0.647912000	-0.035506000
C	-3.348658000	-0.740720000	0.017632000
C	-2.179736000	-1.485240000	0.063604000
C	-0.947317000	-0.851938000	0.057399000
C	-0.885910000	0.541394000	0.002553000
C	-2.067859000	1.286065000	-0.043522000
H	-4.205318000	1.228527000	-0.071554000
H	-4.309300000	-1.241927000	0.022449000
H	-2.220229000	-2.566508000	0.102921000
H	-0.054455000	-1.461421000	0.094789000
H	-1.999169000	2.365643000	-0.085939000
C	0.379744000	1.298946000	-0.013125000
O	0.451805000	2.499037000	-0.055071000
C	1.720092000	0.508899000	0.025868000
F	1.808744000	-0.242562000	1.131935000
F	1.824920000	-0.314174000	-1.034303000
F	2.756251000	1.326201000	0.003445000
O	1.435119000	-3.293395000	-0.125568000
H	1.974494000	-2.703357000	-0.656979000
H	1.938743000	-3.423194000	0.680307000

e. TPH_4 ; E_{ZPE} = -758.400040

C	3.291658000	-0.648169000	-0.039226000
C	3.348540000	0.740249000	0.019416000
C	2.179734000	1.484610000	0.070210000
C	0.947281000	0.851384000	0.063421000
C	0.885696000	-0.541697000	0.002853000
C	2.067568000	-1.286209000	-0.048061000
H	4.204973000	-1.228670000	-0.079018000
H	4.309216000	1.241389000	0.024720000
H	2.220295000	2.565712000	0.113622000
H	0.054604000	1.460781000	0.104909000
H	1.998747000	-2.365599000	-0.094927000
C	-0.379959000	-1.299177000	-0.014557000
O	-0.452071000	-2.499104000	-0.060903000
C	-1.720293000	-0.509289000	0.028380000

F	-1.808179000	0.238260000	1.136906000
F	-1.825862000	0.317604000	-1.029002000
F	-2.756485000	-1.326488000	0.003552000
O	-1.432372000	3.292735000	-0.136909000
H	-1.939598000	3.477391000	0.655837000
H	-1.979305000	2.685355000	-0.640360000

f. TPH_5 ; E_{ZPE} = -758.399292

C	-2.614925000	0.723209000	0.000208000
C	-2.342748000	2.086093000	0.000028000
C	-1.030009000	2.536952000	-0.000037000
C	0.017142000	1.630973000	0.000064000
C	-0.249528000	0.260329000	0.000229000
C	-1.573448000	-0.184174000	0.000286000
H	-3.633388000	0.356537000	0.000236000
H	-3.157513000	2.800534000	-0.000060000
H	-0.819929000	3.599280000	-0.000186000
H	1.033777000	1.998248000	0.000029000
H	-1.777885000	-1.246421000	0.000344000
C	0.804842000	-0.772668000	0.000357000
O	0.592221000	-1.956929000	0.000826000
C	2.290433000	-0.311246000	-0.000148000
F	2.559990000	0.432093000	-1.083474000
F	2.560614000	0.432491000	1.082750000
F	3.111285000	-1.346263000	-0.000193000
O	-4.220417000	-2.216813000	-0.000437000
H	-4.258328000	-2.800170000	0.759907000
H	-4.258719000	-2.799775000	-0.761063000

g. TPH_6 ; E_{ZPE} = -758.399210

C	2.854737000	-1.088136000	-0.388474000
C	3.218125000	-0.171602000	0.591104000
C	2.242961000	0.525563000	1.290852000
C	0.902119000	0.316960000	1.009662000
C	0.532544000	-0.599544000	0.023265000
C	1.519320000	-1.304013000	-0.668888000
H	3.616454000	-1.628936000	-0.935730000
H	4.265134000	0.001181000	0.808484000
H	2.526398000	1.237526000	2.055597000
H	0.154486000	0.869701000	1.561238000
H	1.213563000	-2.008598000	-1.431686000
C	-0.871577000	-0.866597000	-0.354702000
O	-1.212309000	-1.738701000	-1.107359000
C	-1.977674000	0.052729000	0.236033000
F	-2.043228000	-0.072188000	1.568279000
F	-1.715495000	1.343790000	-0.038454000
F	-3.160920000	-0.238697000	-0.265641000
O	1.019344000	2.562933000	-1.582133000
H	1.434474000	1.931714000	-0.989892000
H	0.086676000	2.515242000	-1.362829000

h. TPH_7 ; E_{ZPE} = -758.399196

C	1.964439000	1.937802000	-0.000030000
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C	2.697061000	0.756120000	-0.000248000
C	2.044583000	-0.468336000	-0.000346000
C	0.660681000	-0.519110000	-0.000251000
C	-0.080414000	0.664218000	-0.000044000
C	0.584010000	1.893154000	0.000067000
H	2.473853000	2.893639000	0.000059000
H	3.779834000	0.774125000	-0.000310000
H	2.629257000	-1.379088000	-0.000478000
H	0.166524000	-1.480581000	-0.000332000
H	-0.007022000	2.800257000	0.000234000
C	-1.555755000	0.700300000	0.000071000
O	-2.207943000	1.711373000	0.000215000
C	-2.327092000	-0.650535000	0.000028000
F	-2.017450000	-1.378299000	-1.083202000
F	-2.017190000	-1.378521000	1.083034000
F	-3.633229000	-0.453528000	0.000202000
O	5.270943000	-1.368019000	0.000305000
H	5.769857000	-1.671833000	-0.760352000
H	5.769434000	-1.671887000	0.761218000

2. MLA

a. MLA ; $E_{ZPE} = -382.523571$

C	0.281670000	-0.301116000	-0.046535000
C	-1.116742000	0.161352000	-0.398720000
O	1.205818000	0.618890000	-0.301076000
O	0.516244000	-1.391588000	0.412612000
O	-2.017779000	-0.889565000	-0.188685000
C	-1.515011000	1.387566000	0.408269000
C	2.548501000	0.245263000	0.012120000
H	-1.101193000	0.425602000	-1.465013000
H	-1.500748000	-1.630698000	0.153682000
H	-0.853444000	2.227482000	0.195767000
H	-2.536620000	1.664157000	0.148503000
H	-1.481618000	1.164173000	1.476050000
H	2.643245000	0.023015000	1.075024000
H	2.842035000	-0.633914000	-0.561525000
H	3.163574000	1.099905000	-0.256101000

b. MLA_1; $E_{ZPE} = -458.892138$

O	1.517296000	0.688556000	-1.098642000
C	0.396546000	1.083380000	-0.370356000
C	-0.591522000	-0.057673000	-0.180269000
O	-0.296583000	-1.222469000	-0.036221000
O	-1.846200000	0.379147000	-0.139332000
C	-2.842203000	-0.610318000	0.124070000
C	0.748321000	1.646212000	1.004062000
H	2.004955000	0.012520000	-0.595678000
H	-0.109233000	1.852108000	-0.958846000
H	-3.790589000	-0.080094000	0.132059000
H	-2.835489000	-1.372312000	-0.655084000

