

Electronic Supplementary Information

Mechanistic insights into lysine-targeting covalent inhibition through a theoretical study of ester aminolysis

Volkan Fındık^{a,b}, Manuel F. Ruiz-López^{*a}, and Safiye Sag Erdem^{*b}

^a LPCT, UMR 7019, University of Lorraine, CNRS, 54000 Nancy, France

^b Department of Chemistry, Faculty of Arts and Sciences, Marmara University, 34722 Istanbul, Turkey

Table S1. Cartesian coordinates of stationary points for the reaction of methyamine with methylacetate in water. Optimized geometries at the B3LYP/6-311+G(d,p) level.

RC			
C	-3.21667500	0.07778900	-0.75102600
O	-4.00931000	-0.93815800	-1.06448900
N	5.14041700	-1.54370100	-0.51434900
O	-2.34063700	0.00260000	0.10423300
H	4.53380100	-0.83666400	-0.09852500
H	5.96620300	-1.60102500	0.07405100
O	-0.61289400	2.06317700	0.92915500
H	-1.10465400	2.81688500	1.27550900
H	-1.28215000	1.42025900	0.61562800
O	1.57980900	2.42062300	-0.80890600
H	0.77577100	2.40176600	-0.25285300
H	1.79622200	3.35223700	-0.92367100
O	-0.75399100	-1.75543100	1.76234400
H	-1.39692500	-1.27358400	1.21343900
H	-1.27422200	-2.20765500	2.43574300
O	1.06002900	0.29399400	2.47712700
H	0.51780100	1.01448900	2.10964500
H	0.51204800	-0.49969300	2.32088500
O	3.24809000	0.63741100	0.69637200
H	2.56592500	0.41885300	1.36146300
H	2.79811300	1.27418600	0.11162800
C	-3.52671400	1.32180700	-1.52931000
H	-2.60316500	1.85287000	-1.75746800
H	-4.07065500	1.09198600	-2.44326500
H	-4.14747800	1.97194500	-0.90581300
C	5.52411200	-1.14277000	-1.87498500
H	4.62934900	-1.07651800	-2.49943500
H	6.04691300	-0.17714900	-1.93575400
H	6.17440200	-1.90283500	-2.31609500
C	-3.83912300	-2.18446500	-0.34459300
H	-4.59624500	-2.85049500	-0.74827500
H	-2.84294300	-2.58674200	-0.52475800
H	-3.99940100	-2.02510100	0.72116800
TS (RC-T₁[‡])			
C	-1.21295800	-0.43361000	-0.64731300
O	-2.59759000	-0.37371400	-0.73727500
N	-0.96806300	-0.51023700	1.19465600

O	-0.53677900	0.59081000	-1.00822100
H	0.03885300	-0.67285800	1.34852900
H	-1.14642800	0.44873200	1.49036800
O	2.04358400	0.55492000	-1.70115800
H	2.16057100	0.88015800	-2.60048900
H	1.06254400	0.53154600	-1.52711300
O	3.05614100	-1.81636200	-0.67056900
H	2.80640800	-1.01264100	-1.17373400
H	4.00841000	-1.91264500	-0.77961000
O	-0.19096100	2.64397300	0.70702900
H	-0.41003100	2.00951100	-0.01765100
H	-0.54308000	3.49975800	0.44014200
O	2.51039400	1.86577600	0.81841300
H	2.55290100	1.55727200	-0.10487000
H	1.63112200	2.29029900	0.87331200
O	1.94466900	-0.77448300	1.72702000
H	2.19489700	0.15662100	1.55691300
H	2.38221300	-1.26442500	1.00441100
C	-0.76085500	-1.81542800	-1.08177800
H	0.27860500	-1.98254500	-0.80084400
H	-1.38778100	-2.59869400	-0.65616300
H	-0.84020100	-1.86433300	-2.17080500
C	-1.78697500	-1.45592800	1.97571400
H	-1.49566000	-2.47634000	1.72917000
H	-1.64810600	-1.29990100	3.04796100
H	-2.83769100	-1.31504000	1.72434300
C	-3.19846700	0.92668800	-0.70344400
H	-4.26258800	0.76312200	-0.86513200
H	-3.05404100	1.41034600	0.26707000
H	-2.79461300	1.56602300	-1.48937800

T₁[±]

C	-1.18532800	-0.44065500	-0.54407700
O	-2.58959900	-0.35467400	-0.71704000
N	-0.98645800	-0.47303400	1.10998600
O	-0.48705600	0.57865100	-0.96739200
H	0.03066700	-0.59817800	1.28898600
H	-1.19973900	0.47954900	1.41027800
O	2.04448100	0.46542700	-1.69742200
H	2.14848800	0.73574300	-2.61611900
H	1.06047200	0.46634400	-1.50045400
O	3.00926800	-1.86902200	-0.56874600
H	2.77793400	-1.08115800	-1.10673000
H	3.96482800	-1.96865100	-0.63922300
O	-0.14007100	2.66630000	0.64625600
H	-0.34862200	1.98369400	-0.04660700
H	-0.50544300	3.50080800	0.33422600
O	2.54118900	1.86611100	0.76250200
H	2.57646000	1.52742600	-0.15083100
H	1.67262300	2.31532600	0.80267900
O	1.82142500	-0.70652100	1.71726300
H	2.12908300	0.20611700	1.53435600
H	2.28372900	-1.24287000	1.04316000
C	-0.76970800	-1.81919700	-1.04806000
H	0.25751900	-2.04152700	-0.75642100
H	-1.43045200	-2.60619500	-0.68297800
H	-0.82586000	-1.80065300	-2.13782400
C	-1.77599400	-1.44758700	1.90208700
H	-1.43356700	-2.45539800	1.67653700
H	-1.63479300	-1.24994000	2.96480500
H	-2.82805700	-1.34972300	1.64347800
C	-3.16577800	0.95380400	-0.67941100
H	-4.22200000	0.81920400	-0.90939700
H	-3.07868200	1.41335100	0.31151100
H	-2.70564100	1.60961100	-1.41993700

T₂[±]

C	-1.18537100	-0.44062800	-0.54408100
O	-2.58964600	-0.35461100	-0.71699100
N	-0.98645700	-0.47310100	1.10997900

O	-0.48709000	0.57868400	-0.96736100
H	0.03067200	-0.59825700	1.28895000
H	-1.19973200	0.47946600	1.41032200
O	2.04445700	0.46546200	-1.69739300
H	2.14848700	0.73585700	-2.61606400
H	1.06044800	0.46639000	-1.50044100
O	3.00927600	-1.86902300	-0.56883400
H	2.77792300	-1.08114200	-1.10678200
H	3.96483200	-1.96865400	-0.63934700
O	-0.13995500	2.66638500	0.64624000
H	-0.34857600	1.98374500	-0.04656000
H	-0.50536600	3.50087400	0.33420600
O	2.54124800	1.86601200	0.76259200
H	2.57648700	1.52737200	-0.15075900
H	1.67273500	2.31532200	0.80279300
O	1.82143900	-0.70661000	1.71721700
H	2.12907800	0.20604000	1.53432100
H	2.28374700	-1.24293700	1.04310000
C	-0.76978700	-1.81915200	-1.04814600
H	0.25744400	-2.04151100	-0.75654500
H	-1.43053400	-2.60615800	-0.68308700
H	-0.82596900	-1.80055100	-2.13790800
C	-1.77598300	-1.44768900	1.90204700
H	-1.43357300	-2.45549200	1.67643100
H	-1.63474800	-1.25010300	2.96477200
H	-2.82805100	-1.34979800	1.64347000
C	-3.16579100	0.95387800	-0.67931700
H	-2.70568400	1.60968400	-1.41986200
H	-4.22203000	0.81930300	-0.90924100
H	-3.07862700	1.41341900	0.31160200

TS₁

C	-1.13992700	-0.40932900	-0.47681300
O	-2.56076100	-0.28237900	-0.78657400
N	-0.94929300	-0.53387900	1.00610900
O	-0.43343800	0.66498800	-0.91074000
H	0.70090400	-0.65000900	1.41917700
O	2.00797200	0.49584200	-1.59885400
H	2.17186100	0.85322600	-2.47838600
H	0.98683800	0.50688700	-1.42745600
O	2.94187200	-1.87433300	-0.46310000
H	2.74956100	-1.11124500	-1.04668200
H	3.89521300	-2.00881500	-0.50124800
O	0.04370700	2.66322400	0.59272700
H	-0.27346800	1.91899900	-0.04495500
H	-0.10500000	3.51307100	0.16420300
O	2.34505200	1.60833200	0.75825500
H	2.43708000	1.33901200	-0.20393500
H	1.48222100	2.17351400	0.76571700
O	1.68962200	-0.59105200	1.66503000
H	2.08913400	0.66115700	1.23973700
H	2.16020000	-1.21414700	1.06948800
C	-0.74038500	-1.71471900	-1.17004300
H	0.28878800	-1.97759100	-0.92205400
H	-1.39451300	-2.54080700	-0.88668200
H	-0.81724700	-1.56993700	-2.24878000
C	-1.76171100	-1.54560600	1.70476000
H	-1.42735100	-2.54727000	1.43080300
H	-1.61552400	-1.42722700	2.78026600
H	-2.83010100	-1.46142500	1.48204500
H	-1.15622000	0.38079800	1.40193700
C	-3.17416700	0.94324600	-0.41240900
H	-3.18744900	1.08641000	0.67607100
H	-2.67860400	1.80043400	-0.87690400
H	-4.20634500	0.89357600	-0.76204400

(T⁻...H₃O⁺)₁

C	-1.14126800	-0.40860400	-0.47656300
O	-2.56191400	-0.28128300	-0.78720700
N	-0.95041300	-0.53445800	1.00537800

O	-0.43490500	0.66668000	-0.91021500
H	0.70943900	-0.65389800	1.42378600
O	2.00577500	0.49819100	-1.59721000
H	2.17001900	0.85838200	-2.47555600
H	0.98411400	0.50799600	-1.42609900
O	2.94393100	-1.87506600	-0.46732600
H	2.74928700	-1.11094100	-1.04854900
H	3.89707300	-2.00951700	-0.51012500
O	0.04600900	2.65792400	0.59506300
H	-0.27342000	1.91383900	-0.04401900
H	-0.10290400	3.50905200	0.16909800
O	2.34495300	1.61142400	0.75443100
H	2.43371600	1.33755700	-0.20790100
H	1.47697800	2.17369100	0.76321100
O	1.69566600	-0.59516600	1.67022500
H	2.09768100	0.67251400	1.23852800
H	2.16562300	-1.21654700	1.07303300
C	-0.74105900	-1.71275700	-1.17162100
H	0.28829800	-1.97518600	-0.92395600
H	-1.39459500	-2.53959000	-0.88907900
H	-0.81823700	-1.56680600	-2.25018100
C	-1.76386400	-1.54567700	1.70326500
H	-1.43134400	-2.54758000	1.42785800
H	-1.61651800	-1.42897100	2.77880400
H	-2.83246200	-1.45986800	1.48182600
H	-1.15515500	0.38005700	1.40257600
C	-3.17592600	0.94309100	-0.41000900
H	-3.18947500	1.08341900	0.67882700
H	-2.68064000	1.80170200	-0.87222200
H	-4.20800400	0.89394900	-0.76001900

TS₂

C	-1.15336200	-0.39929700	-0.47695900
O	-2.57096700	-0.26501900	-0.79366500
N	-0.96195400	-0.53737400	0.99864300
O	-0.44167000	0.68001900	-0.90752800
H	0.74460300	-0.67688200	1.44256100
O	2.02804800	0.51419900	-1.60497200
H	2.19434900	0.86870200	-2.48535000
H	1.01606100	0.51950400	-1.44568100
O	2.96554200	-1.86996200	-0.48346900
H	2.76850300	-1.09837900	-1.05307900
H	3.91851300	-2.00297000	-0.53333000
O	0.05346800	2.57633100	0.60866300
H	-0.27351200	1.81477100	-0.06212500
H	-0.09156800	3.44009500	0.20696900
O	2.32779900	1.64926800	0.77069300
H	2.45245300	1.37450100	-0.18222600
H	1.38589200	2.17344600	0.75474400
O	1.71920900	-0.62327800	1.69494500
H	2.13106500	0.73667600	1.24853700
H	2.18844700	-1.22673000	1.08168700
C	-0.74965200	-1.69281200	-1.18785900
H	0.27960200	-1.95570700	-0.94030400
H	-1.40239000	-2.52398300	-0.91679000
H	-0.82490500	-1.53366200	-2.26465600
C	-1.77856200	-1.55260800	1.68562800
H	-1.44989900	-2.55297900	1.40002000
H	-1.62954400	-1.44769700	2.76211000
H	-2.84766500	-1.46190800	1.46714400
H	-1.15827200	0.37283200	1.40916800
C	-3.18653500	0.95256900	-0.39694200
H	-2.68923100	1.81928000	-0.84188700
H	-4.21688400	0.91023800	-0.75264100
H	-3.20470100	1.07290600	0.69407700

T₃⁰

C	-1.24988800	-0.52819000	-0.43610400
O	-2.63411900	-0.40489200	-0.77286700
N	-0.98701500	-0.36835600	0.99679900

O	-0.48823800	0.44270600	-1.13192700
H	0.85327000	-0.52819800	1.52098900
O	2.22203300	0.29149200	-1.76482900
H	2.40466400	0.44936200	-2.69803600
H	1.24502900	0.27149500	-1.67033700
O	3.12504300	-1.88872600	-0.26142300
H	2.94223900	-1.17847100	-0.90925700
H	4.08216100	-1.99798700	-0.25084300
O	-0.15929100	2.65638800	0.42787900
H	-0.47339900	1.29614700	-0.63869900
H	-0.33456300	3.56439500	0.15795600
O	2.46379400	1.92947800	0.63941900
H	2.60637300	1.57408300	-0.25469600
H	0.81817000	2.57104300	0.54302600
O	1.79196100	-0.49698000	1.82106700
H	2.30617900	1.11850700	1.17569900
H	2.27452500	-1.09777700	1.22099300
C	-0.84209900	-1.90272000	-0.94454600
H	0.19596000	-2.10870400	-0.68376100
H	-1.47960100	-2.67722400	-0.51909400
H	-0.95183600	-1.92323000	-2.02935200
C	-1.78377000	-1.21847300	1.89753500
H	-1.48828600	-2.26238000	1.78485900
H	-1.56985900	-0.92001100	2.92465500
H	-2.86258300	-1.14073100	1.72558300
H	-1.11113000	0.60947800	1.25049500
C	-3.25655700	0.85147900	-0.50736000
H	-2.79186800	1.65924700	-1.08025200
H	-4.29434600	0.74741000	-0.82166400
H	-3.23756900	1.10375000	0.55843600

T⁻

C	1.04523300	-0.31628000	-0.07590500
O	1.23625300	-1.70048300	0.40036500
N	1.07048000	0.50567000	1.15186300
O	-0.16260400	-0.18460200	-0.68407400
H	0.58754300	2.25993800	0.71352300
H	0.26705700	0.20485700	1.69941200
O	-0.27525400	2.05046100	-2.30614700
H	-0.21240200	1.17909100	-1.84456900
O	-2.17803500	1.33699800	0.27030800
H	-1.41418700	0.76864400	-0.04124800
H	-2.57411700	1.67766200	-0.54018300
O	-3.78524200	-0.86687100	1.13737200
H	-3.23790400	-1.46141400	0.58764800
H	-3.36292000	-0.00396600	0.97331600
O	-1.95049900	-2.16450600	-0.57586800
H	-1.52280300	-2.97596600	-0.28434400
H	-1.22329300	-1.47428300	-0.60494200
O	0.14910400	3.12109600	0.48853300
H	-0.78717800	2.88206700	0.57551400
H	-0.07303000	2.66848200	-1.58606400
C	2.21818100	0.07489500	-0.99189900
H	2.18658600	1.14852600	-1.18194500
H	3.18704900	-0.17777400	-0.55550400
H	2.12333600	-0.43983200	-1.94857000
C	2.27332300	0.43806800	1.99676100
H	2.07646200	0.98302500	2.92263500
H	2.56736400	-0.58670300	2.24799900
H	3.11109100	0.92868500	1.49784100
C	1.46064200	-2.68861200	-0.59523400
H	1.31914900	-3.66089200	-0.11817800
H	0.75360100	-2.59906600	-1.42707900
H	2.48116700	-2.64594300	-0.99457000

TS₃

C	-0.00643200	-0.96280000	0.16308200
O	-1.95918300	-0.95431400	-0.17968700
N	0.03627500	-0.01977900	1.20813500
O	0.51722300	-0.61840700	-0.94613500

H	2.06171600	0.53069000	1.23882400
H	-0.18302300	0.91094400	0.86201200
O	3.28542000	-1.27834100	-0.99334900
H	2.31985200	-1.21350500	-1.12565300
O	1.36337500	1.87675400	-1.32021000
H	1.00879300	0.94280000	-1.27737600
H	1.61637700	2.04006200	-2.23506500
O	-0.70498100	3.07911000	0.22133600
H	-1.49974800	2.56162300	-0.03463800
H	-0.01392200	2.82290900	-0.41459100
O	-2.85760700	1.43577700	-0.30801800
H	-2.49588200	0.46866000	-0.27625300
H	-3.33124400	1.52422500	-1.14104300
O	2.90458400	0.91636700	0.92961400
H	2.61759500	1.46345600	0.17731300
H	3.43210000	-0.61213500	-0.30041800
C	0.09614900	-2.41659600	0.58090100
H	1.10705500	-2.60310000	0.96025300
H	-0.62451700	-2.68831900	1.34924200
H	-0.05995400	-3.04606200	-0.29391100
C	-0.63451300	-0.28136300	2.48525300
H	-0.54098600	0.61053700	3.10675100
H	-1.69505500	-0.51657100	2.35806400
H	-0.14852400	-1.10418400	3.01145000
C	-2.29290200	-1.66974400	-1.33395700
H	-3.25493400	-1.32721400	-1.74987900
H	-1.53682800	-1.54721600	-2.12851200
H	-2.39725300	-2.75169700	-1.14359400

