

Supplementary Information for

A molecular understanding of the interaction of typical aromatic acids with common aerosol nucleation precursors and their atmospheric implications

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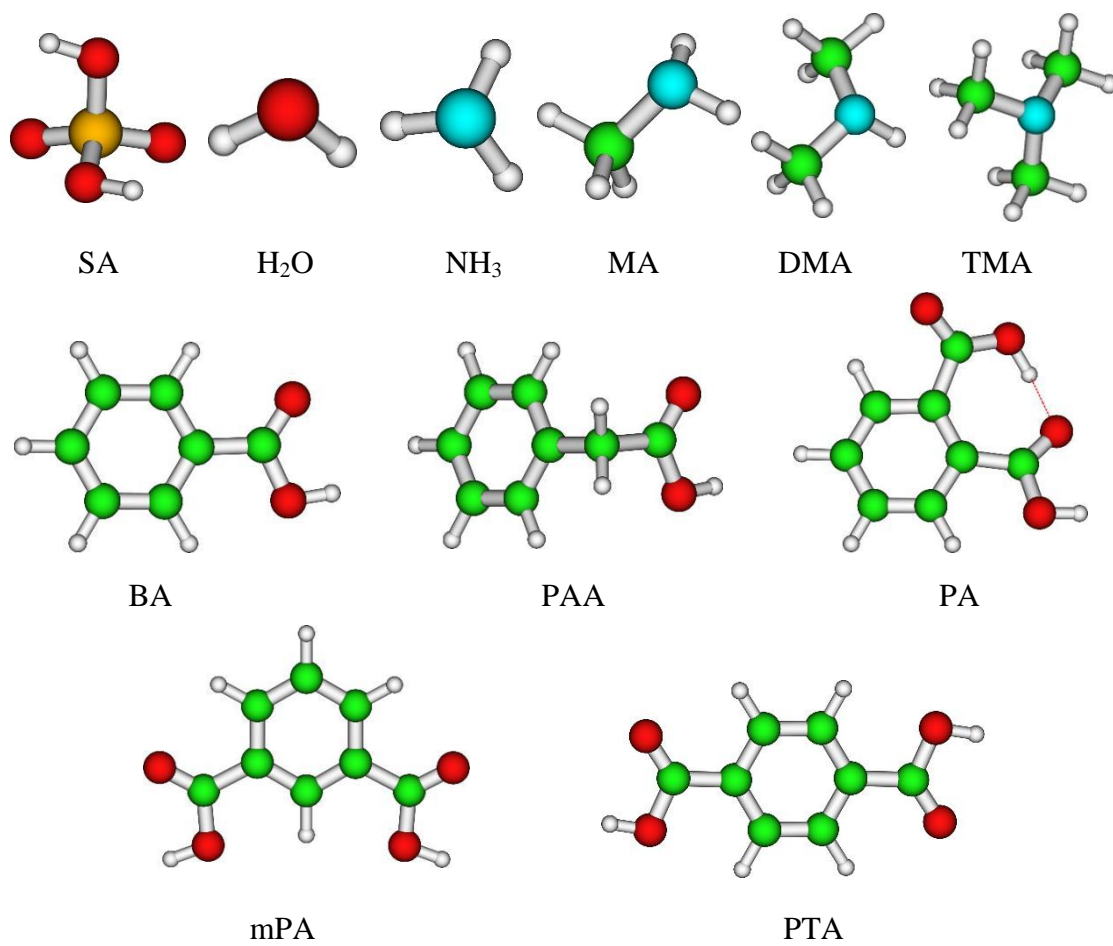


Figure S1.

Table S1. Geometric parameters of the O-H \cdots O intra-molecular hydrogen bonds in the PA-containing complexes.

Conformer	O-H \cdots O			
	$\Delta r(\text{OH})^a$	$r(\text{HB})^b$	$\theta(\text{HB})^c$	$d(\text{O} \cdots \text{O})^d$
PA-SA	-0.0082	1.6032	163.4	2.5733
PA-H ₂ O	0.0012	1.5528	166.4	2.5406
PA-NH ₃	0.0085	1.5228	168.1	2.5221
PA-MA	0.0102	1.5156	168.6	2.5175
PA-DMA	0.0111	1.5124	168.7	2.5155
PA-TMA	0.0118	1.5119	168.4	2.5150

^a $\Delta r(\text{OH}) = r_{\text{dimer}} - r_{\text{monomer}}$, is the OH bond length change in the complexation; ^b The distance of intra-molecular hydrogen bond; ^c The angle of intra-molecular hydrogen bond; ^d The two oxygen atoms contact distance in the O-H \cdots O hydrogen bond.