H	-2.660222000	-1.086494000	1.087699000
H	1.425561000	2.490497000	0.875971000
H	1.252117000	0.885492000	1.604169000
H	-0.143073000	1.984531000	1.535375000
O	2.406663000	-1.493242000	0.428623000
H	1.460241000	-1.673630000	0.290021000
H	2.879471000	-2.198156000	-0.016152000

c. MLA_2 ; E_{ZPE} = -458.890993

O	1.608367000	1.089089000	0.161924000
C	0.309139000	1.087473000	-0.335003000
C	-0.450258000	-0.180791000	0.035552000
O	0.039571000	-1.177591000	0.513485000
O	-1.740841000	-0.092235000	-0.274642000
C	-2.520572000	-1.263029000	-0.030006000
C	-0.390458000	2.335382000	0.172474000
H	2.077173000	0.277011000	-0.097775000
H	0.297884000	1.103187000	-1.438260000
H	-2.132961000	-2.105497000	-0.603086000
H	-2.503469000	-1.517350000	1.029671000
H	-3.530231000	-1.016771000	-0.347411000
H	0.184524000	3.207307000	-0.137649000
H	-0.430535000	2.322257000	1.262808000
H	-1.401648000	2.411672000	-0.222637000
O	2.667457000	-1.470583000	-0.278467000
H	1.815175000	-1.640318000	0.155491000
H	3.340548000	-1.705151000	0.362348000

d. MLA_3 ; E_{ZPE} = -458.890080

O	-1.594198000	1.108447000	-0.178818000
C	-0.303441000	1.087363000	0.337031000
C	0.447973000	-0.188625000	-0.024646000
O	-0.052536000	-1.194751000	-0.471076000
O	1.744554000	-0.098234000	0.260046000
C	2.517556000	-1.273913000	0.018417000
C	0.415678000	2.331867000	-0.150810000
H	-2.083373000	0.303225000	0.061579000
H	-0.307117000	1.097070000	1.441299000
H	2.472371000	-1.549433000	-1.035052000
H	3.535179000	-1.021909000	0.304313000
H	2.145825000	-2.105143000	0.617992000
H	0.474253000	2.324150000	-1.240264000
H	1.420455000	2.398539000	0.261840000
H	-0.158376000	3.206318000	0.153772000
O	-2.751147000	-1.418300000	0.099761000
H	-1.852436000	-1.619358000	-0.209212000
H	-2.886761000	-1.950904000	0.884478000

e. MLA_4 ; E_{ZPE} = -458.889461

O	1.301022000	-0.886368000	-0.295093000
C	0.401181000	0.185259000	-0.454534000
C	-0.978086000	-0.291757000	-0.054157000
O	-1.171996000	-1.368697000	0.454820000

O	-1.924384000	0.599887000	-0.312621000
C	-3.249660000	0.221161000	0.066854000
C	0.824139000	1.394297000	0.365636000
H	0.811007000	-1.591550000	0.151594000
H	0.361705000	0.459080000	-1.515019000
H	-3.887011000	1.053944000	-0.216911000
H	-3.548687000	-0.687323000	-0.455690000
H	-3.300888000	0.047113000	1.141542000
H	0.811773000	1.152759000	1.430062000
H	0.154867000	2.234801000	0.181740000
H	1.840989000	1.675407000	0.092565000
O	3.932947000	0.077472000	0.154894000
H	3.095255000	-0.387340000	0.012612000
H	4.574836000	-0.389010000	-0.381299000

f. MLA_5 ; E_{ZPE} = -458.889456

O	2.014895000	-1.498489000	-0.317379000
C	1.718273000	-0.130548000	-0.321712000
C	0.222575000	0.067012000	-0.199144000
O	-0.541504000	-0.860665000	-0.041689000
O	-0.137684000	1.332723000	-0.284480000
C	-1.540845000	1.608205000	-0.174123000
C	2.461478000	0.589195000	0.793690000
H	1.177008000	-1.966270000	-0.210985000
H	2.011579000	0.306639000	-1.285903000
H	-1.919839000	1.279058000	0.792443000
H	-1.634569000	2.685331000	-0.276699000
H	-2.093138000	1.096971000	-0.961493000
H	2.286774000	1.664171000	0.750111000
H	3.528511000	0.396631000	0.685337000
H	2.141840000	0.211060000	1.766259000
O	-3.396342000	-0.927181000	0.328225000
H	-3.739467000	-1.811743000	0.458348000
H	-2.442503000	-1.036143000	0.212894000

g. MLA_6 ; E_{ZPE} = -458.889381

O	1.439987000	-0.001190000	0.949397000
C	0.534900000	0.477427000	-0.020136000
C	-0.799568000	-0.201154000	0.199283000
O	-0.997559000	-0.967721000	1.110360000
O	-1.703179000	0.136671000	-0.709481000
C	-2.985520000	-0.477897000	-0.563097000
C	0.421702000	1.989847000	0.049794000
H	0.942317000	-0.626370000	1.496886000
H	0.888523000	0.184867000	-1.016662000
H	-3.427165000	-0.210068000	0.396644000
H	-3.589704000	-0.098049000	-1.382206000
H	-2.894628000	-1.562282000	-0.623359000
H	1.411342000	2.425525000	-0.085358000
H	0.037304000	2.298625000	1.023371000
H	-0.238933000	2.363314000	-0.732394000
O	3.349972000	-0.921218000	-0.889675000
H	2.855079000	-0.668993000	-0.095449000

H 4.273006000 -0.808238000 -0.661347000

h. MLA_Pi ; E_{ZPE} = -458.886555

C -0.058274000 -0.220842000 0.309930000
C 1.251278000 0.158576000 -0.346879000
O -0.764075000 -1.076024000 -0.410744000
O -0.394359000 0.208818000 1.389769000
O 1.901718000 1.116629000 0.444753000
C 2.136767000 -1.056872000 -0.573055000
C -2.056958000 -1.398004000 0.102212000
H 0.988391000 0.604122000 -1.313826000
H 1.372173000 1.203447000 1.248537000
H 1.653855000 -1.772634000 -1.238573000
H 3.076175000 -0.732303000 -1.020385000
H 2.360780000 -1.545600000 0.376928000
H -1.979625000 -1.802648000 1.111201000
H -2.678699000 -0.502859000 0.113121000
H -2.468034000 -2.139719000 -0.577364000
O -1.602300000 1.867978000 -0.735446000
H -1.426908000 2.213286000 0.142897000
H -1.662860000 2.638554000 -1.302441000

3. DMI

a. DMI ; E_{ZPE} = -380.853417

N -1.093982000 -0.114925000 0.194653000
C -0.756083000 -1.485156000 -0.101689000
C 0.000005000 0.701082000 0.000151000
C 0.756107000 -1.485153000 0.101603000
N 1.093969000 -0.114892000 -0.194631000
H -1.016584000 -1.739706000 -1.139531000
H 1.270431000 -2.182233000 -0.562344000
H -1.270418000 -2.182300000 0.562180000
H 1.016644000 -1.739783000 1.139416000
O -0.000028000 1.914480000 0.000063000
C 2.422277000 0.384295000 0.014248000
H 3.120169000 -0.084678000 -0.682399000
H 2.412267000 1.459183000 -0.159149000
H 2.771436000 0.195943000 1.038221000
C -2.422270000 0.384275000 -0.014327000
H -3.120246000 -0.084864000 0.682122000
H -2.412312000 1.459126000 0.159301000
H -2.771287000 0.196133000 -1.038389000

b. DMI_1 ; E_{ZPE} = -457.222158

O -0.884937000 -1.096161000 -0.305800000
N -0.065048000 1.032301000 0.106539000
N 1.369061000 -0.637308000 -0.176416000
C 1.236609000 1.653226000 0.031311000
C 2.167212000 0.472407000 0.287239000
C 0.035692000 -0.310174000 -0.141443000
C -1.252699000 1.783356000 -0.197911000