AM...AL⁻

C	2.51359600	-0.04839000	0.18360200
O	-3.73130400	1.28117300	1.19220500
N	2.35750300	1.27668400	0.07358500
O	1.57916600	-0.83818100	-0.07566800
H	-1.92372600	-3.86993500	-1.13356600
H	1.43354900	1.63085500	-0.20300100
O	1.08737600	-3.58235100	0.49824300
H	1.35811500	-2.66123800	0.32654700
O	-0.98375400	-0.89138700	-1.30495300
H	-0.10608400	-0.73149200	-0.91195200
H	-1.51468400	-0.03659900	-1.17644400
O	-0.09594200	2.65155700	-0.57072800
H	-0.97863500	2.16054800	-0.75333700
H	-0.02117900	3.32989100	-1.24941200
O	-2.27429000	1.34522700	-0.97533000
H	-3.16900400	1.32791400	0.35198600
O	-1.62150600	-3.33124700	-0.39488200
H	-1.48515900	-2.41839700	-0.76256600
H	0.15448900	-3.61023100	0.21440900
C	3.86139800	-0.56583000	0.63111900
H	4.64113400	-0.27688900	-0.07880200
H	4.13574400	-0.15035200	1.60414700
H	3.82672300	-1.65084700	0.69968800
C	3.38189900	2.27702700	0.35628600
H	2.96021800	3.25675100	0.13651800
H	3.68744800	2.26351700	1.40598700
H	4.26736700	2.13791300	-0.26864100
H	-3.65162000	2.14859200	1.60073100
C	-2.98082400	1.75810700	-2.11822800
H	-3.23231700	2.83180800	-2.08697200
H	-2.40376500	1.59359600	-3.04407200
H	-3.93163100	1.21277800	-2.23544000

(T⁻...H₃O⁺)₂

C	0.84380800	-0.56935500	0.40149200
O	2.12154300	0.18884000	0.22824000
N	0.41869100	-0.82685500	-1.00070900
O	-0.05364200	0.19727900	1.04390400
H	-1.21301400	-1.24073300	-1.27543800
O	-2.35429200	-0.39562700	1.99429000

H	-2.48197300	0.01742400	2.85525200
H	-1.37746100	-0.26341200	1.72966900
O	1.38997000	2.35331300	-1.39330200
H	1.78379100	1.63380700	-0.85246900
H	1.91125500	2.39806500	-2.20175400
O	-1.16483600	2.20421700	-0.08330000
H	-0.61622500	1.46607600	0.37262700
O	-3.13892100	0.65193400	-0.19085500
H	-2.99039100	0.27824900	0.75683100
H	-2.39636500	1.38126500	-0.28605300
O	-2.19185600	-1.28767100	-1.54562200
H	-2.85545700	-0.13088200	-0.79880100
H	-2.51278700	-2.16960100	-1.32522300
C	1.12679500	-1.88788000	1.13042900
H	0.23861100	-2.52170400	1.07970600
H	1.97271100	-2.42977100	0.70432900
H	1.33552800	-1.68133300	2.18039400
C	1.29991600	-1.67603200	-1.82632900
H	1.23162700	-2.71468100	-1.50053000
H	0.95411200	-1.62767900	-2.86073100
H	2.34724700	-1.36146800	-1.79079800
H	0.36406400	0.09031400	-1.44114900
C	2.77066200	0.59047700	1.43333200
H	3.24805200	-0.25874200	1.93327000
H	3.54347600	1.30865200	1.15427600
H	2.06532700	1.06793400	2.11902400
H	-0.59377300	2.50465800	-0.80787000

TS₄

C	-0.70049900	0.57767700	0.67583400
O	-2.38585700	-0.43491200	-0.02693200
N	-0.41763800	1.19879500	-0.55855200
O	0.04610000	-0.37553200	1.04442900
H	1.36932900	1.71072000	-0.78924500
O	2.57397000	-0.40665200	2.03895100
H	2.74634200	-1.09099900	2.69580500
H	1.59752200	-0.36536900	1.91414200
O	-1.19705800	-1.38423900	-2.03927200
H	-1.77114200	-1.03440500	-1.23443300
H	-1.73819600	-1.37113800	-2.83401400
O	1.08452400	-2.04357800	-0.76360200
H	0.61873500	-1.54263500	-0.04028900
O	3.12853700	-0.64140100	-0.48334800
H	3.08540100	-0.61087100	0.53024400
H	2.31460300	-1.26147700	-0.75449900
O	2.31456000	1.72688200	-1.08709700
H	2.89768300	0.30894600	-0.77891600
H	2.73685800	2.47687700	-0.65181400
C	-1.38529600	1.41108500	1.73090100
H	-0.66439600	2.13724100	2.12455100
H	-2.25303300	1.94727600	1.35396500
H	-1.68944400	0.75745800	2.54674800
C	-1.32255300	2.23963300	-1.07248300
H	-1.26285700	3.13341100	-0.45110900
H	-0.99330600	2.50757400	-2.07719100
H	-2.35772900	1.89312500	-1.11404900
H	-0.28618600	0.47226600	-1.26115400
C	-2.83687000	-1.39257100	0.88478700
H	-3.50773600	-0.95929000	1.64617800
H	-3.40243600	-2.19573700	0.38333800
H	-2.00340400	-1.87807700	1.42343200
H	0.43995700	-1.96594800	-1.50109900

(AM...AL)₁

C	0.11113100	2.30847700	-0.13158600
O	4.20427600	-1.74407900	-0.16822600
N	1.18234300	1.89627600	0.55711100
O	-0.63560200	1.49139800	-0.71872500
H	-4.15660200	-2.42232800	2.44517300
O	-3.36589400	1.10792300	-0.90918900

H	-3.75785800	1.50862400	-1.69254600
H	-2.42911400	1.39654700	-0.89920700
O	1.64108800	-1.10956100	0.80848800
H	3.30957500	-1.54761400	0.16727500
H	1.44348900	-1.46070200	1.68419500
O	-0.37414400	-1.27469700	-0.95663100
H	-0.44779100	-0.29758800	-0.95233400
O	-3.11460800	-1.69219100	-0.71172000
H	-3.34414400	-0.74317000	-0.76407100
H	-1.29453600	-1.58209800	-0.81269400
O	-4.32242800	-2.83231300	1.58812100
H	-3.54759700	-2.03996200	0.08932500
H	-5.27361700	-2.98980600	1.56417800
C	-0.16936400	3.78947900	-0.18713300
H	-0.28809700	4.20292300	0.81752600
H	0.66002300	4.31947300	-0.66302900
H	-1.07815000	3.96173000	-0.75923000
C	2.12013000	2.75806400	1.27319300
H	1.63043700	3.29968300	2.08613000
H	2.89640200	2.12589600	1.70055800
H	2.59420000	3.47804100	0.60288200
H	1.33745400	0.88933600	0.61525800
C	4.21164500	-3.07380500	-0.67989900
H	5.21752400	-3.28042500	-1.04941100
H	3.97003700	-3.81154600	0.09485300
H	3.50659000	-3.19613700	-1.51095500
H	0.87262500	-1.34992700	0.23193600

T₃[±]

C	1.27569600	0.13510000	-0.42057400
O	2.61778500	-0.32261700	-0.15944400
N	0.89197500	0.66553100	1.04132800
O	0.43749700	-0.82178900	-0.73500100
H	-0.00410400	1.18170600	0.95908100
O	-0.02582700	-2.22143700	1.55444900
H	0.18513100	-1.90324400	0.64493000
H	-0.99751400	-2.28712100	1.54281300
O	-2.84627000	-2.15048900	0.94624400
H	-3.34016700	-2.96010700	0.77765900
H	-2.69126200	-1.74657400	0.06679700
O	-2.06680500	-0.82340900	-1.40410400
H	-1.07544900	-0.75710300	-1.21693500
H	-2.16111400	-1.26361800	-2.25627000
O	-3.23159600	1.61397300	-0.97141100
H	-3.23048400	2.15977400	-1.76534500
H	-2.85801800	0.74346200	-1.23999500
O	-1.49938400	2.24824300	1.06365600
H	-2.14700500	2.12138400	0.33345100
H	-1.39444200	3.20031300	1.16605000
C	1.28584900	1.34172500	-1.36413200
H	0.28346300	1.76780200	-1.43651600
H	1.98603400	2.11523100	-1.04412600
H	1.58082300	0.99924000	-2.35727200
C	1.86285500	1.50918300	1.78849300
H	2.02805900	2.43737700	1.24542200
H	1.44499700	1.73554700	2.76939400
H	2.79837300	0.96846600	1.89348700
H	0.68601600	-0.19409400	1.56633700
C	3.17198200	-1.15805400	-1.17378100
H	2.54403800	-2.03361800	-1.35237200
H	3.31001700	-0.61442100	-2.11517700
H	4.14729700	-1.47663100	-0.80584900

TS₅

C	-1.30125600	0.12833400	0.35822600
O	-2.63449100	-0.28456400	0.13396400
N	-0.83638100	0.54904800	-1.02484400
O	-0.49461900	-0.93738600	0.73975500
H	0.03098500	1.09944500	-0.91588200
O	-0.20287800	-1.82177800	-1.55295300

H	-0.35513300	-1.51696000	-0.14550100
H	0.74852800	-1.94917500	-1.68037900
O	2.83781400	-2.06298400	-1.11244800
H	3.27368900	-2.91984300	-1.05386400
H	2.70401500	-1.77768800	-0.18916900
O	2.13867100	-0.98068500	1.44704600
H	1.16216400	-0.90958200	1.32241200
H	2.27730300	-1.47172000	2.26516800
O	3.31415100	1.48599400	1.00969700
H	3.35572100	2.02027000	1.81042600
H	2.94694600	0.61851200	1.28343900
O	1.55243900	2.21067600	-0.98900800
H	2.20726500	2.04919200	-0.27419900
H	1.43914700	3.16618200	-1.03390500
C	-1.18856500	1.26661600	1.36373500
H	-0.16176100	1.63234400	1.40044800
H	-1.85250200	2.08934900	1.09390100
H	-1.45907700	0.90928700	2.35763700
C	-1.77945100	1.32759100	-1.86321100
H	-2.10143900	2.23451400	-1.35049700
H	-1.25767300	1.60254200	-2.77981100
H	-2.64479000	0.71720200	-2.10418500
H	-0.52498600	-0.47197600	-1.49623300
C	-3.31467100	-0.85768100	1.25450100
H	-2.72758400	-1.66333600	1.70035700
H	-3.54409500	-0.10360100	2.01302400
H	-4.24709400	-1.26163400	0.86279600

T₁^o

C	-1.36190700	-0.20960100	-0.28501600
O	-2.67081500	0.29492000	-0.11711200
N	-0.86627900	-0.41735500	1.07659700
O	-0.53645000	0.78038200	-0.90078200
H	0.04496000	-0.87616900	1.01313000
O	-0.07519100	2.32209400	1.43409500
H	-0.47465400	1.52662400	-0.26651900
H	0.89752200	2.32652700	1.34689700
O	2.69864300	2.19178500	0.79655500
H	3.21167900	2.99773500	0.67235500
H	2.64600900	1.77123500	-0.08376300
O	2.13566100	0.76016500	-1.59324200
H	1.16333100	0.67939200	-1.46707700
H	2.26613500	1.16536400	-2.45868100
O	3.40987200	-1.60610000	-0.88735600
H	3.43569400	-2.24415200	-1.60875100
H	3.00531700	-0.79538800	-1.25996100
O	1.73124100	-2.06821700	1.28691900
H	2.34775500	-2.00348500	0.52762400
H	1.58237700	-3.01056600	1.41824900
C	-1.29968200	-1.44766600	-1.17964900
H	-0.28117200	-1.83885600	-1.18522900
H	-1.97079400	-2.22082000	-0.80292700
H	-1.58046200	-1.20913300	-2.20613100
C	-1.72057400	-1.21889400	1.96757500
H	-1.97603200	-2.20591500	1.56049600
H	-1.18046700	-1.36869800	2.90400000
H	-2.64385800	-0.68438500	2.18462000
H	-0.31898400	1.39062000	1.63122800
C	-3.41516200	0.57017600	-1.30574100
H	-2.83951400	1.18666800	-2.00074400
H	-3.73158800	-0.35007300	-1.80518500
H	-4.29904500	1.12064400	-0.98543100

T₂^o

C	1.44396900	-0.48834600	0.31094100
O	1.64900900	0.96783400	0.36028500
N	0.74758000	-0.93938600	-0.83110600
O	0.56555700	-0.68525800	1.42151200
H	-0.07367000	-0.37715700	-1.05353400
O	-1.61515100	-2.42123900	1.61566200

H	-1.31049200	-3.33507200	1.59588400
H	-0.81153900	-1.87097200	1.52303900
O	-3.41270900	-1.64978800	-0.33386900
H	-2.82553700	-1.96111300	0.38975500
H	-4.25246900	-1.43110600	0.08409600
O	-0.24459700	2.69313400	1.46209800
H	0.94628000	-0.26157800	2.20199800
H	0.24552700	3.48622900	1.70512900
O	-2.27230500	2.85689900	-0.39472300
H	-3.10965500	3.02790000	0.04953300
H	-1.58737200	2.86848000	0.30969300
O	-1.90555000	0.34878400	-1.65950100
H	-2.09076600	1.20878500	-1.23539400
H	-2.49146500	-0.29415200	-1.21549800
C	2.77132600	-1.19913500	0.55167300
H	2.60741100	-2.27546500	0.61725400
H	3.49262200	-1.00592600	-0.24282800
H	3.19470800	-0.84769000	1.49373100
C	1.43378200	-1.47744800	-2.00219100
H	1.95836000	-2.40425800	-1.75934400
H	0.67332900	-1.71990300	-2.74587200
H	2.15155000	-0.79179000	-2.47040700
H	0.42029900	2.06447200	1.10833900
C	2.34352900	1.56380900	-0.73928500
H	2.39579300	2.63142400	-0.52729700
H	3.36102200	1.17442000	-0.83162200
H	1.80333800	1.41396800	-1.67745600

TS₆

C	0.93732300	-0.91877800	0.47805000
O	2.28156800	0.58507400	0.10123300
N	0.48123100	-1.34101200	-0.69023300
O	0.01866800	-0.20119200	1.17603100
H	-0.28266400	-0.78632500	-1.10005600
O	-2.64066500	-0.94301900	1.80881300
H	-2.65445600	-1.80762300	2.23398100
H	-1.70155900	-0.74776300	1.63059700
O	-3.91530200	-0.49776500	-0.59863500
H	-3.56970700	-0.68588200	0.30065900
H	-4.67877900	0.07629200	-0.47466300
O	1.01587200	2.18787500	1.40216300
H	0.38390300	0.65468900	1.53567800
H	1.48580400	2.66375000	2.09429300
O	-0.82361200	2.91134900	-0.53145700
H	-1.52690100	3.47602300	-0.19366900
H	-0.20126000	2.77904200	0.21786900
O	-1.54494400	0.44556700	-1.79337200
H	-1.33554000	1.29906200	-1.36493000
H	-2.41707300	0.18288200	-1.43783800
C	1.92764300	-1.72246600	1.26330700
H	1.40949100	-2.58901600	1.68955600
H	2.75093200	-2.06922500	0.64228300
H	2.32459200	-1.11852000	2.07637800
C	1.12642800	-2.35880500	-1.51446700
H	1.15748000	-3.31944200	-0.99687900
H	0.53921000	-2.47525100	-2.42364800
H	2.14325400	-2.07023000	-1.79105200
H	1.70923900	1.58641600	0.81094500
C	2.43230700	0.90571500	-1.25868800
H	2.49222000	1.99346900	-1.40600300
H	3.34553100	0.45885900	-1.67674900
H	1.58277800	0.54875800	-1.86253200

(AM...AL)₂

C	0.52605100	-1.75912500	-0.33787500
O	-4.07709300	-0.04106800	-0.72038700
N	0.88554100	-1.48330900	0.91499100
O	0.43238100	-0.85030700	-1.20528500
H	1.07842200	-0.49970900	1.14700800
O	2.53152600	0.71219900	-2.11585400

H	3.09169200	0.16004600	-2.67220100
H	1.80352500	0.13154400	-1.80778000
O	3.56825300	1.97824200	0.09674400
H	3.27141000	1.56978000	-0.74649600
H	3.73398700	2.90607000	-0.10181800
O	-1.49997600	1.09272200	-1.19051200
H	-0.79852400	0.40184700	-1.22099400
H	-1.46386600	1.54338400	-2.04268400
O	-0.86378300	2.61415100	1.07439900
H	-0.83798400	3.55652300	0.87627300
H	-1.13328100	2.17249700	0.24259600
O	1.46857600	1.21558200	1.80185600
H	0.69790700	1.77686200	1.58496300
H	2.20768100	1.56307300	1.26339700
C	0.23203100	-3.19320700	-0.70027800
H	1.10804500	-3.82422000	-0.52764800
H	-0.58030500	-3.58937700	-0.08506800
H	-0.04996800	-3.24716200	-1.74912500
C	1.02266900	-2.46058000	1.99194000
H	1.76873100	-3.22136200	1.75121500
H	1.34836000	-1.93026300	2.88506800
H	0.07279700	-2.95423200	2.21064500
H	-3.19835700	0.34702300	-0.87887900
C	-4.56076200	0.43079500	0.53491000
H	-4.67369000	1.52137800	0.54532300
H	-5.54146900	-0.01854500	0.69952300
H	-3.90290800	0.13855600	1.36188100

T₄[±]

C	-0.73347200	-0.91860800	-0.49386500
O	-1.99759500	-0.17722700	-0.26220800
N	-0.04215500	-0.68532200	0.91525800
O	0.01746900	-0.42318400	-1.42564800
H	0.90415400	-1.10283100	0.83754200
H	0.11861800	0.33632800	1.00014200
O	1.52811600	1.66928600	-1.36296800
H	1.44157000	2.18142100	-2.17413700
H	0.88798700	0.88338600	-1.42766300
O	-2.24820000	2.34815700	0.97555800
H	-2.74542300	2.93751500	0.39815400
H	-2.22180300	1.48160600	0.51968300
O	0.52306400	2.17596200	1.19774100
H	-0.39729100	2.49504600	1.13063800
H	0.90123700	2.26460400	0.30181900
O	3.85789500	0.42518800	-0.61443200
H	3.09225800	0.95799400	-0.92987000
H	4.44323200	1.04190500	-0.16155700
O	2.69589300	-1.57873900	0.88212200
H	3.18738100	-0.90823900	0.35558600
H	2.97299500	-2.43709300	0.54381500
C	-1.03283600	-2.41756700	-0.62817800
H	-0.10292900	-2.98233000	-0.53221500
H	-1.75211400	-2.77840300	0.10871000
H	-1.43025900	-2.60305300	-1.62628800
C	-0.70947700	-1.17960700	2.14950200
H	-0.73077800	-2.26694900	2.14520300
H	-0.14223800	-0.83445100	3.01373700
H	-1.72248600	-0.78765400	2.19119200
C	-2.87251900	-0.17147900	-1.39355000
H	-3.68414200	0.51970600	-1.16435000
H	-2.34838900	0.16936900	-2.28984700
H	-3.29981100	-1.16260000	-1.57187000