Table S2. Intra-molecular bonded OH-stretching wavenumbers and red shifts of PA-containing complexes.

Conformer	O-H··O		
	$\tilde{\nu}$	$\Delta\nu^a$	f_D/f_M^b
PA-SA	3212	-150	0.6
PA-H ₂ O	3557	266	5.6
PA-NH ₃	2916	146	1.2
PA-MA	2888	175	1.3
PA-DMA	2872	190	1.4
PA-TMA	2861	201	1.4

^a $\Delta\nu^{\sim} = \nu^{\sim}_{\text{monomer}} - \nu^{\sim}_{\text{dimer}}$; ^b f_D/f_M stands for the increase of intensity during the complexation.

Table S3. Atoms in molecules (AIM) parameter analysis for the intra-molecular hydrogen bonds of PA-containing complexes.

Conformer	O-H...O		
	$\Delta q(\text{H})^{\text{a}}$	ρ^{b}	$\nabla^2\rho^{\text{c}}$
PA-SA	-0.0055	0.0606	0.1187
PA-H ₂ O	-0.0019	0.0693	0.1151
PA-NH ₃	-0.0006	0.0751	0.1115
PA-MA	0.0004	0.0766	0.1106
PA-DMA	0.0004	0.0772	0.1098
PA-TMA	0	0.0774	0.1094

^a The change in atomic charge at the H atom; ^b The electron density at the BCPs; ^c The Laplacian electron density at the BCPs.

Table S4. Cartesian coordinates of the minimum energy configurations.

SA			
S	-0.00001300	0.00012800	-0.16197600
O	0.56101100	1.13762800	-0.82892700
O	-0.56122100	-1.13642100	-0.83041000
O	1.09898500	-0.60528800	0.84960800
H	1.68198000	0.12496900	1.13187500
O	-1.09878000	0.60403600	0.85070100
H	-1.68173100	-0.12665200	1.13196500
H ₂ O			
O	0.00000000	0.00000000	0.11885500
H	0.00000000	0.76447500	-0.47541900
H	0.00000000	-0.76447500	-0.47541900
NH ₃			
N	0.00000000	0.00000000	0.11659700
H	0.00000000	0.94392700	-0.27205900
H	-0.81746500	-0.47196300	-0.27205900
H	0.81746500	-0.47196300	-0.27205900
MA			
N	-0.75134800	0.00000000	-0.12321700
H	-1.15393600	0.81569600	0.33692500
H	-1.15393000	-0.81570700	0.33691100
C	0.70767800	0.00000000	0.01802900
H	1.11879700	-0.88173700	-0.48803500
H	1.11877700	0.88182600	-0.48789600
H	1.08365500	-0.00008300	1.05644200
DMA			
N	0.00000800	0.56532300	-0.14865900
H	-0.00003700	1.33959800	0.51313600
C	1.21318600	-0.22288800	0.02025900
H	1.27986700	-0.96466700	-0.78727000
H	2.09276200	0.42729100	-0.05227700
H	1.26349300	-0.77374500	0.98173300
C	-1.21317600	-0.22289300	0.02024700
H	-2.09271100	0.42742200	-0.05158200
H	-1.28027300	-0.96425000	-0.78764000
H	-1.26321100	-0.77422400	0.98147400
TMA			

N	-0.00015400	-0.00012500	-0.37665300
C	0.37496400	1.33481400	0.06073700
H	1.36863800	1.58856000	-0.32834700
H	-0.34264700	2.06874400	-0.32595400
H	0.40404800	1.43286000	1.16842300
C	-1.34357000	-0.34272100	0.06086700
H	-2.05993800	0.39176500	-0.32711400
H	-1.62048800	-1.33043700	-0.32752500
H	-1.44282000	-0.36815000	1.16850800
C	0.96865000	-0.99202600	0.06081400
H	0.69026700	-1.98004800	-0.32581000
H	1.96233600	-0.73885900	-0.32862400
H	1.04142400	-1.06396000	1.16850400
BA			
C	-1.84250600	-1.23403300	0.00002200
C	-0.45009700	-1.20215200	-0.00001900
C	0.22086000	0.02863300	-0.00005300
C	-0.51367800	1.22209600	-0.00003300
C	-1.90426900	1.18548900	0.00000400
C	-2.56994600	-0.04252800	0.00003000
H	-2.36229300	-2.19052000	0.00004800
H	0.12305500	-2.12598800	-0.00002600
H	0.02858200	2.16551100	-0.00005300
H	-2.47175200	2.11442500	0.00001300
H	-3.65857600	-0.07103000	0.00005800
C	1.70267200	0.12356100	-0.00008400
O	2.33648300	1.16154800	0.00007000
O	2.31489300	-1.09583300	0.00001200
H	3.27175800	-0.90451600	0.00010400
PAA			
C	-2.28421400	-1.15641600	-0.18462500
C	-0.98461400	-1.21782000	0.31817600
C	-0.25407900	-0.04704100	0.54692400
C	-0.84565100	1.18856100	0.25749200
C	-2.14384900	1.25129500	-0.24645600
C	-2.86705300	0.07856200	-0.46853800
H	-2.84235500	-2.07610400	-0.35297700
H	-0.53139300	-2.18457800	0.53622800
H	-0.28051200	2.10509100	0.42425800
H	-2.59231300	2.21933700	-0.46411900
H	-3.88215800	0.12746600	-0.85905300
C	1.16748000	-0.10953200	1.07222600