C	1.800714000	-1.992826000	0.013921000
H	1.345845000	2.446570000	0.772346000
H	1.405348000	2.084772000	-0.965420000
H	3.108552000	0.549577000	-0.259130000
H	2.394884000	0.369297000	1.357749000
H	-2.126312000	1.140530000	-0.110071000
H	-1.215548000	2.196166000	-1.214154000
H	-1.356533000	2.609103000	0.508210000
H	1.000145000	-2.655553000	-0.309562000
H	2.027491000	-2.201550000	1.067364000
H	2.693760000	-2.192899000	-0.581107000
O	-3.562252000	-0.717966000	0.348734000
H	-2.645622000	-0.945051000	0.113512000
H	-4.107759000	-1.288833000	-0.192773000

c. DMI_2 ; E_{ZPE} = -457.222157

O	0.885380000	-1.095766000	-0.303439000
N	0.064284000	1.032470000	0.107166000
N	-1.368981000	-0.637778000	-0.176329000
C	-1.237495000	1.652951000	0.030392000
C	-2.168012000	0.471916000	0.285762000
C	-0.035746000	-0.310134000	-0.140326000
C	1.252005000	1.783708000	-0.196516000
C	-1.800389000	-1.993373000	0.013912000
H	-1.405298000	2.084152000	-0.966640000
H	-1.347761000	2.446489000	0.771068000
H	-2.397020000	0.369259000	1.356031000
H	-3.108715000	0.548566000	-0.261788000
H	2.125575000	1.140822000	-0.108532000
H	1.355548000	2.609267000	0.509874000
H	1.215251000	2.196799000	-1.212662000
H	-2.691310000	-2.194807000	-0.583860000
H	-2.030537000	-2.201096000	1.066816000
H	-0.998245000	-2.655843000	-0.306198000
O	3.564255000	-0.717367000	0.346525000
H	4.108876000	-1.287126000	-0.197053000
H	2.647256000	-0.944669000	0.113057000

d. DMI_3 ; E_{ZPE} = -457.222139

O	-0.886518000	-1.113305000	-0.036969000
N	-0.039973000	1.034720000	0.175555000
N	1.363873000	-0.645036000	-0.185167000
C	1.239576000	1.652037000	-0.084543000
C	2.201883000	0.487799000	0.126072000
C	0.040624000	-0.318520000	-0.017384000
C	-1.260822000	1.767759000	-0.024372000
C	1.824545000	-1.989583000	0.011764000
H	1.427806000	2.485207000	0.594307000
H	1.289015000	2.027682000	-1.116270000
H	3.074347000	0.536739000	-0.527398000
H	2.550775000	0.442300000	1.167667000
H	-2.113077000	1.135963000	0.217127000
H	-1.360584000	2.108843000	-1.062388000

H	-1.274640000	2.640688000	0.630736000
H	0.996943000	-2.667505000	-0.189077000
H	2.173087000	-2.152336000	1.039850000
H	2.644491000	-2.213213000	-0.673328000
O	-3.638235000	-0.685907000	-0.032198000
H	-2.695052000	-0.924638000	-0.044422000
H	-4.057224000	-1.350774000	0.514601000

e. DMI_4 ; $E_{ZPE} = -457.219166$

O	-0.500704000	-1.659299000	-1.099510000
N	-1.313012000	0.017308000	0.267258000
N	0.875897000	-0.400969000	0.279906000
C	-0.725720000	1.068843000	1.065126000
C	0.630234000	0.467029000	1.416398000
C	-0.346518000	-0.785356000	-0.274063000
C	-2.587816000	0.178835000	-0.371372000
C	1.943490000	-1.367524000	0.343331000
H	-1.328937000	1.287035000	1.947845000
H	-0.607620000	1.988009000	0.477533000
H	1.410806000	1.221506000	1.517612000
H	0.577904000	-0.118435000	2.344412000
H	-2.768667000	-0.694343000	-0.996075000
H	-2.609795000	1.076593000	-1.000988000
H	-3.380826000	0.256263000	0.375090000
H	1.878920000	-2.007202000	-0.535174000
H	1.868719000	-1.993150000	1.241673000
H	2.908016000	-0.857947000	0.349398000
O	1.572765000	1.942120000	-1.321585000
H	1.657842000	1.844932000	-2.270987000
H	1.394925000	1.048840000	-0.988241000

f. DMI_5 ; $E_{ZPE} = -457.219167$

O	-0.500722000	1.659686000	-1.099173000
N	-1.312676000	-0.017453000	0.267095000
N	0.876175000	0.400919000	0.279616000
C	-0.725303000	-1.069005000	1.064884000
C	0.630524000	-0.466990000	1.416215000
C	-0.346367000	0.785454000	-0.274067000
C	-2.587953000	-0.178343000	-0.370690000
C	1.943818000	1.367407000	0.342943000
H	-0.607037000	-1.988098000	0.477205000
H	-1.328554000	-1.287329000	1.947546000
H	0.577932000	0.118592000	2.344151000
H	1.411228000	-1.221282000	1.517603000
H	-2.610623000	-1.075720000	-1.000815000
H	-2.769051000	0.695235000	-0.994764000
H	-3.380414000	-0.256009000	0.376333000
H	1.878625000	2.007638000	-0.535115000
H	2.908344000	0.857824000	0.348023000
H	1.869650000	1.992470000	1.241727000
O	1.571310000	-1.942664000	-1.321498000
H	1.658344000	-1.845752000	-2.270749000
H	1.394046000	-1.049147000	-0.988460000

4. CON

a. CON_BC1 ; $E_{zPE} = -387.986742$

C	1.317327000	-0.509173000	0.118521000
C	0.458618000	-1.702982000	-0.228332000
C	-0.991732000	1.647445000	-0.119794000
C	-0.931014000	-1.393658000	-0.772118000
C	-1.409914000	0.549290000	0.869633000
C	-1.880475000	-0.758703000	0.236544000
H	0.411781000	-2.343398000	0.655127000
H	-0.847785000	-0.752712000	-1.654364000
H	-1.420187000	1.443732000	-1.107850000
H	-2.225380000	0.918594000	1.496703000
H	1.023331000	-2.253885000	-0.991736000
H	-1.426292000	2.599186000	0.196420000
H	-1.375806000	-2.325603000	-1.131039000
H	-0.585928000	0.351947000	1.561989000
H	-2.838890000	-0.583137000	-0.263757000
H	-2.082563000	-1.478968000	1.036531000
C	1.311083000	0.680983000	-0.818111000
H	0.928043000	0.409832000	-1.804617000
H	2.353201000	0.987418000	-0.929793000
C	0.514104000	1.858433000	-0.246773000
H	0.927668000	2.097174000	0.737976000
H	0.698794000	2.729325000	-0.881737000
O	2.016504000	-0.503664000	1.105339000

b. CON_TBC1 ; $E_{zPE} = -387.98396$

C	0.920067000	-1.620900000	0.472029000
C	-0.499014000	-1.694100000	-0.080888000
C	0.657690000	1.537824000	-0.638582000
C	-1.379906000	-0.465570000	-0.032205000
C	-0.507383000	1.834566000	0.299868000
C	-1.097747000	0.604051000	0.994411000
H	-1.057122000	-2.452604000	0.483779000
O	-2.299512000	-0.343241000	-0.807883000
H	0.290466000	0.982922000	-1.509091000
H	-1.302941000	2.317886000	-0.271837000
H	-0.499011000	-2.040327000	-1.117570000
H	1.009295000	2.494694000	-1.032816000
H	-0.187096000	2.546043000	1.066888000
H	-2.044209000	0.872623000	1.467215000
H	-0.421260000	0.240873000	1.768592000
C	1.904639000	-0.722532000	-0.274208000
H	1.808882000	-0.902197000	-1.351729000
H	2.912244000	-1.054676000	-0.006416000
C	1.839737000	0.784081000	-0.017332000
H	1.873917000	0.970121000	1.063002000
H	2.764591000	1.210249000	-0.414965000
H	0.904054000	-1.343801000	1.531000000
H	1.315779000	-2.640391000	0.448455000