TS₇

C	-0.48623900	1.01414800	0.63672300
O	-2.38950000	-0.03705800	0.02773200
N	0.08198900	0.85641200	-0.74844700
O	-0.00439500	0.29583300	1.48975800
H	1.07165600	1.20874500	-0.69163300
H	0.18044400	-0.18227900	-0.94426700

O	1.72646000	-1.89115700	1.24959300
H	1.71855400	-2.50348000	1.99412000
H	1.09744700	-1.17370200	1.46799600
O	-2.15710000	-2.12623000	-1.17215900
H	-2.53699900	-2.86077800	-0.68075400
H	-2.29184000	-1.07336800	-0.53243000
O	0.39386700	-1.81040900	-1.32993300
H	-0.57918400	-2.08802700	-1.26239600
H	0.84520500	-2.16919400	-0.54972500
O	4.01491700	-0.54317900	0.42569700
H	3.28473300	-1.11762400	0.73934800
H	4.55758700	-1.09221700	-0.15098500
O	2.76224900	1.62711600	-0.68089200
H	3.28782200	0.88970400	-0.29161100
H	3.04016700	2.42872900	-0.22398600
C	-1.18605300	2.30764200	0.92454700
H	-0.42907100	3.10024900	0.95717600
H	-1.92913100	2.56144300	0.17396800
H	-1.65372600	2.24015600	1.90465400
C	-0.60844000	1.51806100	-1.89273100
H	-0.53850100	2.59897200	-1.79397500
H	-0.10366300	1.20653900	-2.80579600
H	-1.64651200	1.19944500	-1.90538200
C	-3.15280800	-0.23909100	1.19557200
H	-3.89589000	-1.03535400	1.04794700
H	-2.52550300	-0.52904700	2.05368400
H	-3.69826900	0.67231400	1.47014200

(AM...AL)₃

C	3.14216200	1.38533400	0.20759800
O	-6.88827500	-0.12489300	-0.24656700
N	3.86840800	0.41550200	-0.36632900
O	2.03722500	1.15996200	0.74295100
H	3.50410100	-0.53885800	-0.34387900
H	-1.92956900	0.60485400	-0.94956300
O	0.13972600	-0.66990800	1.16512000
H	-0.02652500	-0.62339500	2.11422500
H	0.89512600	-0.05000100	0.98959500
O	-4.48991700	0.30321200	1.11805200
H	-4.40585300	1.10704900	1.64179000
H	-6.04572500	0.04481400	0.21739900
O	-2.15923700	-0.06420100	-0.29556700
H	-3.64177400	0.21036700	0.63000900
H	-1.33672600	-0.24046700	0.20901500
O	0.83099500	-3.19422800	0.25636800
H	0.50267000	-2.33272600	0.59256700
H	0.17634200	-3.49731000	-0.38221200
O	3.33867700	-2.46458900	-0.62447500
H	2.46437500	-2.80973800	-0.34001900
H	3.99197300	-3.03579700	-0.20659100
C	3.70637900	2.78729700	0.18815000
H	4.68264500	2.82246400	0.67856500
H	3.84440100	3.13583000	-0.83886700
H	3.01919500	3.45421900	0.70372500
C	5.16787500	0.59431200	-1.00829400
H	5.92705600	0.93788100	-0.30088800
H	5.47924100	-0.37166200	-1.40254400
H	5.11416500	1.30221900	-1.83862300
C	-7.07428300	0.89003400	-1.22811600
H	-7.13565100	1.88855500	-0.77821800
H	-6.26893400	0.89179900	-1.97275200
H	-8.01573400	0.68669200	-1.74151800

Table S2. Cartesian coordinates of stationary points for the reaction of methyamine with phenylacetate in water. Optimized geometries at the B3LYP/6-311+G(d,p) level.

RC

C	-1.88563700	1.73840000	-0.82347000
---	-------------	------------	-------------

O	-2.94965100	0.98962400	-1.16197400
N	4.69415100	-2.21890900	-1.40505100
O	-1.04338400	1.36936000	-0.02264600
H	4.55606800	-1.44067300	-0.75957900
H	3.80124700	-2.69719200	-1.47830200
O	1.18819900	2.76893700	1.00839600
H	0.91780200	3.58920000	1.43747100
H	0.37643400	2.38211700	0.62407800
O	3.45236000	2.65988400	-0.67000400
H	2.65798700	2.81759700	-0.12252900
H	3.96088400	3.47719800	-0.63288200
O	-0.08519200	-0.92747800	1.47298300
H	-0.56803000	-0.25925900	0.95683800
H	-0.73991000	-1.32385000	2.05848500
O	2.21926900	0.43481800	2.36355100
H	1.92442500	1.31599200	2.07332300
H	1.45889100	-0.13920100	2.14623700
O	4.38506800	0.22593200	0.53117400
H	3.67899500	0.18169000	1.20586000
H	4.19192500	1.05524800	0.05682200
C	-1.89035800	3.05941000	-1.52783100
H	-0.89981100	3.50735900	-1.49213400
H	-2.22153400	2.94261900	-2.55943300
H	-2.59924800	3.72010800	-1.02025100
C	5.71222900	-3.13945300	-0.88033400
H	6.66928300	-2.61676000	-0.80452700
H	5.48098200	-3.55965800	0.10927900
H	5.85003800	-3.97361300	-1.57340900
C	-3.14486400	-0.26682000	-0.55073000
C	-3.76578400	-0.32972200	0.69002400
C	-2.78974800	-1.40691500	-1.25848500
C	-4.02682900	-1.58334500	1.24295600
H	-4.04212000	0.58080800	1.20741800
C	-3.05901000	-2.65443900	-0.69538800
H	-2.31669300	-1.31579400	-2.22851300
C	-3.67469300	-2.74406800	0.55307100
H	-4.51059400	-1.64949100	2.21029600
H	-2.78792600	-3.55367100	-1.23572800
H	-3.88332700	-3.71531200	0.98582100

TS (RC-T₁[‡])

C	-0.10000400	0.84643700	-0.80375700
O	1.21882000	1.33488900	-0.84346900
N	-0.59037200	1.43693000	0.99241800
O	-0.29153700	-0.39559500	-0.76296300
H	-1.54742500	1.09469800	1.15598700
H	0.02558200	0.86627100	1.56792200
O	-2.59666000	-1.65559000	-1.40954600
H	-2.49079400	-2.20084600	-2.19699000
H	-1.73779000	-1.18108600	-1.27301600
O	-4.55111700	0.28212000	-0.99533100
H	-3.96934100	-0.45150700	-1.28371500
H	-5.45393900	-0.02880400	-1.12274000
O	0.12166800	-2.01610400	1.41192900
H	0.14447700	-1.48153000	0.58787100
H	0.79164600	-2.70010500	1.30725400
O	-2.66509800	-2.38355800	1.37823000
H	-2.76452200	-2.36363600	0.40973100
H	-1.69535000	-2.38646100	1.50660000
O	-3.33582900	0.38511400	1.57366300
H	-3.14525100	-0.57223500	1.64410000
H	-3.86585800	0.45562200	0.75683100
C	-0.97493600	1.74921900	-1.64237400
H	-2.02557100	1.57121200	-1.41495600
H	-0.73467900	2.80054800	-1.49117000
H	-0.79700000	1.50128600	-2.69261200
C	-0.46539600	2.85967400	1.34984800
H	-1.22698900	3.43268000	0.82136700
H	-0.59325900	3.01762100	2.42412300
H	0.51880200	3.22414700	1.05327700

C	2.27284100	0.50285600	-0.47686800
C	2.67250000	-0.54574600	-1.30472800
C	2.98217200	0.80299700	0.68387000
C	3.78409400	-1.30870100	-0.95190800
H	2.11996300	-0.75445300	-2.21162100
C	4.09685200	0.03632600	1.02667300
H	2.67238300	1.63651700	1.30288700
C	4.49767800	-1.02281000	0.21361700
H	4.09647400	-2.12475700	-1.59366000
H	4.65077500	0.27194000	1.92818800
H	5.36348800	-1.61735800	0.48108300

T₁[±]

C	0.00905400	0.45456900	-0.23799900
O	1.30120700	0.92999400	0.27648200
N	-0.87531000	1.67732100	0.27018900
O	-0.43525200	-0.62553100	0.34001400
H	-1.87169100	1.44405000	0.05285400
H	-0.79310100	1.62836100	1.28846600
O	-2.38335300	-2.19658900	-0.51384100
H	-2.07122400	-3.09763600	-0.65078600
H	-1.58580700	-1.64426700	-0.26835000
O	-3.75448800	-0.63200000	-2.33433300
H	-3.31434400	-1.33110100	-1.80447900
H	-4.58487600	-1.01172400	-2.64129700
O	-1.35560700	-0.35399300	2.82106900
H	-0.88968700	-0.53725600	1.96115400
H	-0.86412900	-0.81552500	3.50870700
O	-3.83179600	-1.00042000	1.66933000
H	-3.48002000	-1.61261100	0.99753100
H	-3.05922600	-0.81992000	2.24229700
O	-3.62816500	1.14913200	-0.16029500
H	-3.81904000	0.48883200	0.53954900
H	-3.77724200	0.65585500	-0.99213100
C	0.01041600	0.45900000	-1.76669500
H	-1.00854400	0.32927600	-2.13557900
H	0.43231300	1.37522200	-2.18082800
H	0.60604700	-0.38448700	-2.11529100
C	-0.56523600	3.05804000	-0.19209600
H	-0.77802100	3.13737100	-1.25540600
H	-1.19820000	3.75637400	0.35428500
H	0.48227700	3.27233800	0.00073500
C	2.45511000	0.21102700	0.08803200
C	2.50931000	-1.16166500	-0.18066800
C	3.64430900	0.93959100	0.22042900
C	3.75111200	-1.78280900	-0.32882300
H	1.59589500	-1.73310600	-0.25630400
C	4.87439600	0.30403300	0.08143500
H	3.58661100	2.00117900	0.43115600
C	4.93720300	-1.06273300	-0.19860900
H	3.78339700	-2.84613700	-0.54043600
H	5.78628800	0.88143100	0.18675300
H	5.89508900	-1.55683400	-0.31136900

T₂[±]

C	0.18854600	0.92063300	0.62127000
O	-1.18632500	1.39425800	0.79041700
N	0.51860000	1.32669400	-0.92184000
O	0.36037200	-0.36017400	0.71478800
H	1.47078900	0.95408400	-1.13322500
O	2.62688500	-1.51668000	1.45360300
H	2.53165700	-1.98062100	2.29244800
H	1.75744100	-1.05603200	1.27275300
O	4.54021700	0.37848800	0.81058700
H	3.97880100	-0.33548700	1.18183000
H	5.44915000	0.06674400	0.87881000
O	-0.15297700	-2.16736700	-1.20895300
H	-0.10527600	-1.52328500	-0.45723300
H	-0.81412200	-2.82318300	-0.96427900
O	2.62639700	-2.46028400	-1.25664000

H	2.75696400	-2.36785800	-0.29535500
H	1.65282100	-2.51461300	-1.34665100
O	3.09556000	0.31199300	-1.61116600
H	2.96707800	-0.66028800	-1.63346000
H	3.71280600	0.44607800	-0.86445200
C	1.03457700	1.80935500	1.52502300
H	2.09445700	1.67538500	1.30223400
H	0.77303100	2.86359300	1.43302900
H	0.85258300	1.49606800	2.55404600
C	0.42271300	2.75163600	-1.33265200
H	1.23405800	3.31169500	-0.87343600
H	0.50876300	2.81664700	-2.41690900
H	-0.53499300	3.15490400	-1.01187400
H	-0.12884900	0.76086600	-1.47302500
C	-2.23116600	0.54948600	0.45865700
C	-2.98972900	0.82917400	-0.67952100
C	-2.58665300	-0.51205600	1.29447100
C	-4.09729800	0.03820900	-0.98902700
H	-2.72465000	1.67242900	-1.30684500
C	-3.69069800	-1.30037400	0.97561800
H	-2.00095200	-0.70774500	2.18292100
C	-4.44784400	-1.03136100	-0.16658800
H	-4.68546300	0.26321100	-1.87158800
H	-3.96402500	-2.12408000	1.62577900
H	-5.30798600	-1.64544600	-0.40723100
T			
C	-0.46757600	-0.87171800	-0.06065200
O	0.80360800	-0.54974200	-0.86603600
N	-1.43749500	-1.20110000	-1.11033100
O	-0.87182600	0.20226400	0.63037400
H	-3.15418000	-1.37239100	-0.29840700
H	-1.57386600	-0.34869100	-1.64818100
O	-2.63122400	-0.52618200	2.66967600
H	-1.90734700	-0.24725400	2.06402200
O	-3.15115200	1.53763900	-0.00751100
H	-2.31460800	1.04231900	0.21949900
H	-3.41957700	1.97230000	0.81008400
O	-1.76924100	3.53013900	-1.56775300
H	-0.96882700	3.36158400	-1.03509000
H	-2.40643000	2.91068700	-1.16948800
O	0.18466900	2.65760500	0.28107200
H	1.14150500	2.58944500	0.19546100
H	-0.13344500	1.72177100	0.40230000
O	-4.03959600	-1.23931300	0.12073100
H	-4.14682400	-0.27852500	0.03016100
H	-3.27539000	-0.89951800	2.04633200
C	-0.16549800	-2.11107200	0.79356700
H	-1.09870500	-2.47844700	1.22376100
H	0.29292300	-2.91025500	0.20928000
H	0.50518500	-1.85038900	1.61007600
C	-1.13707000	-2.31068300	-2.02839800
H	-1.89147500	-2.31528600	-2.81769600
H	-0.14701200	-2.23231500	-2.48954900
H	-1.20506200	-3.26435700	-1.50256000
C	2.01024200	-0.29136400	-0.30255700
C	2.22021400	0.10653100	1.02849000
C	3.12289600	-0.40258200	-1.15609500
C	3.51480400	0.36833900	1.48234800
H	1.37796300	0.22006800	1.69564300
C	4.40554100	-0.12955300	-0.69296000
H	2.95751800	-0.70785500	-2.18333600
C	4.61484100	0.25576300	0.63397500
H	3.65648000	0.67177500	2.51444600
H	5.24683300	-0.22317700	-1.37155800
H	5.61453900	0.46496400	0.99639600
TS₈			
C	-0.59982800	-0.88172400	-0.03975200
O	0.92941500	-0.40524500	-0.91795800

N	-1.41729200	-1.14852500	-1.16847600
O	-0.97046900	0.14153100	0.66291600
H	-3.26694800	-1.39017500	-0.40866900
H	-1.59167500	-0.27533500	-1.65583200
O	-2.82667100	-0.80424000	2.64339100
H	-2.07131400	-0.44319400	2.14127100
O	-3.25963700	1.54046700	0.05902800
H	-2.42376800	1.05957400	0.28965500
H	-3.54901300	1.96247100	0.87638700
O	-1.84654000	3.57864600	-1.44949000
H	-1.04364300	3.38161700	-0.93141200
H	-2.49119100	2.95562800	-1.07183900
O	0.14686400	2.63536700	0.34098700
H	1.09631400	2.55113200	0.19883300
H	-0.17281900	1.70830500	0.44506600
O	-4.13480100	-1.22657700	0.01682400
H	-4.20101100	-0.25801700	-0.03736600
H	-3.42514800	-1.08827900	1.93159300
C	-0.13639300	-2.12330000	0.70373900
H	-1.01251800	-2.60958200	1.14273400
H	0.37234500	-2.83475300	0.05504700
H	0.53394700	-1.83682600	1.51100200
C	-1.07233600	-2.22224800	-2.10885900
H	-1.76895300	-2.17542200	-2.94725500
H	-0.05064600	-2.13314900	-2.48710700
H	-1.19340800	-3.19576300	-1.63193100
C	2.11486600	-0.21688700	-0.34971200
C	2.30587400	0.13926600	1.00774600
C	3.27686200	-0.34689500	-1.15123600
C	3.58720300	0.34068200	1.52176100
H	1.44339500	0.26041700	1.65015400
C	4.54729700	-0.13300500	-0.62772400
H	3.15017000	-0.61914800	-2.19407800
C	4.71988900	0.21030800	0.71725300
H	3.69715400	0.61072800	2.56776000
H	5.41287400	-0.24018700	-1.27444200
H	5.71099600	0.37284600	1.12487800

AM...AL-

C	1.98102900	0.72530300	1.23623300
O	-2.63665200	0.90370900	-1.10273200
N	2.01053900	1.94354700	0.69067000
O	1.94541700	-0.30859800	0.51906900
H	6.10235500	-1.74036600	-0.59992100
H	1.96499000	1.99110500	-0.33214700
O	3.35742500	-2.71205600	1.30204100
H	2.79932700	-1.93558600	1.12032800
O	3.27424300	-0.63938900	-1.89577500
H	2.74608400	-0.52203700	-1.07374500
H	2.75207000	-1.22566400	-2.45665400
O	1.71206600	1.89070600	-2.25959800
H	0.92347800	1.30838800	-2.14303100
H	2.42464000	1.26719700	-2.46467700
O	-0.24279400	0.07948300	-1.62391500
H	-1.19028800	0.35472400	-1.37553100
H	0.18416300	-0.22525100	-0.81149800
O	5.29117500	-2.22893800	-0.77658100
H	4.70811500	-1.61157700	-1.26494600
H	4.09465600	-2.62316900	0.67161000
C	1.99527100	0.61675600	2.74002000
H	2.94464600	0.98560900	3.13837900
H	1.19819900	1.21651500	3.18528200
H	1.86936600	-0.42401800	3.02905700
C	2.03123200	3.20620700	1.42545100
H	2.14694800	4.01255100	0.70331200
H	1.10177100	3.36764600	1.97746600
H	2.86979300	3.24767200	2.12315800
C	-3.57358000	0.20526100	-0.52324400
C	-3.34847500	-1.10383000	-0.00128300
C	-4.89823500	0.71319800	-0.37154300

C	-4.36258700	-1.83141800	0.61564700
H	-2.35494700	-1.53234800	-0.09507200
C	-5.90194400	-0.02499600	0.24779900
H	-5.10973200	1.70674700	-0.75652200
C	-5.65267700	-1.30716700	0.75094700
H	-4.14312400	-2.82480100	0.99768800
H	-6.89556400	0.40527500	0.33999500
H	-6.43795900	-1.87865300	1.23254400