c. CON_CR ; $E_{zPE} = -387.983159$

C	0.749306000	-1.159482000	0.027742000
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C	-0.497736000	-1.361693000	-0.809515000
C	0.293859000	1.838665000	-0.267320000
C	-1.761656000	-0.929109000	-0.071081000
C	-0.897970000	1.421947000	0.620336000
C	-1.991796000	0.576821000	-0.038341000
H	-0.547285000	-2.435754000	-1.012774000
H	-1.707123000	-1.320625000	0.948914000
H	0.046064000	1.679790000	-1.322952000
H	-1.372527000	2.335052000	0.987031000
H	-0.415993000	-0.848745000	-1.770405000
H	0.433918000	2.917336000	-0.163838000
H	-2.626288000	-1.403370000	-0.543005000
H	-0.531470000	0.906030000	1.514181000
H	-2.930924000	0.751086000	0.495146000
H	-2.157352000	0.942341000	-1.058947000
C	1.822869000	-0.241431000	-0.495322000
H	1.805436000	-0.220116000	-1.588187000
H	2.788423000	-0.628073000	-0.164993000
C	1.636528000	1.180477000	0.046281000
H	1.784308000	1.160824000	1.130285000
H	2.441582000	1.795292000	-0.365174000
O	0.858601000	-1.698529000	1.104754000

d. CON_BC2 ; $E_{zPE} = -387.982756$

C	-1.452038000	0.191641000	0.053126000
C	-0.923472000	-0.868909000	0.996416000
C	1.607772000	0.951919000	0.468785000
C	-0.051440000	-1.880564000	0.242672000
C	2.029185000	-0.371291000	-0.181173000
C	0.936174000	-1.272310000	-0.745955000
H	-1.786939000	-1.384538000	1.423276000
H	0.481118000	-2.498469000	0.972125000
H	1.267794000	0.784936000	1.493994000
H	2.629167000	-0.938566000	0.538854000
H	-0.372167000	-0.412054000	1.817485000
H	2.510174000	1.561293000	0.566038000
H	-0.714275000	-2.547854000	-0.312802000
H	2.705515000	-0.132276000	-1.008745000
H	1.426491000	-2.094217000	-1.275943000
H	0.375521000	-0.731657000	-1.515890000
C	-0.900325000	1.590692000	0.181366000
H	-0.956554000	1.885260000	1.235560000
H	-1.550586000	2.250129000	-0.394973000
C	0.551240000	1.759982000	-0.292678000
H	0.606991000	1.536667000	-1.362513000
H	0.781057000	2.823933000	-0.199998000
O	-2.273236000	-0.088693000	-0.788978000

e. CON_TBC2 ; $E_{zPE} = -387.981004$

C	-1.503067000	-0.229764000	0.048318000
C	-1.404221000	1.164236000	-0.521147000
C	1.796767000	-0.872683000	-0.325300000
C	0.049537000	1.626196000	-0.645479000

C	2.045792000	0.417395000	0.457110000
C	0.854881000	1.356880000	0.635089000
H	-1.968303000	1.823413000	0.140522000
H	0.519595000	1.126976000	-1.496178000
H	1.737102000	-0.653999000	-1.396857000
H	2.858952000	0.954958000	-0.042349000
H	-1.888689000	1.173564000	-1.504023000
H	2.692080000	-1.490893000	-0.212734000
H	0.052123000	2.689527000	-0.891952000
H	2.424000000	0.159282000	1.451463000
H	1.219853000	2.295733000	1.058094000
H	0.188844000	0.942133000	1.397756000
C	-0.742501000	-1.344579000	-0.635097000
H	-0.547172000	-1.103934000	-1.683858000
H	-1.404565000	-2.211936000	-0.603037000
C	0.579899000	-1.713599000	0.063612000
H	0.425849000	-1.703185000	1.147118000
H	0.793534000	-2.751996000	-0.199865000
O	-2.145716000	-0.459266000	1.046657000

f. CON_BC1_1 ; E_{ZPE} = -464.355013

C	-0.472965000	-1.019840000	0.151971000
C	0.838274000	-1.759754000	0.197110000
C	0.778424000	1.888928000	0.167718000
C	2.072688000	-0.916274000	0.492904000
C	1.366614000	1.077421000	-0.996048000
C	2.444898000	0.067160000	-0.609702000
H	0.941551000	-2.312368000	-0.739123000
H	1.935405000	-0.380098000	1.435892000
H	1.460572000	1.860248000	1.025219000
H	1.806772000	1.758632000	-1.728615000
H	0.717674000	-2.504063000	0.995316000
H	0.718889000	2.940844000	-0.122682000
H	2.916077000	-1.590959000	0.660904000
H	0.556878000	0.572213000	-1.531826000
H	3.339602000	0.611587000	-0.289618000
H	2.734381000	-0.494249000	-1.504502000
C	-0.745190000	0.047499000	1.182150000
H	-0.085902000	-0.067698000	2.045142000
H	-1.776935000	-0.090762000	1.512370000
C	-0.619440000	1.463863000	0.604075000
H	-1.310082000	1.545962000	-0.239597000
H	-0.985361000	2.159154000	1.363744000
O	-1.310453000	-1.301797000	-0.683702000
O	-3.645261000	0.225678000	-0.386541000
H	-2.907476000	-0.373672000	-0.591807000
H	-4.396155000	-0.119841000	-0.869932000

g. CON_BC1_2 ; E_{ZPE} = -464.354841

C	0.414145000	-1.058357000	0.581403000
C	-1.011215000	-1.552001000	0.614533000
C	-0.328063000	2.007058000	0.104379000
C	-1.766913000	-1.181432000	-0.667941000

C	-0.745394000	1.152566000	-1.091062000
C	-2.012920000	0.307601000	-0.892867000
H	-1.542190000	-1.172691000	1.489942000
H	-1.204784000	-1.584543000	-1.515844000
H	0.630680000	2.479401000	-0.130589000
H	0.086642000	0.509164000	-1.391643000
H	-0.961720000	-2.640557000	0.687427000
H	-1.052634000	2.818811000	0.229811000
H	-2.726785000	-1.704750000	-0.651834000
H	-0.891852000	1.829753000	-1.936164000
H	-2.646033000	0.397307000	-1.779346000
H	-2.608646000	0.711776000	-0.066396000
C	0.791423000	0.124182000	1.432413000
H	1.786016000	0.461172000	1.135322000
H	0.874223000	-0.275959000	2.451908000
C	-0.206025000	1.277609000	1.436386000
H	-1.188806000	0.919506000	1.756355000
H	0.106889000	1.993474000	2.200710000
O	1.231444000	-1.631976000	-0.112739000
O	3.045968000	0.295821000	-1.038081000
H	2.566473000	-0.501700000	-0.759758000
H	3.743007000	-0.014277000	-1.616819000

h. CON_TBC1_1 ; E_{ZPE} = -464.351774

C	0.629074000	1.545363000	-1.169510000
C	-0.696637000	0.799677000	-1.287175000
C	1.115228000	-0.640215000	1.348276000
C	-0.745725000	-0.645721000	-0.870396000
C	1.020697000	-1.827903000	0.394742000
C	0.489699000	-1.492935000	-1.004743000
H	-1.001490000	0.787592000	-2.343015000
O	-1.765422000	-1.130241000	-0.419200000
H	0.108408000	-0.295245000	1.607814000
H	0.361154000	-2.577163000	0.838138000
H	-1.486807000	1.325625000	-0.747279000
H	1.542268000	-1.014273000	2.282383000
H	2.005139000	-2.292307000	0.285862000
H	0.215317000	-2.415409000	-1.520454000
H	1.251956000	-0.985000000	-1.595183000
C	1.180286000	1.723002000	0.244088000
H	0.361747000	2.004969000	0.915808000
H	1.860479000	2.579567000	0.220838000
C	1.948107000	0.551175000	0.860338000
H	2.716825000	0.207949000	0.156741000
H	2.496326000	0.952980000	1.716466000
H	1.390881000	1.082992000	-1.805495000
H	0.461319000	2.538450000	-1.595252000
O	-2.712723000	0.801157000	1.394993000
H	-2.605663000	0.060522000	0.777559000
H	-3.497070000	0.596777000	1.905002000