TS₉

C	0.17674000	-0.80020800	-0.36179300
O	-1.26008600	-1.14959600	-0.70527400
N	0.32437400	-0.70023500	1.11152400
O	0.56946600	0.33735100	-0.94814000
H	1.95153500	-0.32200900	1.48974500
O	3.03678100	0.57124100	-1.72804400
H	3.13168200	0.79590100	-2.66021400
H	2.04782000	0.41182700	-1.54060300
O	4.42933000	-1.32270400	-0.19681500
H	4.11066700	-0.73721200	-0.91315300
H	5.39164600	-1.27591900	-0.21633100
O	0.72334600	2.69234200	0.08927300
H	0.54529300	1.79074500	-0.34809500
H	0.47034900	3.38000300	-0.53663700
O	3.17641000	2.08100900	0.45132700
H	3.33519400	1.70081400	-0.45727500
H	2.24236500	2.48991000	0.36887700
O	2.90121400	-0.00973400	1.68888700
H	3.06183900	1.16207600	1.08407400
H	3.50308500	-0.61592200	1.20034000
C	0.89557100	-2.04495300	-0.89307900
H	1.95352000	-2.00413900	-0.63289900
H	0.46932200	-2.96772200	-0.49879800
H	0.80004800	-2.05728500	-1.97948500
C	-0.17484300	-1.81720300	1.93456700
H	0.44268800	-2.70230000	1.77937000
H	-0.09368200	-1.53224700	2.98491700
H	-1.21685300	-2.07293900	1.71953900
H	-0.13618800	0.15676200	1.40543400
C	-2.34855500	-0.40476600	-0.38102100
C	-2.34354400	0.90528000	0.12056900
C	-3.58679100	-1.03917900	-0.59453000
C	-3.55221300	1.54580600	0.40964700
H	-1.42032900	1.44345500	0.26691100
C	-4.78067600	-0.38740100	-0.31070200
H	-3.58620300	-2.05065300	-0.98483800
C	-4.77487400	0.91394800	0.19989400
H	-3.52542900	2.55877000	0.79731400
H	-5.72067700	-0.89996300	-0.48528300
H	-5.70488200	1.42248500	0.42539200

T⁻...H₃O⁺

C	0.17135200	-0.79342700	-0.36720700
O	-1.26406000	-1.13613400	-0.72876900
N	0.30573700	-0.69246300	1.10291100
O	0.57377500	0.34335500	-0.95431000
H	1.98141500	-0.32796100	1.51978800
O	3.04148900	0.56819100	-1.71284300
H	3.14473600	0.80351700	-2.64162600
H	2.04916000	0.40781400	-1.53372300
O	4.44331000	-1.34286200	-0.19408800
H	4.11877900	-0.75321100	-0.90336600
H	5.40536300	-1.29793600	-0.22551100
O	0.75263700	2.67297800	0.09558700
H	0.56178600	1.77037300	-0.34694700
H	0.50259500	3.36891900	-0.52258200
O	3.18298700	2.08047600	0.43533300
H	3.33306100	1.67358700	-0.46895400
H	2.23049700	2.47801700	0.35422200
O	2.92191200	-0.02555100	1.72664400

H	3.09279100	1.21687000	1.07215000
H	3.51727600	-0.63122500	1.23413500
C	0.89048900	-2.03948900	-0.89413800
H	1.94757800	-1.99849100	-0.63058200
H	0.46242900	-2.96088200	-0.49868400
H	0.79811900	-2.05486100	-1.98080000
C	-0.21260500	-1.80132500	1.92363700
H	0.39323200	-2.69520800	1.77213400
H	-0.13153800	-1.51696000	2.97420700
H	-1.25750000	-2.04411900	1.70596300
H	-0.14203000	0.17211500	1.39361200
C	-2.35335800	-0.39797300	-0.39251600
C	-2.34919600	0.91700700	0.09610100
C	-3.59047100	-1.04205500	-0.58171900
C	-3.55729100	1.55300800	0.39696900
H	-1.42666500	1.46121700	0.22315100
C	-4.78417000	-0.39450300	-0.28730200
H	-3.58922900	-2.05741600	-0.96182700
C	-4.77890100	0.91164400	0.21084800
H	-3.53132300	2.56979100	0.77455500
H	-5.72348600	-0.91431300	-0.44315500
H	-5.70869900	1.41665200	0.44500700

TS₁₀

C	0.31130300	-0.74425300	-0.45451900
O	-1.43101300	-1.05680000	-1.04815300
N	0.19054600	-0.64328400	0.96002500
O	0.73364000	0.32494600	-1.03832900
H	1.93739800	-0.29711900	1.61902800
O	3.33473000	0.49298700	-1.60580500
H	3.57307700	0.71310000	-2.51383600
H	2.34534200	0.35725400	-1.57463800
O	4.40202700	-1.50412900	0.11969100
H	4.22954600	-0.91986700	-0.64239300
H	5.35968500	-1.59397000	0.17971100
O	0.90951500	2.71743100	0.02039800
H	0.69951100	1.84354500	-0.43030300
H	0.71696400	3.42676700	-0.60356700
O	3.29058200	2.04287000	0.53430300
H	3.51098300	1.61230800	-0.34332900
H	2.36097900	2.46874300	0.37333100
O	2.85941000	-0.03155000	1.87053500
H	3.13148100	1.21710800	1.18239300
H	3.45059900	-0.67920800	1.42428200
C	0.83143300	-2.07154600	-0.97032200
H	1.88061400	-2.17856800	-0.68010900
H	0.27006600	-2.92105100	-0.58807100
H	0.76742800	-2.06710800	-2.05748900
C	-0.39921400	-1.74455900	1.73616600
H	0.25394600	-2.61683600	1.70543600
H	-0.47892100	-1.42180100	2.77486300
H	-1.39023900	-2.02659100	1.37272100
H	-0.24102300	0.24552800	1.19801300
C	-2.47094600	-0.39006800	-0.56517200
C	-2.44737800	0.99206100	-0.25880200
C	-3.69555200	-1.07403500	-0.35598100
C	-3.58021600	1.63861000	0.23714400
H	-1.54349500	1.55889400	-0.43815600
C	-4.82220300	-0.41487100	0.12338900
H	-3.73502800	-2.13381700	-0.58676200
C	-4.77697300	0.94885400	0.43323900
H	-3.52643600	2.69981900	0.46089900
H	-5.74426500	-0.97089800	0.26338500
H	-5.65468300	1.45957000	0.81243600

AM...H₃O⁺...AL⁻

C	0.72974800	1.21331300	0.31829700
O	-3.10820500	0.61015300	0.26852900
N	0.30617000	2.38112100	-0.17060000
O	1.75297900	0.65542400	-0.15957800

H	7.31086700	0.07640500	-0.05110800
H	0.87101100	2.78718300	-0.90439000
O	3.08621200	-1.57755700	0.42358500
H	2.55052100	-2.37973200	0.45382200
H	2.46403400	-0.80787000	0.32015200
O	5.30514400	-1.13273000	2.17285000
H	4.45010400	-1.36858600	1.76646100
H	5.48943700	-1.81432800	2.82885600
O	3.56095700	1.06196500	-2.13080400
H	2.80693400	1.05879200	-1.49069800
H	3.18329500	1.13482300	-3.01536600
O	4.77661300	-1.07171500	-1.49798900
H	4.11908300	-1.41954600	-0.81204100
H	4.35893000	-0.19297400	-1.84557300
O	6.83099500	-0.76011000	-0.03844800
H	5.65649800	-0.88623300	-0.99045300
H	6.43455700	-0.85613700	0.86138000
C	-0.05197900	0.59061900	1.43904400
H	-0.07560700	1.26296800	2.30129500
H	-1.08861000	0.41824600	1.12320500
H	0.41332300	-0.34819400	1.73210900
C	-0.86337200	3.13557800	0.28694000
H	-0.67153100	3.61367200	1.25145000
H	-1.06763800	3.91175100	-0.44886200
H	-1.73330800	2.48094500	0.36280400
C	-4.19274200	-0.06493100	0.06816100
C	-4.20401200	-1.31139000	-0.64063700
C	-5.47381700	0.37532700	0.53883500
C	-5.37438700	-2.03373000	-0.85068000
H	-3.25686200	-1.68674400	-1.01949900
C	-6.63568400	-0.35795800	0.31966500
H	-5.51908900	1.31535000	1.08283400
C	-6.60910900	-1.57338500	-0.37595400
H	-5.32579700	-2.97366100	-1.39495300
H	-7.58103800	0.02267500	0.69843700
H	-7.51775400	-2.14075400	-0.54283400

(AM...AL) :

C	-4.24781600	-1.60284900	0.55232000
O	3.67333500	-1.00667700	0.54577500
N	-4.96548100	-1.23707200	-0.51929700
O	-3.65411700	-0.76937000	1.26773600
H	-5.05229200	-0.23909200	-0.72173600
H	-0.19072400	1.15167500	-0.86092300
O	-2.58169500	1.67704400	1.20782200
H	-2.51046900	1.92178700	2.13819700
H	-3.03262300	0.79270700	1.19120000
O	2.13455400	1.04393400	1.44000100
H	1.87105400	0.98170400	2.36460400
H	3.14144600	-0.23570400	0.85539900
O	-0.08934100	1.65413100	-0.04502000
H	1.31381700	1.24580200	0.93473500
H	-0.96813900	1.63631700	0.39084600
O	-4.04815000	3.42347400	-0.36794600
H	-3.47340800	2.88196000	0.21448500
H	-3.45335300	3.93808400	-0.92441100
O	-5.59158100	1.45254600	-1.52475800
H	-5.08901500	2.21583900	-1.16540500
H	-6.52077700	1.69584700	-1.45320900
C	-4.17459000	-3.07674200	0.87819700
H	-5.17292900	-3.49438200	1.03193100
H	-3.71150700	-3.63163300	0.05782100
H	-3.58309600	-3.21234100	1.78079300
C	-5.69204000	-2.14144000	-1.40618900
H	-6.49398200	-2.66880400	-0.88302600
H	-6.13665200	-1.54257100	-2.19939300
H	-5.02726800	-2.87721500	-1.86440800
C	4.89174400	-0.61973000	0.08130500
C	5.29564100	0.72158600	0.04865800
C	5.76285300	-1.61542800	-0.37787200

C	6.55917700	1.05371000	-0.43974000
H	4.62084500	1.49155800	0.40527000
C	7.02171200	-1.27018400	-0.86304800
H	5.44120800	-2.65037900	-0.34781000
C	7.43045500	0.06504300	-0.89810800
H	6.86110200	2.09534000	-0.46037100
H	7.68727100	-2.05079500	-1.21537900
H	8.41100500	0.32935200	-1.27614000

T₃[±]

C	0.10315000	0.48318000	-0.48308500
O	1.32753800	0.90674100	0.22079500
N	-0.85717300	1.64686000	0.04496400
O	-0.38522400	-0.64897200	-0.07755100
H	-1.77249500	1.50281700	-0.42359500
O	-1.37235000	-0.09158700	2.42083900
H	-0.99384500	-0.50994200	1.61531900
H	-2.31649300	-0.33959900	2.41184900
O	-4.12820600	-0.79216000	2.19465000
H	-4.26875600	-1.00299000	1.24848500
H	-4.45957500	-1.55325700	2.68340100
O	-1.98319400	-2.32125200	-1.34209900
H	-1.32273900	-1.70413900	-0.91354700
H	-1.74342600	-3.21167900	-1.06414800
O	-4.28444400	-1.20186800	-0.56731400
H	-5.05965500	-1.58563100	-0.99284300
H	-3.49652500	-1.72543200	-0.87355600
O	-3.42861400	1.37055300	-1.20996400
H	-3.84108900	0.50341000	-1.01063400
H	-4.08232300	2.03598000	-0.96829900
C	0.27834800	0.66395900	-1.99175900
H	-0.68812800	0.54716800	-2.48569900
H	0.70070400	1.63612300	-2.24863500
H	0.94721100	-0.11202700	-2.36358100
C	-0.44985200	3.07083900	-0.08671800
H	-0.36908900	3.33062200	-1.13988400
H	-1.21323200	3.69407900	0.37892100
H	0.50520500	3.21715000	0.40909700
H	-1.01115500	1.40231500	1.03388000
C	2.48277800	0.17409500	0.15937100
C	2.58432400	-1.14288400	-0.30622800
C	3.62926900	0.82968200	0.63074800
C	3.82856800	-1.77737400	-0.30652200
H	1.70332600	-1.66778100	-0.64418000
C	4.85976300	0.18102100	0.63178800
H	3.53687200	1.84797000	0.99049800
C	4.97038900	-1.12892000	0.15947400
H	3.89564200	-2.79671900	-0.67137900
H	5.73595000	0.70394300	0.99929700
H	5.92937300	-1.63361300	0.15720500

TS₁₁

C	0.11866200	0.41453800	-0.31787800
O	1.30952400	0.85381900	0.35546700
N	-0.85268900	1.53501500	0.00172500
O	-0.40390300	-0.72944100	0.24248900
H	-1.67697700	1.40545500	-0.60787500
O	-1.45102200	0.39881100	2.14119800
H	-0.87241500	-0.42166900	1.18090500
H	-2.39958300	0.20321400	2.20679900
O	-4.36710400	-0.27774300	2.02276700
H	-4.44244700	-0.65032200	1.12208900
H	-4.72917700	-0.95018100	2.60961800
O	-2.04230100	-2.59043900	-0.93235600
H	-1.38558500	-1.96816000	-0.54416000
H	-1.91631000	-3.43019400	-0.47698400
O	-4.33363900	-1.17972900	-0.64860100
H	-5.09888400	-1.59318200	-1.06435200
H	-3.57251800	-1.80042200	-0.76899800
O	-3.24877100	1.20307400	-1.63538700

H	-3.73884300	0.40876400	-1.33764800
H	-3.88645200	1.92525400	-1.62427100
C	0.33245100	0.25643500	-1.81569000
H	-0.62314400	0.05054000	-2.29930900
H	0.76480400	1.16059000	-2.24620400
H	1.00600600	-0.57858900	-2.00731000
C	-0.37814700	2.93337600	-0.11591200
H	0.01888900	3.13299600	-1.11184500
H	-1.23094400	3.58801900	0.06374900
H	0.38978600	3.12396800	0.62815600
H	-1.22133900	1.22850600	1.08102200
C	2.50375100	0.17045600	0.22485500
C	2.61036200	-1.22305200	0.24936100
C	3.65225400	0.96146900	0.13864200
C	3.87324600	-1.81188500	0.16898800
H	1.72124500	-1.83091400	0.33523200
C	4.90736000	0.36072000	0.07380800
H	3.54740700	2.03987600	0.12417400
C	5.02453100	-1.02992000	0.08377300
H	3.95223300	-2.89332600	0.18393800
H	5.79329400	0.98237600	0.00867200
H	6.00067700	-1.49734800	0.02821500

T₁^o

C	0.18562600	0.53557700	-0.31592500
O	1.33051700	0.78810700	0.51891300
N	-0.75824600	1.57696000	0.07514400
O	-0.39665200	-0.71262600	0.00270800
H	-1.62064900	1.43460500	-0.45526200
O	-1.60872700	0.07466100	2.38063700
H	-0.78551800	-0.63916700	0.90553200
H	-2.56557000	-0.11968500	2.30681600
O	-4.32452700	-0.56679600	2.01855400
H	-4.43620900	-0.84584500	1.08625600
H	-4.69239100	-1.27918400	2.55265700
O	-2.10164400	-2.36745100	-1.44236000
H	-1.42242700	-1.82507300	-0.98918900
H	-1.90947600	-3.28318500	-1.21199400
O	-4.41301300	-1.15131200	-0.71065200
H	-5.19322400	-1.52608100	-1.13513800
H	-3.64186900	-1.70022200	-0.99519100
O	-3.48140400	1.43008500	-1.38070800
H	-3.91449900	0.57819700	-1.17713900
H	-4.10113300	2.10801300	-1.09052900
C	0.55520400	0.50420600	-1.79652300
H	-0.35419100	0.39643900	-2.38970900
H	1.05720000	1.42808900	-2.08474500
H	1.21586700	-0.33478500	-2.01647100
C	-0.31761900	2.96974000	-0.08928900
H	-0.04080500	3.22608900	-1.11990200
H	-1.14010700	3.62080300	0.21172300
H	0.53369900	3.17044600	0.55958700
H	-1.45252300	0.87173400	1.83254200
C	2.52784600	0.12893700	0.30722800
C	2.63628000	-1.26469700	0.31754500
C	3.66981400	0.92030800	0.16844900
C	3.89152500	-1.85511100	0.16956900
H	1.74935100	-1.87097900	0.43846500
C	4.92065300	0.31971700	0.03491800
H	3.56530600	1.99889700	0.16860600
C	5.03671200	-1.07064700	0.02981700
H	3.97225500	-2.93651600	0.17395100
H	5.80318900	0.94076800	-0.07021500
H	6.00879300	-1.53760500	-0.07814200

T₂^o

C	0.46447900	1.22597300	-0.37479000
O	1.44445800	0.48296500	-1.20866400
N	1.05947700	2.15505600	0.53194900
O	-0.21805800	0.30619400	0.43873100

H	-5.96760000	0.57822200	0.42609000
H	1.60629200	1.65569900	1.22506500
O	-1.97015600	-1.52588200	-0.68090700
H	-1.68307800	-2.38874200	-1.00077900
H	-0.73898000	-0.32651100	-0.10238100
O	-4.08189800	-0.53377900	-2.08409600
H	-2.68120700	-1.22083000	-1.29623100
H	-4.51862300	-1.05538300	-2.76627800
O	-1.83551400	0.86129300	2.64697800
H	-1.16750400	0.78676600	1.93503700
H	-1.34998400	0.76674700	3.47371500
O	-3.54573300	-1.15515600	1.71153300
H	-2.96985600	-1.45386200	0.98401300
H	-3.02122700	-0.45797900	2.15673100
O	-5.63611900	-0.28766000	0.16461300
H	-4.94956100	-0.53250800	0.82959000
H	-4.74403500	-0.40808600	-1.36592600
C	-0.44138300	1.88784800	-1.40345200
H	-1.19670400	2.48579200	-0.89216100
H	0.13007000	2.52746700	-2.07569900
H	-0.93432800	1.11984300	-2.00038900
C	1.79765300	3.28776100	-0.02894400
H	1.10855300	4.01061600	-0.46925000
H	2.32403300	3.78672200	0.78536900
H	2.53248700	3.00400100	-0.79326200
C	2.35126400	-0.35046200	-0.58218800
C	2.09269300	-1.72271600	-0.52522200
C	3.55683600	0.14953100	-0.08196500
C	3.02928600	-2.58685000	0.03863200
H	1.16491900	-2.10253400	-0.93517500
C	4.48882800	-0.72092300	0.48586100
H	3.77387100	1.20751300	-0.15732200
C	4.22850000	-2.08901200	0.55148300
H	2.82244400	-3.65065300	0.07475900
H	5.42300500	-0.32579500	0.86920600
H	4.95590700	-2.76259000	0.98964100

TS₁₂

C	0.36099900	1.61410500	0.19083800
O	1.63271200	0.81780700	-1.31380700
N	1.18477800	1.97137800	1.16985800
O	-0.33790800	0.51645200	0.45497000
H	-5.94906300	-0.34446600	1.19120500
H	1.45735400	1.23225300	1.80439800
O	-2.04203300	-0.43174900	-1.33218200
H	-1.72579200	-0.74423400	-2.18801000
H	-0.91674300	0.23491400	-0.30792900
O	-4.39045400	0.88128500	-1.47872300
H	-2.87115000	0.08698300	-1.50018700
H	-4.88630800	0.92369300	-2.30372700
O	-1.51446500	-0.98081600	2.66856900
H	-0.96193000	-0.43091900	2.08958100
H	-0.90018300	-1.54037000	3.15723700
O	-3.24261800	-2.08911000	0.73443100
H	-2.77392600	-1.73267900	-0.04068300
H	-2.69503300	-1.80075700	1.49199200
O	-5.60187500	-0.72657900	0.37786800
H	-4.80942200	-1.25320200	0.63635600
H	-4.94800700	0.37431700	-0.84375200
C	-0.18056900	2.62633000	-0.76661400
H	-0.92330600	3.23868600	-0.24420500
H	0.60916200	3.26868800	-1.14744000
H	-0.66081800	2.12448600	-1.60310500
C	2.01081300	3.17424800	1.15155300
H	1.38826600	4.06746800	1.09318300
H	2.57536600	3.20878400	2.08105800
H	2.70826300	3.16252300	0.31038300
C	2.33703700	-0.20235200	-0.88394100
C	1.94960000	-1.54477400	-1.15253700
C	3.52411000	-0.02903100	-0.11991400

C	2.70263500	-2.62530100	-0.70363100
H	1.04896000	-1.70956500	-1.73587000
C	4.26850800	-1.11867300	0.32867600
H	3.85975200	0.98126200	0.08953600
C	3.86866500	-2.42693000	0.04429200
H	2.37795500	-3.63521700	-0.93694000
H	5.17368300	-0.94470400	0.90328000
H	4.45181300	-3.27164700	0.39329000

AM⁺...AL⁻

C	0.27593200	1.78058600	0.30720100
O	1.77228900	0.82726500	-1.46309500
N	1.16662200	2.06619000	1.22581700
O	-0.39079600	0.66874900	0.48913300
H	-5.85789000	-0.67553600	1.31174900
H	1.38186300	1.32986500	1.88649700
O	-2.06904000	-0.14533800	-1.31116900
H	-1.75250600	-0.31933600	-2.20569700
H	-1.01079100	0.43762600	-0.27338500
O	-4.49397300	0.98489900	-1.22585600
H	-2.94293400	0.32360600	-1.38928800
H	-5.02201300	1.09886000	-2.02368100
O	-1.30345500	-1.32569400	2.50933300
H	-0.81768500	-0.64280800	2.02220000
H	-0.63084700	-1.93057400	2.84299300
O	-3.09297500	-2.19215600	0.50753100
H	-2.67877900	-1.69773800	-0.22041900
H	-2.51873500	-1.99950200	1.27549000
O	-5.52950100	-0.92284100	0.44049500
H	-4.70267700	-1.43754100	0.59284800
H	-4.99428700	0.36573400	-0.64446300
C	-0.14905300	2.77384200	-0.71691800
H	-0.87188900	3.45740100	-0.25734500
H	0.69910900	3.34643700	-1.08212000
H	-0.62508800	2.26817000	-1.55258700
C	2.00461400	3.26422600	1.25066500
H	1.39008700	4.16326400	1.21621000
H	2.56439800	3.26036400	2.18290100
H	2.70349600	3.26187800	0.41228300
C	2.37089300	-0.21919600	-0.98770900
C	1.93526700	-1.55060000	-1.28191400
C	3.50423000	-0.12398800	-0.11874100
C	2.57725400	-2.66910100	-0.76132700
H	1.07832300	-1.67015700	-1.93926400
C	4.13555900	-1.25286500	0.39698700
H	3.87891900	0.86624600	0.12335200
C	3.68458700	-2.54046000	0.08668100
H	2.21029500	-3.65939000	-1.01830000
H	4.99590500	-1.12794800	1.04938000
H	4.18129700	-3.41598000	0.48938700

T₄[±]

C	0.23801000	-0.79096800	-0.23151700
O	-0.86033500	-0.05903700	0.55626300
N	1.32040300	-0.84542000	0.92132600
O	0.70183200	-0.13309500	-1.22900300
H	2.16832200	-1.25753700	0.48601600
H	1.57245700	0.13948600	1.13452300
O	2.40812500	1.83308000	-1.30090400
H	2.14404800	2.49823100	-1.94581300
H	1.69634000	1.11856800	-1.29638200
O	-0.52467100	2.35832900	2.04754400
H	-1.06046400	3.06373800	1.66832400
H	-0.72726600	1.56008300	1.52285500
O	2.16911400	1.88696300	1.49549800
H	1.30832200	2.28447200	1.72954500
H	2.32244200	2.12543300	0.56156600
O	4.70961700	0.34495500	-1.54281900
H	3.95113000	0.97068900	-1.50846100
H	5.47104100	0.82974800	-1.20618900

O	3.81659100	-1.82767700	-0.10443600
H	4.20768400	-1.10080500	-0.64035200
H	3.88082300	-2.62176500	-0.64608300
C	-0.24597200	-2.21219000	-0.52217300
H	0.60190800	-2.81094400	-0.86178100
H	-0.70930400	-2.69656000	0.33789100
H	-0.97359100	-2.16660500	-1.33253000
C	1.01509100	-1.55881100	2.19047900
H	0.92251900	-2.62562700	2.00048400
H	1.83475900	-1.38880900	2.88827400
H	0.08862200	-1.17045500	2.60500300
C	-2.12966700	-0.03167700	0.01383000
C	-2.38618900	0.51899300	-1.24645800
C	-3.18437700	-0.51456800	0.79320300
C	-3.69621700	0.56537500	-1.72289800
H	-1.56254000	0.89702200	-1.83680300
C	-4.49198500	-0.44924100	0.31387300
H	-2.96883100	-0.93421000	1.76902900
C	-4.75325100	0.08573300	-0.94803800
H	-3.89104500	0.98895100	-2.70212300
H	-5.30543100	-0.82191100	0.92649300
H	-5.76960600	0.13273900	-1.32171700

TS₁₃

C	-0.44473700	0.93835500	-0.56877900
O	1.04153600	0.37629800	0.79257800
N	-1.44553400	1.11439300	0.55858300
O	-0.64624200	-0.02932500	-1.28840200
H	-2.36755300	1.29093100	0.08942000
H	-1.56101600	0.18538800	1.02772400
O	-2.22222100	-2.25353800	-0.86876700
H	-1.91678400	-3.04673400	-1.32354200
H	-1.59371700	-1.53351000	-1.09802200
O	0.56153800	-1.33027900	2.80135600
H	1.19096100	-2.05727800	2.75084300
H	0.79703200	-0.70826000	2.05803300
O	-1.98793100	-1.35509600	1.82651400
H	-1.12315900	-1.56902300	2.23946800
H	-2.08127600	-1.94236000	1.05660200
O	-4.69247400	-1.07175800	-1.35826400
H	-3.88646100	-1.60890200	-1.20575700
H	-5.40178900	-1.51114300	-0.87633400
O	-3.98144800	1.46255600	-0.58557400
H	-4.31174300	0.58646700	-0.89235400
H	-4.11604200	2.07332700	-1.31870600
C	0.20910700	2.19866000	-1.05626400
H	-0.53793900	2.77026800	-1.61907000
H	0.60154700	2.81805700	-0.25479100
H	1.01587400	1.92817200	-1.73547300
C	-1.21057700	2.16757600	1.58716800
H	-1.28828000	3.15150500	1.13043500
H	-1.98078900	2.06290900	2.34993800
H	-0.22523400	2.01998700	2.01812700
C	2.19362900	0.07341300	0.19651900
C	2.39957900	-1.18453800	-0.41601000
C	3.26439000	0.99658400	0.16272700
C	3.61401700	-1.49853300	-1.02386500
H	1.59094800	-1.90700300	-0.39942600
C	4.47519200	0.67331300	-0.44452500
H	3.12563200	1.96578300	0.63045800
C	4.66186200	-0.57529900	-1.04471100
H	3.74425300	-2.47369100	-1.48294300
H	5.28115300	1.40060600	-0.44860700
H	5.60627800	-0.82431100	-1.51517600

(AM⁺N...AL⁻)₁

C	0.71357200	-0.93662400	-0.65859800
O	-1.28940400	0.30987100	0.72738600
N	1.43176600	-0.97431400	0.65272500
O	1.03990500	-0.06600600	-1.42451400

H	2.39542200	-1.36218200	0.44508000
H	1.60642200	0.02635200	0.94916800
O	3.08445400	1.92205300	-1.22342300
H	3.06270400	2.66922600	-1.83273100
H	2.34799000	1.33543800	-1.47471900
O	-0.45634500	2.57651900	1.64013100
H	-0.72478200	3.30821700	1.07493500
H	-0.84973300	1.73390700	1.22944500
O	2.05791800	1.60646300	1.43807600
H	1.20114200	2.09187400	1.52842500
H	2.49560000	1.98004700	0.65440500
O	5.29939700	0.24682700	-0.93274500
H	4.60932100	0.92914700	-1.06496500
H	5.99743900	0.66891900	-0.41971600
O	3.99251200	-1.86897000	0.19080600
H	4.53408700	-1.15383900	-0.21997000
H	4.14693100	-2.66455900	-0.33081700
C	-0.18647100	-2.08104600	-0.97483400
H	0.39956600	-3.00672100	-0.98488000
H	-0.97510400	-2.18400600	-0.23060900
H	-0.62266600	-1.92143000	-1.95834300
C	0.82510100	-1.73944800	1.78379000
H	0.78995100	-2.79796900	1.53684700
H	1.46328100	-1.59273800	2.65342200
H	-0.16949700	-1.33950000	1.96232000
C	-2.50371300	0.17928600	0.24872800
C	-3.04504900	1.08826400	-0.70335900
C	-3.35308100	-0.88960600	0.64988300
C	-4.33471500	0.93739000	-1.20548600
H	-2.42341500	1.91386700	-1.03759400
C	-4.63977500	-1.03273900	0.13678600
H	-2.97688400	-1.59631500	1.38375500
C	-5.14913900	-0.12347600	-0.79545300
H	-4.70983500	1.65570100	-1.92900600
H	-5.25578900	-1.86232500	0.47209300
H	-6.15239200	-0.23696400	-1.19010300

(AM⁺N...AL⁻)₂

C	-1.44732400	-0.96990300	1.07396400
O	1.80798100	0.26244200	-0.06389200
N	-1.70235500	-0.91836400	-0.39724400
O	-2.25365800	-0.40707600	1.76944600
H	-2.67314700	-1.30531900	-0.56115100
H	-1.78536400	0.12529900	-0.64098200
O	-3.98168500	1.78519100	1.01340300
H	-4.23723000	2.44406600	1.66995200
H	-3.51378900	1.08177100	1.49568300
O	0.59990000	2.50766900	-0.40693800
H	0.76777100	3.08787100	0.34271500
H	1.13774500	1.65280900	-0.24142200
O	-1.89888800	1.70964900	-0.95890300
H	-1.02106800	2.10879100	-0.71969700
H	-2.56132600	2.05821900	-0.33818700
O	-5.85191600	0.33697700	-0.48607600
H	-5.28922300	0.95562600	0.02252200
H	-6.18079400	0.83491100	-1.24279000
O	-4.23677100	-1.81165300	-0.97786600
H	-4.88575300	-1.08447800	-0.82660200
H	-4.59659400	-2.59431300	-0.54556800
C	-0.21276200	-1.65263900	1.52907400
H	-0.16547300	-2.67500900	1.14630000
H	0.64844900	-1.10167500	1.11456200
H	-0.18531200	-1.65475800	2.61623400
C	-0.72634800	-1.56140000	-1.32904400
H	-0.70773000	-2.63598200	-1.16065800
H	-1.07053600	-1.36141600	-2.34222300
H	0.25718800	-1.12013300	-1.17037800
C	3.11064200	0.12139800	-0.06540200
C	4.00234100	1.23167100	-0.03973900
C	3.71628300	-1.16737700	-0.08949700

C	5.38395600	1.05851900	-0.03833800
H	3.58152500	2.23244800	-0.02060100
C	5.09897300	-1.32609900	-0.08629100
H	3.06683400	-2.03739900	-0.11144400
C	5.95365800	-0.21864300	-0.06091600
H	6.02683600	1.93417800	-0.01813600
H	5.51721100	-2.32867000	-0.10479300
H	7.03005600	-0.34703200	-0.05889400
TS₁₄			
C	-1.56428400	-1.09808600	1.06431200
O	1.85776700	0.20553200	-0.07039600
N	-1.75783100	-0.95988100	-0.36289100
O	-2.43066500	-0.65197600	1.79104400
H	-2.74898200	-1.19699500	-0.58990200
H	-1.73489200	0.28043900	-0.58778000
O	-3.81649400	1.73405600	1.07672700
H	-3.95357800	2.40897600	1.75241300
H	-3.49804600	0.93601800	1.53871900
O	0.59343900	2.34909500	-0.33842100
H	0.72075800	2.91703800	0.42885500
H	1.18789400	1.49253900	-0.19891600
O	-1.76444600	1.51358100	-0.79534000
H	-0.84243800	1.91830800	-0.57691600
H	-2.43717500	1.87745100	-0.18223000
O	-5.87103800	0.69522200	-0.53802200
H	-5.24650000	1.19855100	0.02046300
H	-6.13506400	1.29209200	-1.24698000
O	-4.40008100	-1.54212300	-1.18303600
H	-4.99976800	-0.78607800	-0.99270200
H	-4.84744900	-2.32899600	-0.85270000
C	-0.28740800	-1.70102200	1.54158900
H	-0.18296800	-2.72368300	1.16890100
H	0.55696100	-1.12086300	1.14143100
H	-0.27592300	-1.70019500	2.62916300
C	-0.82609200	-1.64367100	-1.30052500
H	-0.86657300	-2.72490400	-1.16957500
H	-1.14382200	-1.39590300	-2.31236600
H	0.18570700	-1.27402200	-1.13757300
C	3.16784300	0.11800900	-0.08058300
C	4.01346100	1.26215000	-0.07237900
C	3.81902400	-1.14636900	-0.09804700
C	5.40086400	1.14210300	-0.08088800
H	3.55540600	2.24643800	-0.05969000
C	5.20673400	-1.25207900	-0.10513500
H	3.20238300	-2.04004700	-0.10711300
C	6.01816300	-0.11242800	-0.09675500
H	6.00962300	2.04185600	-0.07420200
H	5.66294600	-2.23789400	-0.11840700
H	7.09862800	-0.19969200	-0.10263600

Table S3. Cartesian coordinates of stationary points for the reaction of methyammine with *p*-nitrophenyl acetate in water. Optimized geometries at the B3LYP/6-311+G(d,p) level.

RC			
C	0.87327200	-2.79783500	-0.52613600
O	2.09224800	-2.41739100	-0.97162100
N	-5.66790900	3.03017600	-1.31417100
O	0.16286100	-2.06913200	0.13988100
H	-5.38305800	2.21830000	-0.76606700
H	-4.84680600	3.62018500	-1.40929300
O	-2.41614700	-2.65256400	1.20702100
H	-2.40684500	-3.45126300	1.74761700
H	-1.51459300	-2.56006800	0.84277000
O	-4.48304800	-2.15423900	-0.65496100
H	-3.78989300	-2.45085900	-0.03321700
H	-5.15977000	-2.83955200	-0.63838600
O	-0.27942600	0.65020700	1.16395200

H	0.03997500	-0.19244600	0.80124600
H	0.42119900	0.96168900	1.74783400
O	-2.83960300	0.02829800	2.19299700
H	-2.77366400	-0.93029300	2.03707300
H	-1.96987500	0.36326400	1.89981300
O	-4.95116100	0.49130700	0.35133300
H	-4.23508000	0.46102800	1.01602500
H	-4.90823900	-0.38737600	-0.06800600
C	0.55209400	-4.19671400	-0.94498300
H	-0.49755500	-4.41189700	-0.76039300
H	0.79108000	-4.33883700	-1.99934000
H	1.17199200	-4.88742700	-0.36688700
C	-6.73295300	3.76436400	-0.61722800
H	-7.61092300	3.12096900	-0.51681900
H	-6.46083000	4.11856900	0.38769000
H	-7.03174400	4.63417100	-1.20831200
C	2.59203200	-1.15318500	-0.64433200
C	3.27886200	-0.98591100	0.55388600
C	2.46488900	-0.12889400	-1.57613000
C	3.84773000	0.24942900	0.83555000
H	3.37157000	-1.81002600	1.24913000
C	3.03432900	1.10738800	-1.29910600
H	1.93275000	-0.30072700	-2.50261800
C	3.71452500	1.27679100	-0.09572200
H	4.38877500	0.41512600	1.75601400
H	2.95491200	1.92554900	-2.00034100
N	4.31976600	2.58501800	0.19926000
O	4.21658500	3.47278300	-0.64175800
O	4.89830800	2.72610300	1.27241200

TS (RC-T₁[±])