i. CON_TBC1_2 ; E_{ZPE} = -464.352362

C	2.018822000	-1.184839000	0.413924000
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C	0.705385000	-1.780439000	-0.079836000
C	0.540782000	1.642710000	-0.612667000
C	-0.565373000	-0.978260000	0.042636000
C	-0.595888000	1.480728000	0.389957000
C	-0.665038000	0.109195000	1.075128000
H	0.498137000	-2.696693000	0.489418000
O	-1.500081000	-1.224744000	-0.695149000
H	0.360853000	0.995547000	-1.478969000
H	-1.548777000	1.655777000	-0.112951000
H	0.782761000	-2.095420000	-1.123550000
H	0.485094000	2.662976000	-1.000423000
H	-0.506090000	2.242599000	1.169589000
H	-1.629522000	0.015326000	1.577820000
H	0.126403000	0.010602000	1.818148000
C	2.561837000	0.015106000	-0.358978000
H	2.488301000	-0.187026000	-1.434282000
H	3.632197000	0.081579000	-0.142139000
C	1.952172000	1.387585000	-0.070666000
H	1.973856000	1.574217000	1.009874000
H	2.627041000	2.128408000	-0.507445000
H	1.949006000	-0.934228000	1.477095000
H	2.761977000	-1.985109000	0.355296000
O	-3.760755000	0.309687000	-0.061776000
H	-4.569747000	-0.011836000	-0.460557000
H	-3.060995000	-0.286977000	-0.378513000

j. CON_CR_1 ; E_{ZPE} = -464.351431

O	1.059610000	-1.465410000	-0.333214000
C	0.431994000	-0.919819000	0.554050000
C	1.002402000	0.240376000	1.315731000
H	2.078905000	0.093942000	1.417380000
H	0.550033000	0.291492000	2.309209000
C	0.755226000	1.559740000	0.569446000
H	1.340301000	1.546304000	-0.353934000
H	1.176245000	2.357099000	1.187049000
C	-0.703767000	1.883330000	0.256627000
H	-0.758686000	2.958512000	0.070506000
H	-1.319126000	1.713467000	1.147661000
C	-1.322652000	1.154289000	-0.954871000
H	-0.529182000	0.705956000	-1.562274000
H	-1.783749000	1.909001000	-1.595940000
C	-2.392678000	0.100386000	-0.656276000
H	-3.052529000	0.020001000	-1.525143000
H	-3.024847000	0.458301000	0.165094000
C	-1.894617000	-1.303627000	-0.336098000
H	-1.362727000	-1.716765000	-1.197864000
H	-2.758330000	-1.950406000	-0.161402000
C	-0.968237000	-1.386216000	0.875393000
H	-0.869270000	-2.431457000	1.184537000
H	-1.381748000	-0.830575000	1.719277000
H	2.645386000	-0.640719000	-0.813670000
O	3.390626000	-0.030026000	-0.943728000
H	4.001414000	-0.491429000	-1.518964000

k. CON_CR_2 ; E_{ZPE} = -464.351434

C	-0.431883000	-0.920345000	0.554170000
C	0.968548000	-1.386651000	0.874925000
C	0.703542000	1.883442000	0.257094000
C	1.894552000	-1.303257000	-0.336836000
C	1.322360000	1.154858000	-0.954689000
C	2.392437000	0.100903000	-0.656556000
H	0.869892000	-2.432112000	1.183379000
H	1.362451000	-1.716076000	-1.198629000
H	1.319140000	1.713550000	1.147958000
H	1.783409000	1.909813000	-1.595508000
H	1.382268000	-0.831429000	1.718980000
H	0.758134000	2.958683000	0.071196000
H	2.758389000	-1.950029000	-0.162704000
H	0.528854000	0.706736000	-1.562210000
H	3.052188000	0.020838000	-1.525534000
H	3.024707000	0.458579000	0.164843000
C	-1.002042000	0.239822000	1.316106000
H	-0.549350000	0.290750000	2.309451000
H	-2.078495000	0.093286000	1.418163000
C	-0.755294000	1.559423000	0.570125000
H	-1.340587000	1.546156000	-0.353117000
H	-1.176360000	2.356501000	1.188061000
O	-1.059806000	-1.466195000	-0.332711000
O	-3.390293000	-0.029200000	-0.944469000
H	-2.645571000	-0.640395000	-0.813915000
H	-4.001592000	-0.490855000	-1.519011000

l. CON_BC2_1 ; E_{ZPE} = -464.351082

C	-0.548824000	1.020832000	0.170519000
C	-0.639813000	-0.130563000	1.140909000
C	2.424155000	-0.082475000	0.328687000
C	-0.539567000	-1.480361000	0.411859000
C	1.971491000	-1.416560000	-0.273999000
C	0.510767000	-1.551548000	-0.689347000
H	-1.614531000	-0.071018000	1.631343000
H	-0.352608000	-2.258821000	1.157449000
H	2.135304000	-0.019276000	1.380878000
H	2.221616000	-2.218880000	0.428594000
H	0.129615000	-0.037577000	1.906036000
H	3.517261000	-0.087013000	0.334862000
H	-1.515528000	-1.694404000	-0.027141000
H	2.579730000	-1.600926000	-1.165984000
H	0.398009000	-2.515794000	-1.193295000
H	0.274540000	-0.804109000	-1.454918000
C	0.699031000	1.862096000	0.169290000
H	0.913177000	2.150464000	1.204442000
H	0.484348000	2.765278000	-0.403287000
C	1.944535000	1.171901000	-0.409186000
H	1.768766000	0.942625000	-1.464511000
H	2.738712000	1.921675000	-0.396485000
O	-1.453935000	1.255861000	-0.606494000

O	-3.686853000	-0.383941000	-0.152107000
H	-2.990815000	0.243152000	-0.412524000
H	-4.491936000	-0.050674000	-0.549055000

m. CON_BC2_2 ; E_{ZPE} = -464.350786

C	-0.660482000	0.824055000	-0.757596000
C	0.688340000	1.477187000	-0.933636000
C	1.378805000	-1.577632000	-0.462696000
C	1.404523000	1.590604000	0.420001000
C	1.961734000	-0.926632000	0.796938000
C	1.311324000	0.354470000	1.307709000
H	0.520875000	2.477881000	-1.339371000
H	2.453021000	1.845509000	0.239090000
H	1.749830000	-1.075815000	-1.360548000
H	3.031293000	-0.750939000	0.636790000
H	1.290149000	0.923276000	-1.652414000
H	1.788956000	-2.589549000	-0.516802000
H	0.964123000	2.429115000	0.963873000
H	1.898018000	-1.660112000	1.607345000
H	1.775192000	0.600806000	2.267323000
H	0.259115000	0.162017000	1.542381000
C	-0.862223000	-0.558344000	-1.312837000
H	-0.487899000	-0.568458000	-2.342459000
H	-1.932727000	-0.764810000	-1.326409000
C	-0.149530000	-1.667743000	-0.520216000
H	-0.575851000	-1.707235000	0.485659000
H	-0.435255000	-2.606524000	-0.999411000
O	-1.536521000	1.400146000	-0.142229000
O	-3.007591000	-0.611016000	1.154801000
H	-2.669215000	0.195739000	0.733575000
H	-3.711676000	-0.319738000	1.734800000

n. CON_TBC2_1 ; E_{ZPE} = -464.349146

C	-0.633464000	-1.061604000	0.280121000
C	0.576284000	-1.946985000	0.407477000
C	1.133864000	1.810786000	0.435447000
C	1.874563000	-1.156579000	0.224517000
C	1.979886000	1.248058000	-0.707433000
C	1.827857000	-0.241536000	-1.009071000
H	0.486650000	-2.732689000	-0.344099000
H	2.071425000	-0.566281000	1.122296000
H	1.564854000	1.517706000	1.398926000
H	3.029359000	1.465440000	-0.481831000
H	0.556142000	-2.417410000	1.396972000
H	1.236320000	2.899171000	0.400543000
H	2.699345000	-1.867786000	0.153623000
H	1.749099000	1.802081000	-1.622760000
H	2.603879000	-0.528334000	-1.722511000
H	0.883991000	-0.399201000	-1.539909000
C	-0.741102000	0.157865000	1.157826000
H	-0.137003000	0.038445000	2.060851000
H	-1.790705000	0.228368000	1.449832000
C	-0.356443000	1.471676000	0.447156000

H	-0.773333000	1.469403000	-0.563750000
H	-0.882977000	2.268177000	0.975949000
O	-1.497783000	-1.306988000	-0.539408000
O	-3.508788000	0.660479000	-0.523983000
H	-4.314895000	0.393888000	-0.966741000
H	-2.898253000	-0.088981000	-0.626510000

o. CON_TBC2_2 ; E_{ZPE} = -464.348693

C	-0.656640000	1.014642000	0.415092000
C	-0.927128000	-0.105344000	1.381135000
C	2.439056000	-0.033348000	-0.362386000
C	0.119684000	-1.217498000	1.255805000
C	1.795257000	-1.378176000	-0.702391000
C	0.369941000	-1.617889000	-0.206177000
H	-1.926216000	-0.493517000	1.180961000
H	1.053655000	-0.899122000	1.725170000
H	2.732480000	-0.015449000	0.692712000
H	2.450300000	-2.161951000	-0.307199000
H	-0.915664000	0.309590000	2.395402000
H	3.380018000	0.017641000	-0.917747000
H	-0.227821000	-2.071197000	1.839699000
H	1.799663000	-1.505810000	-1.789561000
H	0.130291000	-2.672942000	-0.353794000
H	-0.332181000	-1.083873000	-0.852816000
C	0.684079000	1.702196000	0.453666000
H	1.163854000	1.573564000	1.427100000
H	0.477224000	2.764749000	0.311080000
C	1.639246000	1.234953000	-0.661633000
H	1.075774000	1.132979000	-1.594034000
H	2.348631000	2.049285000	-0.825093000
O	-1.474513000	1.354561000	-0.417692000
O	-3.401590000	-0.642767000	-0.854941000
H	-4.135922000	-0.385941000	-1.413261000
H	-2.846231000	0.150420000	-0.776219000

Table S2 : Singlet excited states.

Complex	Electron promotion	Etat	Lambda	f	Shift ($\Delta\lambda_{\text{monohydraté}} - \Delta\lambda_{\text{isolés}}$)
TPH	42 → 45	S1	319.23	f=0.0001	
	44 → 45	S2	270.59	f=0.0237	
	43 → 45	S3	245.03	f=0.2788	
	43 → 46	S4	197.06	f=0.0802	
	42 → 46	S5	194.26	f=0.0000	
TPH_1	47 → 50 (HOMO-2 → LUMO)	S1	310.02	0.0003	-9.21
	49 → 50 (HOMO → LUMO)	S2	281.15	0.0253	10.56
	48 → 50 (HOMO-1 → LUMO)	S3	250.69	0.2835	5.66
	46 → 50 (HOMO-3 → LUMO)	S4	245.41	0.0135	48.35
	45 → 50 (HOMO-4 → LUMO)	S5	198.24	0.0008	3.98
TPH_2	46 → 50 (HOMO-3 → LUMO)	S1	310.93	f=0.0001	-8.3
	48 → 50 (HOMO-1 → LUMO)	S2	278.09	f=0.0236	7.5
	49 → 50 (HOMO → LUMO)	S3	274.37	f=0.0107	29.34
	47 → 50 (HOMO-2 → LUMO)	S4	249.5	f=0.3062	52.44
	47 → 51 (HOMO-2 → LUMO+1)	S5	197.7	f=0.0652	3.44
MLA	27 → 29	S1	201.96	f=0.0012	
	28 → 29	S2	190.4	f=0.0328	
MLA_1	33 → 34 (HOMO → LUMO)	S1	211.94	f=0.0049	9.98
MLA_2	33 → 34 (HOMO → LUMO)	S1	211.7	f=0.0033	-9.74
	32 → 34 (HOMO-1 → LUMO)	S2	190.25	f=0.0079	0.15
DMI	31 → 32	S1	224.88	f=0.0002	
	31 → 33	S2	210.56	f=0.0765	
	31 → 34	S3	202.68	f=0.0453	
	31 → 34	S4	199.92	f=0.0235	
	31 → 35	S5	198.84	f=0.0002	
DMI_1	36 → 37 (HOMO → LUMO)	S1	220.97	f=0.0003	-3.91
	36 → 38 (HOMO → LUMO+1)	S2	205.68	f=0.0962	-4.88
	36 → 40 (HOMO → LUMO+3)	S3	198.47	f=0.0489	-4.21
	36 → 39 (HOMO → LUMO+2)	S4	195.84	f=0.0021	-4.08
	35 → 37 (HOMO-1 → LUMO+1)	S5	193.52	f=0.0055	-5.32
DMI_2	36 → 37 (HOMO → LUMO)	S1	220.99	f=0.0003	-3.89
	36 → 38 (HOMO → LUMO+1)	S2	205.69	f=0.0962	-4.87
	36 → 40 (HOMO → LUMO+3)	S3	198.48	f=0.0489	-4.2
	36 → 39 (HOMO → LUMO+2)	S4	195.85	f=0.0021	-4.07
	35 → 37 (HOMO-1 → LUMO+1)	S5	193.52	f=0.0055	-5.32