C	-1.10968000	0.93002100	-0.83525900
O	0.11789000	1.63237800	-0.86676500
N	-1.67581800	1.49701900	1.01896300
O	-1.10172900	-0.31368100	-0.75984800
H	-2.54554200	0.98517700	1.21677700
H	-0.94645500	1.07222600	1.58712500
O	-3.22683300	-1.93841800	-1.35482300
H	-3.07150700	-2.46930000	-2.14401200
H	-2.44436000	-1.34705400	-1.25208900
O	-5.43895700	-0.30759200	-0.86375700
H	-4.76515000	-0.94618900	-1.17447500
H	-6.28913600	-0.74892300	-0.96594900
O	-0.39599600	-1.93807000	1.38611200
H	-0.46640200	-1.38143900	0.58407300
H	0.33695000	-2.54264500	1.22720200
O	-3.11810500	-2.65609600	1.43913400
H	-3.24668700	-2.65394200	0.47417600
H	-2.15358100	-2.53022200	1.53956000
O	-4.19414500	-0.02182000	1.68089200
H	-3.85291600	-0.93711900	1.73691000
H	-4.74499300	-0.03059900	0.87515900
C	-2.12569800	1.68883800	-1.64933800
H	-3.13074300	1.35097900	-1.39999300
H	-2.04416000	2.76356500	-1.49698500
H	-1.93347200	1.47251900	-2.70453700
C	-1.81440200	2.92592900	1.34072700
H	-2.67511300	3.33361300	0.81028600
H	-1.95798700	3.09072700	2.41261300
H	-0.91935200	3.46077700	1.01986500
C	1.30592500	0.99556600	-0.59587000
C	1.74258000	-0.10172400	-1.34661500
C	2.11757700	1.55105000	0.39665600
C	2.98763400	-0.65468600	-1.08787700
H	1.11508400	-0.50999400	-2.12549600
C	3.36682900	1.00569200	0.65500200
H	1.76609800	2.40939800	0.95436300
C	3.78453400	-0.09679700	-0.08800800
H	3.34615000	-1.50084000	-1.65660500
H	4.00781000	1.42174800	1.41907700

N	5.09985700	-0.67992600	0.18189100
O	5.80330600	-0.15792200	1.04482600
O	5.44399600	-1.66696000	-0.46571000

T₁[‡]

C	1.02980800	0.68422500	0.31228900
O	-0.23408500	1.36232100	-0.13797200
N	2.03759400	1.70208400	-0.36608500
O	1.21252300	-0.48504900	-0.20503900
H	2.99669300	1.29059900	-0.25984600
H	1.81358600	1.64381500	-1.36127800
O	2.89999200	-2.33926100	0.71749300
H	2.44194300	-3.13833100	1.00026500
H	2.20061200	-1.68191000	0.45229200
O	4.67083900	-0.81106500	2.20481200
H	4.07989100	-1.49020100	1.81576700
H	5.44897500	-1.28285700	2.52104500
O	1.86394600	-0.89933900	-2.78750800
H	1.48466900	-0.76672200	-1.88298400
H	1.24359100	-1.46020600	-3.26502300
O	4.32430300	-1.69724900	-1.70127400
H	3.95321900	-2.15957200	-0.92828900
H	3.53483300	-1.49051500	-2.24202700
O	4.64947900	0.66666200	-0.18684400
H	4.64452000	-0.09883800	-0.80112600
H	4.79451600	0.26029200	0.69164900
C	1.13930700	0.80946300	1.82972000
H	2.14943400	0.54254200	2.14641900
H	0.90060900	1.81186700	2.18439900
H	0.44366600	0.10566300	2.28665400
C	2.04727300	3.13019200	0.05852400
H	2.41412400	3.19754900	1.07958500
H	2.71639900	3.68045300	-0.60165600
H	1.04042000	3.53312600	-0.01088300
C	-1.44190100	0.77495200	-0.04699100
C	-1.68481600	-0.52695200	0.42958400
C	-2.52397900	1.57097100	-0.47439800
C	-2.98359000	-1.00767800	0.48316700
H	-0.86510100	-1.15939600	0.73146200
C	-3.81657100	1.08981500	-0.42241800
H	-2.32127100	2.56905000	-0.84165000
C	-4.04259400	-0.20359900	0.06018100
H	-3.17960600	-2.00643000	0.84758800
H	-4.64757400	1.69994500	-0.74714700
N	-5.39840800	-0.71696300	0.11972300
O	-6.31987700	0.00853700	-0.26278200
O	-5.57962900	-1.85856800	0.55053400

T₂[‡]

C	-1.03136000	0.68995700	-0.30915400
O	0.23337600	1.36597000	0.14282300
N	-2.03808400	1.70392800	0.37652300
O	-1.21308100	-0.48212800	0.20174800
H	-2.99716000	1.29149900	0.27226800
H	-1.81009700	1.64251200	1.37055100
O	-2.89546400	-2.33386000	-0.73777700
H	-2.43709100	-3.12905600	-1.03081500
H	-2.19658300	-1.67863500	-0.46677200
O	-4.68061200	-0.79681200	-2.19887200
H	-4.08507300	-1.47713900	-1.81906400
H	-5.46047500	-1.26825800	-2.51133900
O	-1.84889400	-0.93755900	2.78152500
H	-1.47599300	-0.78490700	1.87749000
H	-1.22564500	-1.50974000	3.24151200
O	-4.31399200	-1.71354600	1.69025700
H	-3.94665600	-2.16861400	0.91127600
H	-3.52246400	-1.51751600	2.23201300
O	-4.64827200	0.66546700	0.20260700
H	-4.63561400	-0.10533600	0.81022100
H	-4.79611100	0.26622100	-0.67863200

C	-1.14297800	0.82379200	-1.82571500
H	-2.15378700	0.55938700	-2.14240400
H	-0.90412900	1.82796200	-2.17522500
H	-0.44849800	0.12205500	-2.28754500
C	-2.05111300	3.13358000	-0.04264400
H	-2.42066600	3.20424000	-1.06250200
H	-2.71943900	3.68030400	0.62128500
H	-1.04473600	3.53793000	0.02572400
C	1.44061400	0.77799300	0.04929100
C	1.68278200	-0.52121600	-0.43512200
C	2.52327400	1.57037400	0.48213000
C	2.98109700	-1.00281600	-0.49076300
H	0.86280800	-1.15114000	-0.74144300
C	3.81543900	1.08836800	0.42798200
H	2.32125500	2.56641600	0.85525700
C	4.04061400	-0.20234000	-0.06224300
H	3.17640000	-1.99950100	-0.86116300
H	4.64683800	1.69575100	0.75684100
N	5.39591800	-0.71662800	-0.12410100
O	6.31783800	0.00540100	0.26391000
O	5.57633600	-1.85564300	-0.56210400

TS₁₅

C	-1.13012100	0.73226600	-0.27709900
O	0.25841700	1.41932900	0.14829100
N	-2.09404100	1.66457500	0.31096800
O	-1.21816800	-0.46597900	0.25896500
H	-3.69516800	0.97499700	0.23775000
H	-1.94394500	1.63553000	1.31720000
O	-2.81427800	-2.32120300	-0.65282200
H	-2.38373800	-3.15540600	-0.87103900
H	-2.09604100	-1.65216700	-0.41800100
O	-4.67147700	-0.81690200	-2.12814500
H	-4.05734800	-1.50914900	-1.81175800
H	-5.44716500	-1.27732600	-2.46721800
O	-1.98217600	-0.87446400	2.70970500
H	-1.53418600	-0.68816200	1.82340700
H	-1.43185000	-1.50069600	3.19290900
O	-4.14636000	-1.55972200	1.51957700
H	-3.75346400	-2.10453500	0.78232300
H	-3.35337700	-1.35968000	2.13337300
O	-4.59130000	0.50658200	0.27826300
H	-4.39953400	-0.60370200	1.00919200
H	-4.77081900	0.18287700	-0.63479800
C	-1.13968000	0.78128400	-1.80395500
H	-2.13168100	0.49808000	-2.16299000
H	-0.89504800	1.77122200	-2.18842500
H	-0.41674500	0.06654800	-2.19539600
C	-2.09404300	3.06886200	-0.14014100
H	-2.47222400	3.13422700	-1.16070100
H	-2.77232100	3.63149100	0.50322500
H	-1.10289800	3.52816200	-0.09534000
C	1.44238500	0.82766900	0.06285800
C	1.67445600	-0.49508600	-0.38544700
C	2.55545300	1.61198100	0.45949400
C	2.96292700	-0.99410700	-0.44391900
H	0.84034000	-1.12163500	-0.65817400
C	3.83812000	1.11198500	0.40184000
H	2.37400000	2.62168600	0.80675600
C	4.04459200	-0.19735600	-0.05459300
H	3.14032600	-2.00419600	-0.78690800
H	4.68204700	1.71768400	0.70151600
N	5.38355500	-0.72739500	-0.12089800
O	6.32570000	-0.00861700	0.23431400
O	5.54835600	-1.88291100	-0.53084800

T⁻...H₃O⁺

C	-1.13012100	0.73226600	-0.27709900
O	0.25841700	1.41933000	0.14829000
N	-2.09404100	1.66457500	0.31096800

O	-1.21816800	-0.46597900	0.25896400
H	-3.69516800	0.97499600	0.23774900
H	-1.94394500	1.63553100	1.31720000
O	-2.81427700	-2.32120300	-0.65282200
H	-2.38373800	-3.15540600	-0.87103800
H	-2.09604100	-1.65216700	-0.41800100
O	-4.67147700	-0.81690200	-2.12814500
H	-4.05734700	-1.50914900	-1.81175800
H	-5.44716500	-1.27732600	-2.46721800
O	-1.98217600	-0.87446400	2.70970500
H	-1.53418600	-0.68816100	1.82340700
H	-1.43185000	-1.50069500	3.19290900
O	-4.14636000	-1.55972200	1.51957700
H	-3.75346400	-2.10453500	0.78232200
H	-3.35337700	-1.35968000	2.13337200
O	-4.59130000	0.50658200	0.27826300
H	-4.39953300	-0.60370200	1.00919200
H	-4.77081900	0.18287700	-0.63479800
C	-1.13968000	0.78128400	-1.80395500
H	-2.13168100	0.49808000	-2.16299000
H	-0.89504800	1.77122200	-2.18842500
H	-0.41674600	0.06654700	-2.19539600
C	-2.09404400	3.06886300	-0.14014100
H	-2.47222500	3.13422700	-1.16070200
H	-2.77232100	3.63149200	0.50322500
H	-1.10289800	3.52816200	-0.09534100
C	1.44238500	0.82766900	0.06285700
C	1.67445700	-0.49508600	-0.38544700
C	2.55545300	1.61198100	0.45949400
C	2.96292700	-0.99410700	-0.44392000
H	0.84034100	-1.12163500	-0.65817400
C	3.83811900	1.11198500	0.40183900
H	2.37400000	2.62168700	0.80675600
C	4.04459100	-0.19735700	-0.05459300
H	3.14032500	-2.00419700	-0.78690700
H	4.68204700	1.71768400	0.70151500
N	5.38355500	-0.72739500	-0.12089800
O	6.32570000	-0.00861700	0.23431300
O	5.54835600	-1.88291100	-0.53084800

TS₁₆

C	-1.16693400	0.73991700	-0.28203800
O	0.29088200	1.45052500	0.13701300
N	-2.09247300	1.67200300	0.33374500
O	-1.22485100	-0.45394700	0.24297200
H	-3.74892100	0.97414400	0.26866000
H	-1.94144400	1.62293600	1.33844400
O	-2.82341400	-2.32853400	-0.67065300
H	-2.40204700	-3.16562800	-0.89648300
H	-2.09977600	-1.66781500	-0.44752100
O	-4.69999200	-0.79771300	-2.12343000
H	-4.08383800	-1.49360600	-1.82250400
H	-5.47218700	-1.25480900	-2.47479400
O	-1.98587000	-0.91775100	2.68886100
H	-1.53506500	-0.70891000	1.81075400
H	-1.43260500	-1.54734800	3.16462400
O	-4.13529800	-1.60532800	1.51291200
H	-3.74416400	-2.12730900	0.75480700
H	-3.33112700	-1.40002400	2.12164800
O	-4.63287700	0.50182200	0.30800600
H	-4.41257300	-0.66841300	1.04583000
H	-4.80916800	0.18963000	-0.60835400
C	-1.16747000	0.81610300	-1.80441800
H	-2.15942600	0.54035500	-2.17121000
H	-0.92076800	1.81165100	-2.17132000
H	-0.44453300	0.10592000	-2.20354300
C	-2.09665800	3.08034900	-0.10085500
H	-2.49343300	3.15875600	-1.11338000
H	-2.76197500	3.63638700	0.56127200
H	-1.10346200	3.53569300	-0.06851300

C	1.46457400	0.85615900	0.05809500
C	1.68885200	-0.46772200	-0.40224600
C	2.59033900	1.62183600	0.46807400
C	2.97044100	-0.98091200	-0.45869300
H	0.84966300	-1.08230300	-0.68722900
C	3.86626600	1.10741400	0.41117100
H	2.41991400	2.63048100	0.82435700
C	4.06154900	-0.20102000	-0.05660000
H	3.13812100	-1.98965500	-0.81074400
H	4.71600300	1.70023800	0.72045300
N	5.39113600	-0.74451100	-0.12169500
O	6.34222600	-0.04027800	0.24371500
O	5.54624700	-1.89949100	-0.54121500

AM...H₃O⁺...AL⁻

C	-1.16693400	0.73991700	-0.28203800
O	0.29088200	1.45052500	0.13701300
N	-2.09247300	1.67200300	0.33374500
O	-1.22485100	-0.45394700	0.24297200
H	-3.74892100	0.97414400	0.26866000
H	-1.94144400	1.62293600	1.33844400
O	-2.82341400	-2.32853400	-0.67065300
H	-2.40204700	-3.16562800	-0.89648300
H	-2.09977600	-1.66781500	-0.44752100
O	-4.69999200	-0.79771300	-2.12343000
H	-4.08383800	-1.49360600	-1.82250400
H	-5.47218700	-1.25480900	-2.47479400
O	-1.98587000	-0.91775100	2.68886100
H	-1.53506500	-0.70891000	1.81075400
H	-1.43260500	-1.54734800	3.16462400
O	-4.13529800	-1.60532800	1.51291200
H	-3.74416400	-2.12730900	0.75480700
H	-3.33112700	-1.40002400	2.12164800
O	-4.63287700	0.50182200	0.30800600
H	-4.41257300	-0.66841300	1.04583000
H	-4.80916800	0.18963000	-0.60835400
C	-1.16747000	0.81610300	-1.80441800
H	-2.15942600	0.54035500	-2.17121000
H	-0.92076800	1.81165100	-2.17132000
H	-0.44453300	0.10592000	-2.20354300
C	-2.09665800	3.08034900	-0.10085500
H	-2.49343300	3.15875600	-1.11338000
H	-2.76197500	3.63638700	0.56127200
H	-1.10346200	3.53569300	-0.06851300
C	1.46457400	0.85615900	0.05809500
C	1.68885200	-0.46772200	-0.40224600
C	2.59033900	1.62183600	0.46807400
C	2.97044100	-0.98091200	-0.45869300
H	0.84966300	-1.08230300	-0.68722900
C	3.86626600	1.10741400	0.41117100
H	2.41991400	2.63048100	0.82435700
C	4.06154900	-0.20102000	-0.05660000
H	3.13812100	-1.98965500	-0.81074400
H	4.71600300	1.70023800	0.72045300
N	5.39113600	-0.74451100	-0.12169500
O	6.34222600	-0.04027800	0.24371500
O	5.54624700	-1.89949100	-0.54121500

(AM...AL)₁

C	-2.88594700	-1.45405700	1.22897200
O	0.70817600	0.38637200	1.59155000
N	-2.64382100	-2.06565300	0.06102600
O	-3.72958300	-0.53792300	1.33080300
H	-3.20224400	-1.78714300	-0.74864000
H	-2.27281900	3.63863100	-0.96805800
O	-4.55031600	1.57663500	-0.07245900
H	-5.31487100	1.90857300	0.41333500
H	-4.26598400	0.74863500	0.39683100
O	-0.30471000	2.84313200	1.51145000
H	-0.45892700	3.27588300	2.35833300

H	0.33118000	1.30655100	1.54946800
O	-2.45887800	3.40687000	-0.05161000
H	-1.09462900	3.03399100	0.95191900
H	-3.20160300	2.76536200	-0.07844800
O	-5.07547500	0.87375400	-2.70492800
H	-4.91499500	1.21400200	-1.79878300
H	-4.67768900	1.51436200	-3.30457800
O	-3.97378700	-1.64952500	-2.52641700
H	-4.39144200	-0.77344300	-2.67548900
H	-4.63233500	-2.30114200	-2.78980900
C	-2.08933200	-1.89328300	2.43459600
H	-2.07349900	-2.97990700	2.53997800
H	-1.05510600	-1.55035800	2.33388200
H	-2.52232300	-1.44558500	3.32671600
C	-1.67519300	-3.13678600	-0.15559300
H	-1.95625100	-4.05322000	0.37053300
H	-1.64772500	-3.34972100	-1.22313300
H	-0.67267400	-2.84127900	0.16043400
C	1.88378500	0.29078200	0.95720300
C	2.52384100	-0.96258700	0.95132300
C	2.48755100	1.38551000	0.30897400
C	3.73793600	-1.12245000	0.31205400
H	2.05005900	-1.79608300	1.45453900
C	3.70359900	1.22663100	-0.33102500
H	1.99325600	2.34880500	0.31703000
C	4.32519900	-0.02548900	-0.32846800
H	4.23584100	-2.08186900	0.30288300
H	4.17532900	2.06043500	-0.83184400
N	5.59885800	-0.18979500	-0.99996200
O	6.10471100	0.78908300	-1.55610400
O	6.13180800	-1.30301900	-0.99138000

T₃[±]

C	-0.93384300	0.68561900	-0.58551100
O	0.27964500	1.31575400	0.05125100
N	-2.02237200	1.64454300	0.06452500
O	-1.16143600	-0.52086600	-0.19445000
H	-2.93409600	1.36291900	-0.34878800
O	-2.08659700	-0.18453300	2.38650600
H	-1.69741800	-0.54857100	1.56325800
H	-2.97411200	-0.58881800	2.44507200
O	-4.67892000	-1.34428600	2.35153200
H	-4.84989800	-1.56375600	1.41233500
H	-4.82593400	-2.16034200	2.84183500
O	-2.56545400	-2.44448100	-1.37691400
H	-1.98320800	-1.73501200	-0.99169400
H	-2.15943200	-3.28557000	-1.14129800
O	-4.95959200	-1.73049400	-0.40329600
H	-5.69266400	-2.22856100	-0.78265500
H	-4.12412900	-2.11294100	-0.78026200
O	-4.57407000	0.95696100	-1.03230500
H	-4.82875700	0.03171500	-0.82975800
H	-5.31498000	1.50424400	-0.74923600
C	-0.88487900	0.95296400	-2.08839700
H	-1.84640000	0.68655800	-2.53148500
H	-0.65430400	1.99272100	-2.32158400
H	-0.11760900	0.31984900	-2.53402500
C	-1.87528900	3.12266600	-0.02838400
H	-1.92198600	3.42841600	-1.07112000
H	-2.69768200	3.58423500	0.51771400
H	-0.92589900	3.41813600	0.40794200
H	-2.06287600	1.34114100	1.04977500
C	1.48808900	0.72833700	0.03141700
C	1.77993500	-0.52631300	-0.53806800
C	2.52322900	1.47071400	0.63725300
C	3.07780600	-1.01049500	-0.50882700
H	0.99434100	-1.12071400	-0.97684100
C	3.81498300	0.98608000	0.66730600
H	2.28471700	2.43178000	1.07503100
C	4.08983900	-0.25827200	0.08938900

H	3.30979600	-1.97224100	-0.94474200
H	4.60922400	1.55666900	1.12770100
N	5.44477400	-0.77372700	0.11432000
O	6.32387800	-0.09471600	0.65181400
O	5.66970500	-1.87151200	-0.40240700

TS₁₇

C	-0.92306100	0.58723600	-0.50033200
O	0.27141100	1.24511800	0.03125800
N	-2.00643700	1.55210000	-0.07039400
O	-1.16336700	-0.60332700	0.11592200
H	-2.86020100	1.28891800	-0.58765600
O	-2.17972500	0.34815200	2.07791100
H	-1.61263100	-0.34545300	1.13980900
H	-3.07377200	-0.00040700	2.24731100
O	-4.86627200	-0.73318400	2.31865300
H	-5.01326400	-1.14807300	1.44484100
H	-5.05453400	-1.42000200	2.96725500
O	-2.60711600	-2.71286200	-0.87477700
H	-2.01664300	-1.98991900	-0.56138400
H	-2.28991300	-3.51917200	-0.45331300
O	-5.04881400	-1.69903300	-0.31013200
H	-5.77996400	-2.24305500	-0.62447700
H	-4.21492900	-2.18725300	-0.52414400
O	-4.50280700	0.81291100	-1.42898400
H	-4.81594600	-0.04385400	-1.07280800
H	-5.24251200	1.42293600	-1.33365200
C	-0.83379200	0.46753300	-2.01497700
H	-1.78389000	0.09559500	-2.40091800
H	-0.61747000	1.43470700	-2.46975900
H	-0.04846800	-0.23339200	-2.29595000
C	-1.77328200	3.00459100	-0.23913900
H	-1.50724300	3.25189300	-1.26820700
H	-2.69934900	3.51887100	0.01831600
H	-0.98196000	3.33243300	0.42931400
H	-2.21299100	1.16948200	1.08972600
C	1.49948300	0.67760800	0.02614500
C	1.77970500	-0.66846100	-0.26403500
C	2.54898500	1.55252200	0.36390900
C	3.09143100	-1.11764400	-0.23211600
H	0.98190300	-1.35816200	-0.48841400
C	3.85398600	1.10271400	0.40153400
H	2.31398800	2.58485300	0.58950900
C	4.11990900	-0.23573300	0.09728500
H	3.31851500	-2.15085500	-0.45463700
H	4.66327600	1.77214700	0.65652500
N	5.49152700	-0.71647100	0.12910300
O	6.38460300	0.07650900	0.43399100
O	5.70861000	-1.89726500	-0.14982900

T₁⁰

C	-0.87302600	0.74852700	-0.51896300
O	0.30376300	1.23706300	0.19321000
N	-1.92148000	1.64316700	-0.05385600
O	-1.19382600	-0.55335400	-0.11263400
H	-2.80280900	1.33610000	-0.47271200
O	-2.25768400	0.04043500	2.33958800
H	-1.52191100	-0.51145500	0.82104600
H	-3.16981400	-0.31523400	2.39560300
O	-4.83518600	-1.04236600	2.33894700
H	-5.01013600	-1.35760500	1.42789700
H	-5.00952300	-1.79363400	2.91634400
O	-2.74983700	-2.53421500	-1.33988600
H	-2.12485500	-1.87154400	-0.98292800
H	-2.37556600	-3.39594900	-1.12525500
O	-5.13836500	-1.69775700	-0.35506600
H	-5.88936700	-2.20629600	-0.68185300
H	-4.32507400	-2.12171800	-0.72207600
O	-4.69774600	0.96980300	-1.17907600
H	-4.97306800	0.07270400	-0.90686600

H	-5.39977200	1.55679900	-0.87826900
C	-0.62650400	0.74440300	-2.02497400
H	-1.55124200	0.46627600	-2.53308300
H	-0.32370800	1.73583600	-2.36109100
H	0.14873600	0.03118700	-2.30334300
C	-1.74233300	3.08065400	-0.30656100
H	-1.63585700	3.33328800	-1.36895500
H	-2.62207000	3.59948700	0.07725100
H	-0.86837000	3.44857700	0.22920000
H	-2.32320600	0.87326200	1.83262500
C	1.53105500	0.67060400	0.11593300
C	1.79667600	-0.65171300	-0.27880300
C	2.59038000	1.50434100	0.51893600
C	3.10309500	-1.11703800	-0.28479100
H	0.99108600	-1.31309200	-0.55567300
C	3.89088300	1.03863900	0.51927500
H	2.36691400	2.51835600	0.82504700
C	4.14125600	-0.27435100	0.11055300
H	3.31853100	-2.13276700	-0.58555400
H	4.70799200	1.67737300	0.82338800
N	5.50804100	-0.77160000	0.10298700
O	6.41010900	-0.01369300	0.46450600
O	5.71105700	-1.93033000	-0.26437400

T₂^o

C	-0.74602800	1.62762600	-0.22656500
O	0.36011800	1.33131000	-1.22933800
N	-0.35248400	2.51743200	0.80391500
O	-1.07423900	0.42825100	0.40541900
H	-6.68249800	-0.88007600	0.86641500
H	0.29944400	2.06927900	1.43741700
O	-2.44563300	-1.52208400	-0.95560700
H	-1.99237200	-2.18097800	-1.49396500
H	-1.49826600	-0.20440700	-0.21846300
O	-4.88767600	-0.85652400	-1.94085300
H	-3.28282000	-1.29587700	-1.43174600
H	-5.26084400	-1.30779700	-2.70590000
O	-2.49558000	0.05103900	2.80651200
H	-1.92356100	0.31191900	2.05824100
H	-1.90478600	-0.07301700	3.55750700
O	-3.76113000	-2.11754000	1.54949400
H	-3.22348000	-2.09226900	0.73711100
H	-3.37473800	-1.41287200	2.10886900
O	-6.17527500	-1.54109500	0.38290900
H	-5.37431000	-1.72727000	0.92790800
H	-5.47139100	-1.07520000	-1.17822800
C	-1.85203500	2.16974300	-1.11734800
H	-2.71396300	2.43058300	-0.50207800
H	-1.51841200	3.05184400	-1.66272400
H	-2.14249800	1.40888000	-1.84173500
C	0.05018500	3.87723500	0.44612100
H	-0.81462300	4.45644300	0.11835300
H	0.45204400	4.35795900	1.33817600
H	0.81109600	3.91799700	-0.34377000
C	1.47023300	0.66063300	-0.81557100
C	1.60329800	-0.69725500	-1.14225800
C	2.51028100	1.31772000	-0.14054000
C	2.74836300	-1.39537800	-0.79470500
H	0.80341100	-1.18932800	-1.68002000
C	3.65845900	0.62518900	0.21737600
H	2.43058000	2.37361500	0.07831800
C	3.76388400	-0.72577200	-0.11003600
H	2.86056300	-2.44115700	-1.04366800
H	4.46772200	1.12198800	0.73368000
N	4.97304700	-1.45664500	0.26372600
O	5.85608100	-0.85428400	0.87330400
O	5.05707400	-2.64460000	-0.04584400

TS₁₈

C	-0.86126400	1.77593600	0.01319000
---	-------------	------------	------------

O	0.40722300	1.50023300	-1.22904400
N	-0.34659600	2.49508600	1.04812300
O	-1.16564400	0.51878200	0.41383600
H	-6.53617200	-1.40493600	1.12665200
H	0.19895200	1.94826600	1.70104200
O	-2.52358600	-1.12406900	-1.22075500
H	-2.09957100	-1.53903500	-1.98086700
H	-1.61175600	-0.00497300	-0.30052800
O	-5.08536000	-0.39968800	-1.69977400
H	-3.42643600	-0.84141200	-1.51543200
H	-5.52506600	-0.62476800	-2.52696600
O	-2.17497700	-0.71313000	2.80707100
H	-1.72646800	-0.18612700	2.12286900
H	-1.47971500	-1.00804900	3.40590400
O	-3.49181500	-2.54348800	1.11988400
H	-3.05534100	-2.25366900	0.29915500
H	-3.07293800	-1.99463800	1.81318900
O	-6.05340000	-1.84501800	0.41862800
H	-5.18692100	-2.11721200	0.80286800
H	-5.56707900	-0.88146600	-0.98824300
C	-1.83947800	2.46230400	-0.90548700
H	-2.72986500	2.73045300	-0.33130500
H	-1.40711500	3.36158300	-1.33920000
H	-2.12315000	1.78907600	-1.71211500
C	0.04073200	3.89490700	0.90823900
H	-0.83450000	4.52074100	0.72930400
H	0.49818300	4.21406500	1.84337000
H	0.75733300	4.04718500	0.09420500
C	1.46626300	0.79201100	-0.87726000
C	1.62470900	-0.53262800	-1.35654200
C	2.48414200	1.32531000	-0.04685700
C	2.73460200	-1.28586100	-1.02842900
H	0.85571300	-0.94343900	-1.99910900
C	3.59470100	0.57315500	0.29226500
H	2.40397200	2.34720200	0.29958700
C	3.71615300	-0.73167500	-0.19664700
H	2.85169000	-2.29507000	-1.39849400
H	4.37289600	0.98544900	0.91969300
N	4.87788400	-1.51877400	0.15582700
O	5.72996700	-1.02019300	0.89885800
O	4.97771400	-2.66395000	-0.29721200

(AM⁺o...AL⁻)₁

C	-1.39032200	2.02164800	0.35231200
O	0.73084600	1.68281600	-1.49949600
N	-0.74061500	2.67103100	1.28119900
O	-1.52439900	0.73920900	0.52627700
H	-6.24277200	-2.37795400	1.18002400
H	-0.34296100	2.11485600	2.02914700
O	-2.67723700	-0.68286300	-1.26150800
H	-2.25635100	-0.78420800	-2.12384400
H	-1.98779300	0.25504800	-0.24213500
O	-5.32801300	-0.46505800	-1.37692900
H	-3.65477000	-0.55758600	-1.41411000
H	-5.80273100	-0.57278500	-2.20852600
O	-1.82123300	-1.40496100	2.66257500
H	-1.53744000	-0.61711900	2.17676300
H	-1.02895800	-1.73587900	3.10134200
O	-3.07491200	-2.90532600	0.63126100
H	-2.79405800	-2.33935400	-0.10691300
H	-2.65266200	-2.49485700	1.41204500
O	-5.78463300	-2.53297600	0.34686500
H	-4.84803100	-2.73269500	0.57936700
H	-5.63285200	-1.19102000	-0.78299400
C	-2.03067400	2.72478400	-0.79237200
H	-2.97138200	3.16787100	-0.44924200
H	-1.38614900	3.51684300	-1.16698500
H	-2.24462600	2.02452400	-1.59517900
C	-0.48864300	4.11470900	1.29836800
H	-1.42384900	4.66803400	1.21981500

H	-0.01464900	4.35616600	2.24607700
H	0.17904500	4.39556900	0.48278500
C	1.68711000	0.95085900	-1.11270300
C	1.83909300	-0.41906900	-1.55690500
C	2.69969400	1.42538300	-0.19239400
C	2.87131800	-1.21343200	-1.13078200
H	1.10033500	-0.80695700	-2.25017500
C	3.73024400	0.62717600	0.23156000
H	2.62152500	2.44897600	0.15781300
C	3.83463900	-0.70573900	-0.22847600
H	2.96338100	-2.23474200	-1.47647200
H	4.47563300	1.00410100	0.91966100
N	4.89481200	-1.52519900	0.21006800
O	5.74074400	-1.06344700	1.00828500
O	4.97483600	-2.70309000	-0.20467800

(AM⁺...AL⁻)₂

C	-2.74742700	1.45175500	0.01683800
O	1.11832800	0.79895100	-1.32485400
N	-3.50259600	1.51651800	1.07534500
O	-2.87024800	0.37077700	-0.70853200
H	-3.96617400	0.62357400	1.33509200
O	-5.31854100	-0.74005100	-1.89198900
H	-5.79547600	-0.06201800	-2.38385000
H	-4.52339800	-0.30398800	-1.54448500
O	-6.41525700	-1.97152200	0.32882800
H	-6.13422100	-1.59283400	-0.53094000
H	-6.58200100	-2.90635200	0.16655700
O	-0.82852100	-0.73167500	-1.55766600
H	-1.99657900	0.02339300	-1.17943900
H	-0.86471100	-1.10625200	-2.44577100
O	-1.79325400	-2.24952200	0.76669400
H	-1.56628100	-3.18559200	0.77228600
H	-1.38977100	-1.88129600	-0.03936400
O	-4.21711200	-1.10380100	1.82712300
H	-3.43519900	-1.55700300	1.45786800
H	-4.99009900	-1.49294300	1.36936300
C	-1.80270700	2.52215400	-0.40473900
H	-2.17215500	2.97126600	-1.33099700
H	-1.68446000	3.29526600	0.34969700
H	-0.82748700	2.07537400	-0.62225200
C	-3.62208500	2.65175300	1.99376800
H	-3.72038900	3.58549100	1.44326800
H	-4.51976200	2.50092400	2.58929400
H	-2.75914700	2.70449000	2.65991700
H	0.04757100	-0.15240700	-1.47822100
C	2.27908900	0.47585800	-0.86886100
C	3.31542800	1.45769300	-0.74663700
C	2.60306100	-0.86026600	-0.46298400
C	4.56248900	1.13366400	-0.26793800
H	3.09039300	2.47445800	-1.04754300
C	3.85146400	-1.18322700	0.01522300
H	1.83851600	-1.62463000	-0.54168600
C	4.84438000	-0.19102700	0.11789400
H	5.33516000	1.88600700	-0.18348400
H	4.08171600	-2.19620100	0.31694100
N	6.13664200	-0.52768900	0.61291500
O	6.37149700	-1.70368700	0.94512900
O	7.00229400	0.36169600	0.70208600

T₄[±]

C	1.19052200	-0.32257400	0.84953900
O	0.07780700	0.73457400	0.39576500
N	2.37823500	0.69965400	0.95854000
O	1.44082700	-1.20716800	-0.02415800
H	3.20972900	0.12067800	1.19800700
H	2.56289900	1.05182900	-0.00333800
O	2.97716400	-1.13886300	-2.17124900
H	2.58957500	-1.63354700	-2.90161000
H	2.33661100	-1.19014300	-1.40556400

O	0.50707900	2.71782500	-1.75827400
H	-0.16325200	2.62684600	-2.44479500
H	0.24985500	2.09742400	-1.05510000
O	3.06928300	1.62925900	-1.69102900
H	2.23983800	2.06256300	-1.96842500
H	3.07669200	0.75651700	-2.12637500
O	5.36511800	-1.82932700	-0.96932700
H	4.56981800	-1.62389200	-1.50873300
H	6.11627800	-1.46885200	-1.45309000
O	4.78244700	-0.74253800	1.49252200
H	5.06193800	-1.16906600	0.65061000
H	4.81485100	-1.43237300	2.16427800
C	0.78849000	-0.78756000	2.24687700
H	1.63229100	-1.32052700	2.69114000
H	0.49236700	0.02995500	2.90374900
H	-0.04091300	-1.48824200	2.15879300
C	2.29159500	1.85022100	1.89985600
H	2.28898300	1.48765600	2.92503000
H	3.16479400	2.48336400	1.74551700
H	1.38467600	2.41328900	1.69782600
C	-1.20479100	0.34191500	0.25930600
C	-1.59701400	-0.96632900	-0.08749800
C	-2.19036600	1.33305100	0.44031700
C	-2.94000200	-1.26928500	-0.23702800
H	-0.84397000	-1.72341700	-0.24915700
C	-3.53033800	1.03362000	0.28034600
H	-1.88156300	2.33432800	0.71389400
C	-3.90022400	-0.27175700	-0.05534100
H	-3.24904800	-2.27002300	-0.50513700
H	-4.28791000	1.79151800	0.42231800
N	-5.30631500	-0.59534200	-0.22008300
O	-6.13893300	0.30221700	-0.07060100
O	-5.61519200	-1.75521500	-0.50330800

TS₁₉

C	1.25565900	-0.33330000	0.89958400
O	0.03513300	0.79462900	0.27901300
N	2.38591200	0.72400100	0.92467000
O	1.48488500	-1.25262600	0.09158200
H	3.24455200	0.19278300	1.19292100
H	2.55466700	1.02133500	-0.06086000
O	3.05416400	-1.30816200	-2.09590500
H	2.69515300	-1.86923000	-2.79240300
H	2.41569300	-1.34009000	-1.33900100
O	0.52355300	2.59778500	-1.89166600
H	-0.14330800	2.46395900	-2.57428200
H	0.26566600	2.01660800	-1.14990100
O	3.05769200	1.49653900	-1.75067500
H	2.22989700	1.91468400	-2.05917200
H	3.08676000	0.61240200	-2.15884900
O	5.47384700	-1.80898000	-0.83998000
H	4.67672200	-1.67692300	-1.39725300
H	6.21318900	-1.44822000	-1.34152400
O	4.81783800	-0.58804100	1.53403500
H	5.12608700	-1.05731900	0.72511900
H	4.87008400	-1.22872200	2.25177600
C	0.73871700	-0.64327200	2.29139600
H	1.54214100	-1.13055300	2.85143300
H	0.40869900	0.24007200	2.83453500
H	-0.08870300	-1.34638800	2.21048600
C	2.26715600	1.92447000	1.79939700
H	2.29870200	1.62208700	2.84350000
H	3.11290800	2.57809100	1.58945800
H	1.33493800	2.43678500	1.58108100
C	-1.23352000	0.40315100	0.18440900
C	-1.62120100	-0.92920500	-0.09583200
C	-2.24406400	1.38266400	0.33866600
C	-2.95870400	-1.26183300	-0.20615700
H	-0.86027400	-1.68365500	-0.23593000
C	-3.57953600	1.05303900	0.21861700