CON_BC1	35 → 36	S1	289.07	f=0.0000	
	35 → 37	S2	204.4	f=0.0057	
	35 → 38	S3	192.3	f=0.0053	
	35 → 39	S4	191.52	f=0.0017	
CON_1	40 → 41 (HOMO → LUMO)	S1	279.2	f=0.0000	-9.87
	39 → 41 (HOMO-1 → LUMO)	S2	195.22	f=0.0068	-9.18
	40 → 42 (HOMO → LUMO+1)	S3	192.21	f=0.0077	-0.09
CON_2	40 → 41 (HOMO → LUMO)	S1	280.93	f=0.0001	-8.14
	40 → 42 (HOMO → LUMO+1)	S2	192.46	f=0.0069	-11.94
	39 → 41 (HOMO-1 → LUMO)	S3	192.41	f=0.0022	0.11
CON_TBC1	35 → 36	S1	291.54	f=0.0001	
	35 → 37	S2	205.05	f=0.0059	
	35 → 39	S3	193.33	f=0.0028	
	35 → 38	S4	192.26	f=0.0039	
	35 → 40	S5	188.63	f=0.0172	
CON_TBC1_1	40 → 41 (HOMO → LUMO)	S1	284.89	f=0.0001	-6.65
	40 → 42 (HOMO → LUMO+1)	S2	193.84	f=0.0069	-11.21
	39 → 41 (HOMO-1 → LUMO)	S3	191.39	f=0.0034	-1.94
CON_TBC1_2	40 → 41 (HOMO → LUMO)	S1	281.32	f=0.0000	-10.22
	39 → 41 (HOMO-1 → LUMO+1)	S2	196.4	f=0.0048	-8.65
	40 → 42 (HOMO → LUMO+1)	S3	192.67	f=0.0074	-0.66
CON_CR	35 → 36	S1	293.46	f=0.0001	
	35 → 37	S2	202.57	f=0.0048	
	35 → 38	S3	191.25	f=0.0020	
	35 → 39	S4	190.87	f=0.0009	
CON_CR_1	40 → 41 (HOMO → LUMO)	S1	283.54	f=0.0002	-9.92
	39 → 41 (HOMO-1 → LUMO+1)	S2	197.58	f=0.0053	-4.99
	40 → 42 (HOMO → LUMO+1)	S3	191.11	f=0.0061	-0.14
CON_CR_2	40 → 41 (HOMO → LUMO)	S1	283.54	f=0.0002	-9.92
	39 → 41 (HOMO-1 → LUMO+1)	S2	197.58	f=0.0053	-4.99
	40 → 42 (HOMO → LUMO+1)	S3	191.11	f=0.0061	-0.14
CON_BC2	35 → 36	S1	294.19	f=0.0000	
	35 → 37	S2	202.89	f=0.0046	
	35 → 38	S3	193.16	f=0.0006	
	35 → 39	S4	191.42	f=0.0074	
CON_BC2_1	40 → 41 (HOMO → LUMO)	S1	284.16	f=0.0000	-10.03
	39 → 41 (HOMO-1 → LUMO+1)	S2	198.04	f=0.0038	-4.85
	40 → 42 (HOMO → LUMO+1)	S3	190.69	f=0.0061	-2.47

CON_BC2_2	40 → 41 (HOMO → LUMO)	S1	286.06	f=0.0002	-8.13
	39 → 41 (HOMO-1 → LUMO+1)	S2	194.09	f=0.0039	-8.8
	40 → 42 (HOMO → LUMO+1)	S3	192.11	f=0.0078	-1.05
CON_TBC2	35 → 36	S1	292.02	f=0.0000	
	35 → 37	S2	202.74	f=0.0069	
	35 → 38	S3	193.65	f=0.0004	
CON_TBC2_1	40 → 41 (HOMO → LUMO)	S1	282.02	f=0.0001	-10
	39 → 41 (HOMO-1 → LUMO+1)	S2	196.2	f=0.0066	-6.54
	40 → 42 (HOMO → LUMO+1)	S3	190.83	f=0.0092	-2.82
CON_TBC2_2	40 → 41 (HOMO → LUMO)	S1	282.99	f=0.0002	-9.03
	39 → 41 (HOMO-1 → LUMO+1)	S2	195.94	f=0.0035	-6.8
	40 → 42 (HOMO → LUMO+1)	S3	190.94	f=0.0079	-2.71

Table S3: Triplet excited states.

Complex	Electron promotion	Etat	Lambda	Shift
TPH	43 → 45	T1	394.66	
	42 → 45	T2	379.17	
	44 → 45	T3	326.79	
	44 → 46	T4	282.52	
	43 → 46	T5	237.42	
TPH_1	47 → 50 (HOMO-2 → LUMO)	T1	363.37	-31.29
	49 → 50 (HOMO → LUMO)	T2	342.64	-36.53
	49 → 51 (HOMO → LUMO+1)	T3	283.97	-42.82
	46 → 50 (HOMO-3 → LUMO)	T4	247.27	-35.25
TPH_2	47 → 50 (HOMO-2 → LUMO)	T1	400.8	6.14
	46 → 50 (HOMO-3 → LUMO)	T2	365.3	-13.87
	48 → 50 (HOMO-1 → LUMO)	T3	337.68	10.89
	48 → 51 (HOMO-1 → LUMO+1)	T4	283.67	1.15
	49 → 50 (HOMO → LUMO)	T5	274.9	37.48
MLA	27 → 29	T1	223.65	
	26 → 29	T2	206.61	
	28 → 29	T3	196.28	
MLA_1	32 → 34 (HOMO-1 → LUMO+1)	T1	234.44	10.79
	30 → 34 (HOMO-3 → LUMO+1)	T2	207.33	0.72
	32 → 34 (HOMO-1 → LUMO+1)	T3	195.23	-1.05
MLA_2	33 → 34 (HOMO → LUMO+1)	T1	234.28	10.63
	30 → 34 (HOMO-3 → LUMO+1)	T2	206.83	0.22
	33 → 34 (HOMO → LUMO+1)	T3	198.16	1.88
DMI	31 → 32	T1	229.29	
	31 → 33	T2	217.52	
	30 → 41	T3	213.2	
	30 → 32	T4	208.78	
	30 → 32	T5	201.14	
DMI_1	36 → 37 (HOMO → LUMO)	T1	225.27	-4.02
	36 → 38 (HOMO → LUMO+1)	T2	219.11	1.59
	35 → 45 (HOMO-1 → LUMO+9)	T3	209.98	-3.22
	36 → 38 (HOMO → LUMO+2)	T4	204.58	-4.2
	36 → 39 (HOMO → LUMO+3)	T5	198.16	-2.98
DMI_2	36 → 37 (HOMO → LUMO)	T1	225.28	-4.01
	36 → 38 (HOMO → LUMO+1)	T2	219.1	1.58
	35 → 45 (HOMO-1 → LUMO+9)	T3	209.95	-3.25
	36 → 38 (HOMO → LUMO+2)	T4	204.59	-4.19
	36 → 39 (HOMO → LUMO+3)	T5	198.17	-2.97

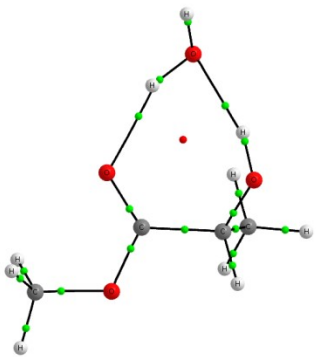
CON_BC1	35 → 36	T1	337.9	
	34 → 36	T2	231.02	
	35 → 37	T3	206.33	
	35 → 38	T4	193.95	
	35 → 39	T5	192.27	
CON_BC1_1	40 → 41 (HOMO → LUMO)	T1	322.37	-15.53
	38 → 41 (HOMO-2 → LUMO)	T2	229.23	-1.79
	39 → 41 (HOMO-1 → LUMO)	T3	196.5	-9.83
	40 → 42 (HOMO → LUMO+1)	T4	194.13	0.18
CON_BC1_2	40 → 41 (HOMO → LUMO)	T1	324.77	-13.13
	38 → 41 (HOMO-2 → LUMO)	T2	229.95	-1.07
	40 → 42 (HOMO → LUMO+1)	T3	194.49	-11.84
	39 → 41 (HOMO-1 → LUMO)	T4	193.46	-0.49
CON_TBC1	35 → 36	T1	340.62	
	30 → 36	T2	230.27	
	35 → 37	T3	207.03	
	35 → 39	T4	195	
	35 → 38	T5	192.93	
CON_TBC1_1	40 → 41 (HOMO → LUMO)	T1	329.73	-10.89
	33 → 41 (HOMO-7 → LUMO+1)	T2	227.88	-2.39
	40 → 42 (HOMO → LUMO+1)	T3	195.92	-11.11
	39 → 41 (HOMO-1 → LUMO)	T4	191.71	-3.29
CON_TBC1_2	40 → 41 (HOMO → LUMO)	T1	324.6	-16.02
	33 → 41 (HOMO-7 → LUMO+1)	T2	227.82	-2.45
	39 → 41 (HOMO-1 → LUMO)	T3	197.51	-9.52
	40 → 42 (HOMO → LUMO+1)	T4	194.64	-0.36
CON_CR	35 → 36	T1	342.73	
	34 → 36	T2	233.61	
	35 → 37	T3	204.7	
	35 → 38	T4	192.74	
	35 → 39	T5	191.72	
CON_CR_1	40 → 41 (HOMO → LUMO)	T1	327.22	-15.51
	38 → 41 (HOMO-2 → LUMO+1)	T2	232.06	-1.55
	39 → 41 (HOMO-1 → LUMO)	T3	198.57	-6.13
	40 → 42 (HOMO → LUMO+1)	T4	193.43	0.69
CON_CR_2	40 → 41 (HOMO → LUMO)	T1	327.22	-15.51
	38 → 41 (HOMO-2 → LUMO+1)	T2	232.06	-1.55
	39 → 41 (HOMO-1 → LUMO)	T3	198.57	-6.13
	40 → 42 (HOMO → LUMO+1)	T4	193.43	0.69

CON_BC2	35 → 36	T1	345.96	
	31 → 37	T2	229.4	
	35 → 37	T3	204.93	
	35 → 38	T4	194.08	
	35 → 39	T5	192.97	
CON_BC2_1	40 → 41 (HOMO → LUMO)	T1	329.94	-16.02
	38 → 41 (HOMO-2 → LUMO+1)	T2	227.1	-2.3
	39 → 41 (HOMO-1 → LUMO)	T3	199.72	-5.21
	40 → 42 (HOMO → LUMO+1)	T4	192.78	-1.3
CON_BC2_2	40 → 41 (HOMO → LUMO)	T1	332.45	-13.51
	35 → 41 (HOMO-5 → LUMO+1)	T2	227.91	-1.49
	40 → 42 (HOMO → LUMO+1)	T3	194.32	-10.61
	39 → 41 (HOMO-1 → LUMO)	T4	194.24	0.16
CON_TBC2	35 → 36	T1	343.48	
	32 → 36	T2	228.18	
	35 → 37	T3	204.73	
	35 → 38	T4	194.46	
	35 → 39	T5	191.2	
CON_TBC2_1	40 → 41 (HOMO → LUMO)	T1	327.43	-16.05
	31 → 41 (HOMO-9 → LUMO+1)	T2	226.01	-2.17
	39 → 41 (HOMO-1 → LUMO)	T3	197.38	-7.35
	40 → 42 (HOMO → LUMO+1)	T4	192.81	-1.65
CON_TBC2_2	40 → 41 (HOMO → LUMO)	T1	328.69	-14.79
	29 → 41 (HOMO-11 → LUMO+1)	T2	226.42	-1.76
	39 → 41 (HOMO-1 → LUMO)	T3	195.92	-8.81
	40 → 42 (HOMO → LUMO+1)	T4	192.94	-1.52

Table S4: Vibrational and Topological characterisation of the monohydrated complexes. Electron densities $\rho(r)$ at the intermolecular bond critical points are given in a.u. Scaled vibrational frequencies are given in cm^{-1} (Scaling factor: 0.9604).

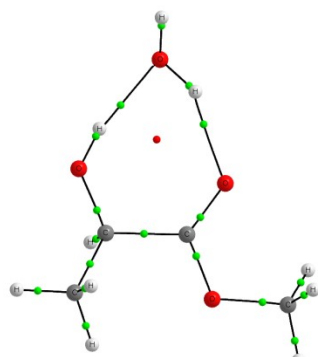
TPH_1				TPH_2				TPH_3				TPH_4				TPH_5			
BCP	$\rho(r)$	$\nu_{\text{sym}}(\text{O-H})$	$\nu \text{ C=O}$	BCP	$\rho(r)$	$\nu_{\text{sym}}(\text{O-H})$	$\nu \text{ C=O}$	BCP	$\rho(r)$	$\nu_{\text{sym}}(\text{O-H})$	$\nu \text{ C=O}$	BCP	$\rho(r)$	$\nu_{\text{sym}}(\text{O-H})$	$\nu \text{ C=O}$	BCP	$\rho(r)$	$\nu_{\text{sym}}(\text{O-H})$	$\nu \text{ C=O}$
O-H(W)	0.023	3608.77	1727.19	O-H(W)	0.02	3645.34	1730.77	F-H(W)	0.007	3697.25	1738.33	F-H(W)	0.023	3697.16	1738.33	O(W)-H	0.006	3701.72	1738.65
O(W)-H	0.01			O(W)-H	0.01	O(W)-H	0.007												
				O(W)-F	0.004														
BCP	$\rho(r)$	$\nu_{\text{sym}}(\text{O-H})$	$\nu \text{ C=O}$	BCP	$\rho(r)$	$\nu_{\text{sym}}(\text{O-H})$	$\nu \text{ C=O}$												
F-H(W)	0.008	3693.06	1747.41	O(W)-H	0.006	3701.62	1738.58												
				O(W)-H	0.007														

MLA_1



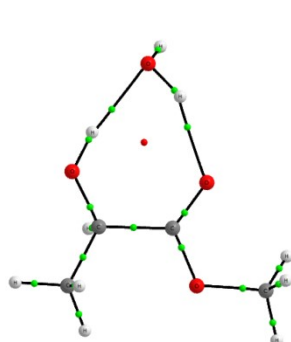
BCP	$\rho(r)$	$v_{sym}(O-H)$	$v C=O$
O-H(W)	0.03	3491.55	1723.52
O(W)-H	0.03		

MLA_2



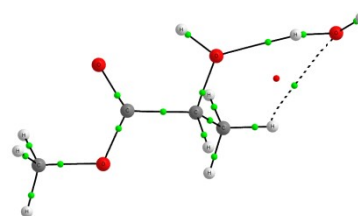
BCP	$\rho(r)$	$v_{sym}(O-H)$	$v C=O$
O-H(W)	0.03	3524.43	1723.15
O(W)-H	0.03		

MLA_3



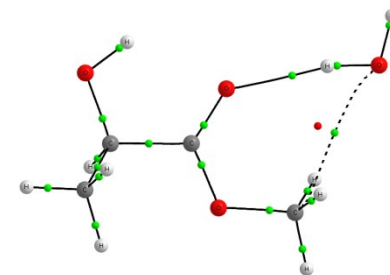
BCP	$\rho(r)$	$v_{sym}(O-H)$	$v C=O$
O-H(W)	0.03	3531.39	1736.81
O(W)-H	0.03		

MLA_4



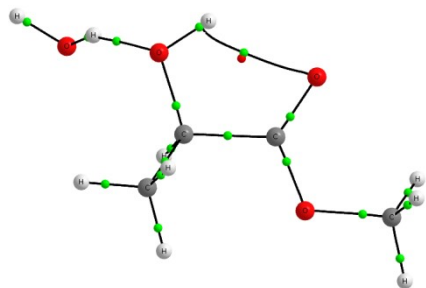
BCP	$\rho(r)$	$v_{sym}(O-H)$	$v C=O$
O-H(W)	0.03	3547.87	1721.46
O(W)-H	0.006		

MLA_5



BCP	$\rho(r)$	$v_{sym}(O-H)$	$v C=O$
O-H(W)	0.02	3582.02	1715.86

MLA_6



BCP	$\rho(r)$	$v_{sym}(O-H)$	$v C=O$
O-H(W)	0.03	3531.39	1735.80