H	-1.94963900	2.40175700	0.55810300
C	-3.93630000	-0.27340900	-0.05086900
H	-3.25526000	-2.27870800	-0.42360300
H	-4.34821500	1.80367100	0.33970200
N	-5.33329500	-0.62549000	-0.17385500
O	-6.18251600	0.26228000	-0.04151100
O	-5.63059800	-1.80190400	-0.40693400

(AM⁺N...AL⁻)₁

C	2.03867300	-1.24224300	-0.49287800
O	-0.49174200	0.66298200	-0.34472500
N	2.43408400	-0.65798100	0.82207200
O	2.57950500	-0.79401700	-1.46816600
H	3.36849300	-1.09967300	1.07717400
H	2.66503200	0.36860800	0.66434500
O	4.69944000	1.15675500	-1.68053400
H	4.92070900	1.55750100	-2.52953700
H	4.01254900	0.49135200	-1.85857100
O	0.63418400	3.02013300	0.09556800
H	0.43941700	3.59015000	-0.65580600
H	0.14146400	2.16472500	-0.06493400
O	3.09391700	1.97737000	0.52598300
H	2.26885500	2.47447400	0.30844200
H	3.67186100	2.02355200	-0.25469200
O	6.59342500	-0.17258600	-0.09354700
H	6.02909300	0.36383800	-0.68678000
H	7.19321800	0.44694400	0.33672900
O	4.89973800	-1.61310600	1.48160000
H	5.57740400	-1.13640400	0.94456300
H	5.10031400	-2.55308500	1.40883200
C	1.07534400	-2.37698800	-0.46955600
H	1.47261200	-3.19014700	0.14523400
H	0.12724000	-2.05873200	-0.03356000
H	0.91704200	-2.72684200	-1.48675700
C	1.48797600	-0.78159600	1.97355800
H	1.34989300	-1.82804600	2.23383100
H	1.93422700	-0.25580700	2.81543100
H	0.54342600	-0.31796000	1.69891300
C	-1.75069400	0.44729300	-0.25377800
C	-2.39060800	-0.59910000	-1.00541500
C	-2.60275900	1.22723800	0.60451800
C	-3.73865900	-0.84313000	-0.90484800
H	-1.77686800	-1.19542600	-1.67079500
C	-3.95045700	0.98133300	0.70371700
H	-2.15106200	2.02428100	1.18438600
C	-4.53609900	-0.05793000	-0.04766600
H	-4.20213200	-1.63288200	-1.48104900
H	-4.57451800	1.57667100	1.35689700
N	-5.92881900	-0.31157000	0.05655300
O	-6.62155200	0.39311700	0.81652200
O	-6.43209200	-1.23433400	-0.61377200

(AM⁺N...AL⁻)₂

C	-2.76995500	-1.21873200	0.94511200
O	0.70618900	0.27442900	0.07295900
N	-2.95166300	-0.92779000	-0.50723400
O	-3.64170500	-0.82684700	1.67628200
H	-3.92756900	-1.23475300	-0.77348700
H	-2.99308400	0.14775100	-0.58513700
O	-5.19473200	1.60138300	1.27473600
H	-5.43122000	2.17406600	2.01471600
H	-4.81483500	0.79457800	1.66065900
O	-0.61367800	2.56121300	-0.10228000
H	-0.43764900	3.08943100	0.68345700
H	-0.06481200	1.72729900	-0.01151000
O	-3.11332800	1.74075500	-0.67047200
H	-2.24328500	2.13725800	-0.41202000
H	-3.76952900	2.00076200	-0.00015200
O	-7.05774000	0.57013900	-0.54858600
H	-6.49910100	1.05428400	0.09205700

H	-7.31863700	1.21445400	-1.21602600
O	-5.49908400	-1.53395900	-1.35419900
H	-6.12320600	-0.81460700	-1.09908000
H	-5.92941400	-2.36474600	-1.12322600
C	-1.51854000	-1.90615500	1.35594900
H	-1.42308600	-2.87256300	0.85417400
H	-0.65849500	-1.29166800	1.05520800
H	-1.52935900	-2.04642700	2.43427000
C	-1.95597700	-1.45265700	-1.48945900
H	-1.96534700	-2.54016500	-1.48254900
H	-2.25497300	-1.09510900	-2.47308700
H	-0.96802300	-1.06917200	-1.24120500
C	1.98266800	0.18827700	0.02797300
C	2.65381900	-1.07814700	0.15264400
C	2.82627200	1.34112400	-0.14897900
C	4.02262900	-1.17981800	0.11119100
H	2.04375600	-1.96463500	0.28427600
C	4.19501800	1.23665100	-0.19065200
H	2.35305400	2.31116500	-0.25086600
C	4.81253300	-0.02408000	-0.06019700
H	4.50859400	-2.14150200	0.20876700
H	4.81189000	2.11543600	-0.32376800
N	6.22680000	-0.12932900	-0.10097300
O	6.91084800	0.90175200	-0.25503700
O	6.75885800	-1.25075500	0.01819700

TS₂₀

C	-2.65202100	-1.21907800	0.94528200
O	0.85612000	0.31938200	0.07305800
N	-2.81360100	-0.92569400	-0.45851200
O	-3.54684700	-0.88031000	1.69574300
H	-3.79413100	-1.15228500	-0.73684100
H	-2.82801900	0.35613400	-0.55085200
O	-4.95488600	1.54798600	1.22308000
H	-5.11125700	2.15234100	1.95886800
H	-4.63820600	0.70986000	1.60961000
O	-0.55679600	2.48629700	-0.12617100
H	-0.43220100	3.03897600	0.65305600
H	0.05936200	1.68889400	-0.02544800
O	-2.90802200	1.57739100	-0.62817200
H	-2.01193100	1.99919300	-0.38583700
H	-3.59238300	1.84839000	0.02342400
O	-6.97273800	0.64492200	-0.52426900
H	-6.37021500	1.10270000	0.09366800
H	-7.25423000	1.30911500	-1.16325400
O	-5.42139600	-1.45057800	-1.41131700
H	-6.04860700	-0.74385500	-1.13856400
H	-5.85473100	-2.28721200	-1.20974000
C	-1.37437400	-1.84817600	1.39123400
H	-1.24508300	-2.82742900	0.92194300
H	-0.52834200	-1.22220000	1.08060100
H	-1.39011200	-1.95776300	2.47318800
C	-1.84712900	-1.47805400	-1.44471100
H	-1.86754700	-2.56766700	-1.44514400
H	-2.14304100	-1.11674400	-2.42857600
H	-0.84555800	-1.11712700	-1.21653300
C	2.13323100	0.22662200	0.02954600
C	2.79182300	-1.04516500	0.15423500
C	2.98401500	1.37270800	-0.14490800
C	4.15981700	-1.15847600	0.11412500
H	2.17342600	-1.92594900	0.28438200
C	4.35227000	1.25676000	-0.18554800
H	2.51880200	2.34683700	-0.24565200
C	4.95847200	-0.00902200	-0.05571000
H	4.63773700	-2.12417700	0.21131600
H	4.97663100	2.13042700	-0.31709400
N	6.37278000	-0.12630600	-0.09568600
O	7.06497400	0.89880000	-0.24905900
O	6.89443500	-1.25203700	0.02355600

Table S4. Calculated energies (a.u) of stationary points for the methylamine + methylacetate reaction at different levels of theory. MP2/aug-cc-pVTZ calculations are carried out on B3LYP/6-311+G(d,p) optimized geometries.

	E _{B3LYP/6-311+G(d,p)}	E _{MP2/aug-cc-PVTZ}	ZPE _{B3LYP/6-311+G(d,p)}	H _{B3LYP/6-311+G(d,p)}	TΔS _{B3LYP/6-311+G(d,p)}	G _{B3LYP/6-311+G(d,p)}	G _{MP2/aug-cc-PVTZ}
RC	-746.756613	-745.336070	-746.478127	-746.451358	0.089114	-746.540472	-745.119928
TS(RC-T₁[‡])	-746.741750	-745.337222	-746.460033	-746.436905	0.073567	-746.510472	-745.105944
T₁[‡]	-746.742324	-745.341883	-746.459004	-746.436037	0.072699	-746.508736	-745.108295
T₂[‡]	-746.742324	-745.341882	-746.459002	-746.436035	0.072689	-746.508724	-745.108282
TS₁	-746.713552	-745.317716	-746.434324	-746.414093	0.065983	-746.480076	-745.084240
(T⁻...H₃O⁺)₁	-746.713552	-745.317710	-746.434292	-746.414063	0.065976	-746.480039	-745.084197
TS₂	-746.713472	-745.317611	-746.434540	-746.414319	0.065923	-746.480242	-745.084381
T₃⁰	-746.742125	-745.343888	-746.458634	-746.435825	0.072026	-746.507851	-745.109614
T⁻	-746.262600	-744.868057	-745.993594	-745.971042	0.072824	-746.043866	-744.649323
TS₃	-746.256940	-744.854639	-745.991066	-745.968168	0.073471	-746.041639	-744.639339
AM...AL⁻	-746.296319	-744.879784	-746.033200	-746.007737	0.087433	-746.095170	-744.678635
(T⁻...H₃O⁺)₂	-746.711171	-745.314867	-746.431884	-746.410280	0.069761	-746.480041	-745.083737
TS₄	-746.699054	-745.293237	-746.421823	-746.399808	0.070687	-746.470495	-745.064678
(AM...AL)₁	-746.770178	-745.349826	-746.491940	-746.465203	0.089566	-746.554769	-745.134417
T₃[‡]	-746.737069	-745.341882	-746.455234	-746.431478	0.076415	-746.507893	-745.112706
TS₅	-746.716909	-745.318396	-746.439680	-746.416731	0.074173	-746.490904	-745.092390
T₁⁰	-746.735200	-745.342583	-746.453715	-746.429593	0.076971	-746.506564	-745.113947
T₂⁰	-746.730484	-745.327352	-746.450090	-746.425568	0.078162	-746.503730	-745.100598
TS₆	-746.713172	-745.303526	-746.437182	-746.413447	0.075555	-746.489002	-745.079356
(AM...AL)₂	-746.772189	-745.353049	-746.493886	-746.467514	0.087451	-746.554965	-745.135825
T₄[‡]	-746.735921	-745.340713	-746.453808	-746.430444	0.073933	-746.504377	-745.109169
TS₇	-746.710983	-745.302966	-746.435715	-746.412282	0.074521	-746.486803	-745.078786
(AM...AL)₃	-746.768269	-745.354128	-746.491104	-746.464004	0.092711	-746.556715	-745.142574

Table S5. Calculated energies (a.u) of stationary points for the methylamine + phenylacetate reaction at different levels of theory. MP2/aug-cc-pVTZ calculations are carried out on B3LYP/6-311+G(d,p) optimized geometries.

	E _{B3LYP/6-311+G(d,p)}	E _{MP2/aug-cc-pVTZ}	ZPE _{B3LYP/6-311+G(d,p)}	H _{B3LYP/6-311+G(d,p)}	TΔS _{B3LYP/6-311+G(d,p)}	G _{B3LYP/6-311+G(d,p)}	G _{MP2/aug-cc-pVTZ}
RC	-938.539121	-936.676970	-938.209198	-938.179177	0.099010	-938.278187	-936.413920
TS(RC-T₁[‡])	-938.526778	-936.679586	-938.193393	-938.166958	0.083079	-938.250037	-936.402845
T₁[‡]	-938.529109	-936.687252	-938.193560	-938.167580	0.082269	-938.249849	-936.406730
T₂[‡]	-938.529009	-936.688645	-938.193429	-938.167520	0.080927	-938.248447	-936.408084
T⁻	-938.054329	-936.219011	-937.733320	-937.707454	0.081069	-937.788523	-935.953205
TS₈	-938.051964	-936.210755	-937.732541	-937.706313	0.082983	-937.789296	-935.948087
AM...AL⁻	-938.089911	-936.230260	-937.771646	-937.743583	0.092675	-937.836258	-935.976607
TS₉	-938.500700	-936.663530	-938.169108	-938.145613	0.074790	-938.220403	-936.383234
T...H₃O⁺	-938.500732	-936.663613	-938.168213	-938.143970	0.076593	-938.220563	-936.383444
TS₁₀	-938.497145	-936.653714	-938.164957	-938.140429	0.077781	-938.218210	-936.374779
AM...H₃O⁺...AL⁻	-938.519470	-936.654465	-938.188626	-938.161451	0.088878	-938.250329	-936.385324
(AM...AL)₁	-938.565440	-936.697861	-938.235335	-938.205876	0.099994	-938.305870	-936.438291
T₃[‡]	-938.527285	-936.683245	-938.192782	-938.166284	0.083429	-938.249713	-936.405673
TS₁₁	-938.505653	-936.665609	-938.176762	-938.151122	0.081161	-938.232283	-936.392239
T₁⁰	-938.525099	-936.682517	-938.191409	-938.164533	0.084876	-938.249409	-936.406826
T₂⁰	-938.526633	-936.682561	-938.192763	-938.166062	0.085631	-938.251693	-936.407622
TS₁₂	-938.515881	-936.660885	-938.184385	-938.157247	0.085760	-938.243007	-936.388011
AM⁺_O...AL⁻	-938.516385	-936.658870	-938.185394	-938.157003	0.090456	-938.247459	-936.389944
T₄[‡]	-938.524096	-936.682614	-938.190189	-938.163550	0.083265	-938.246815	-936.405333
TS₁₃	-938.519536	-936.672033	-938.187151	-938.160625	0.083443	-938.244068	-936.396565
(AM⁺_N...AL⁻)₁	-938.520623	-936.667789	-938.188927	-938.161578	0.085841	-938.247419	-936.394585
(AM⁺_N...AL⁻)₂	-938.520639	-936.662859	-938.189865	-938.162512	0.087232	-938.249744	-936.391964
TS₁₄	-938.517735	-936.660063	-938.191912	-938.165271	0.086365	-938.251636	-936.393964

Table S6. Calculated energies (a.u) of stationary points for the methylamine + *p*-nitrophenyl acetate reaction at different levels of theory. MP2/aug-cc-pVTZ calculations are carried out on B3LYP/6-311+G(d,p) optimized geometries.

	E _{B3LYP/6-311+G(d,p)}	E _{MP2/aug-cc-pVTZ}	ZPE _{B3LYP/6-311+G(d,p)}	H _{B3LYP/6-311+G(d,p)}	TΔS _{B3LYP/6-311+G(d,p)}	G _{B3LYP/6-311+G(d,p)}	G _{MP2/aug-cc-pVTZ}
RC	-1143.104901	-1140.914703	-1142.772662	-1142.740125	0.105098	-1142.845223	-1140.655909
TS(RC-T₁[‡])	-1143.095665	-1140.918049	-1142.760488	-1142.731130	0.090917	-1142.822047	-1140.644430
T₁[‡]	-1143.102297	-1140.929539	-1142.764258	-1142.735723	0.088389	-1142.824112	-1140.653711
T₂[‡]	-1143.102210	-1140.929509	-1142.764339	-1142.735722	0.088446	-1142.824168	-1140.651467
TS₁₅	-1143.079635	-1140.907072	-1142.745893	-1142.719370	0.082883	-1142.802253	-1140.629690
T...H₃O⁺	-1143.079635	-1140.907072	-1142.745893	-1142.719370	0.082884	-1142.802254	-1140.629690
TS₁₆	-1143.079596	-1140.905026	-1142.745257	-1142.718555	0.083223	-1142.801778	-1140.627208
AM...H₃O⁺...AL⁻	-1143.111074	-1140.910685	-1142.777722	-1142.747818	0.097267	-1142.845085	-1140.644696
(AM..AL)₁	-1143.139755	-1140.944955	-1142.807279	-1142.775455	0.104107	-1142.879562	-1140.684762
T₃[‡]	-1143.100874	-1140.926295	-1142.764491	-1142.735228	0.090571	-1142.825799	-1140.651220
TS₁₇	-1143.077354	-1140.907572	-1142.747550	-1142.719269	0.087584	-1142.806853	-1140.637071
T₁⁰	-1143.096652	-1140.923869	-1142.760891	-1142.731359	0.090909	-1142.822268	-1140.649486
T₂⁰	-1143.096678	-1140.922819	-1142.761007	-1142.731556	0.092567	-1142.824123	-1140.650264
TS₁₈	-1143.094315	-1140.913005	-1142.760151	-1142.730633	0.093385	-1142.824018	-1140.642708
(AM⁺_o...AL⁻)₁	-1143.106878	-1140.910866	-1142.773877	-1142.742547	0.101181	-1142.843728	-1140.647716
(AM⁺_o...AL⁻)₂	-1143.116478	-1140.920993	-1142.785971	-1142.754954	0.098423	-1142.853377	-1140.657892
T₄[‡]	-1143.096232	-1140.924017	-1142.760332	-1142.730794	0.090104	-1142.820898	-1140.648683
TS₁₉	-1143.095857	-1140.920419	-1142.760288	-1142.731353	0.088653	-1142.820006	-1140.644568
(AM⁺_N...AL⁻)₁	-1143.106214	-1140.916327	-1142.772333	-1142.742073	0.094578	-1142.836651	-1140.646764
(AM⁺_N...AL⁻)₂	-1143.107104	-1140.913938	-1142.773788	-1142.743493	0.095416	-1142.838909	-1140.645744
TS₂₀	-1143.103657	-1140.911158	-1142.774280	-1142.744878	0.093681	-1142.838559	-1140.646060

Table S7. Calculated imaginary frequencies at B3LYP/6-311+G(d,p) level for all the transition structures reported in this work (cm⁻¹).

methyl acetate, MA

TS(RC- T₁[‡])	191.0 <i>i</i>
TS₁	64.8 <i>i</i>
TS₂	191.3 <i>i</i>
TS₃	207.6 <i>i</i>
TS₄	207.8 <i>i</i>
TS₅	611.9 <i>i</i>
TS₆	318.9 <i>i</i>
TS₇	715.3 <i>i</i>

phenyl acetate, PA

TS(RC- T₁[‡])	203.0 <i>i</i>
TS₈	202.5 <i>i</i>
TS₉	174.0 <i>i</i>
TS₁₀	200.8 <i>i</i>
TS₁₁	861.0 <i>i</i>
TS₁₂	129.1 <i>i</i>
TS₁₃	104.2 <i>i</i>
TS₁₄	921.0 <i>i</i>

p-nitrophenyl acetate, PNPA

TS(RC- T₁[‡])	193.8 <i>i</i>
TS₁₅	115.5 <i>i</i>
TS₁₆	111.2 <i>i</i>
TS₁₇	1357.2 <i>i</i>
TS₁₈	272.0 <i>i</i>
TS₁₉	147.3 <i>i</i>
TS₂₀	930.5 <i>i</i>