H	1.34997100	-1.07776200	1.55078400
H	1.34211600	0.69014500	1.79952200
C	2.16025300	0.09113100	-0.05645500
O	2.62089000	1.15523300	-0.40743400
O	2.46451900	-1.08313400	-0.67458600
H	3.06374200	-0.85283100	-1.41094400

PA

C	0.03597800	2.74881600	-0.08870300
C	-0.93732000	1.76235600	-0.01763600
C	-0.60519700	0.39325900	0.00036000
C	0.76643000	0.01048500	-0.01499000
C	1.72336000	1.03354800	-0.06374800
C	1.37851100	2.37894000	-0.11720800
H	-0.25521200	3.79692800	-0.11807900
H	-1.98562100	2.04374800	0.01191200
H	2.76591500	0.72561600	-0.04391400
H	2.15975000	3.13516200	-0.17071500
C	1.41016300	-1.37940200	0.07496000
O	2.57575900	-1.47067300	0.40907300
O	0.70647400	-2.45916100	-0.25205900
H	-0.25941800	-2.23406000	-0.40734800
C	-1.75179200	-0.54959800	0.00459300
O	-1.73397000	-1.73505700	-0.32025500
O	-2.91742700	0.01811500	0.38224300
H	-3.59289900	-0.68360300	0.31036500

mPA

C	-0.00001600	2.30150000	-0.00002600
C	-1.20551700	1.60491100	-0.00010200
C	-1.20997900	0.20358500	-0.00017400
C	-0.00001500	-0.49799300	-0.00013100
C	1.20993000	0.20354400	0.00002200
C	1.20545000	1.60487300	0.00006900
H	0.00002800	3.38960900	-0.00003300
H	-2.16097300	2.12578000	-0.00011900
H	-0.00008500	-1.58372500	-0.00028800
H	2.16088700	2.12578300	0.00020500
C	2.52656000	-0.48816300	0.00004700
O	3.60449000	0.07340000	-0.00080100
O	2.41243100	-1.84530500	0.00112800
H	3.32714800	-2.18527500	0.00087700
C	-2.52650500	-0.48815300	0.00000900
O	-3.60451100	0.07331000	0.00104600

O	-2.41233200	-1.84534900	-0.00113500
H	-3.32707900	-2.18524500	-0.00081200
PTA			
C	-0.72259100	-1.19839100	0.00002600
C	-1.39599800	0.03161900	0.00012100
C	-0.66607100	1.22746000	0.00018100
C	0.72259300	1.19839400	0.00011100
C	1.39600000	-0.03161600	0.00001800
C	0.66607200	-1.22745900	-0.00000600
H	-1.29203900	-2.12423500	-0.00000500
H	-1.21024300	2.16952200	0.00028200
H	1.29203600	2.12424100	0.00014400
H	1.21024800	-2.16951700	-0.00005900
C	2.88115200	-0.12363400	-0.00003500
O	3.51230500	-1.16216300	-0.00026600
O	3.48629900	1.09655400	0.00010200
H	4.44512900	0.91436000	0.00002300
C	-2.88115200	0.12363200	0.00024500
O	-3.51230700	1.16216100	-0.00055200
O	-3.48630000	-1.09655600	0.00018700
H	-4.44513000	-0.91436300	-0.00011900
BA-SA			
C	4.38759400	1.12589000	0.08334200
C	3.00007900	1.20170900	0.00636000
C	2.23847300	0.02495800	-0.04205900
C	2.87672400	-1.22307400	-0.01412400
C	4.26362000	-1.29242500	0.06247900
C	5.01964600	-0.11890200	0.11117100
H	4.97836200	2.03913700	0.12141000
H	2.49789400	2.16552800	-0.01614000
H	2.26994500	-2.12487600	-0.05332700
H	4.75806600	-2.26171700	0.08366000
H	6.10543600	-0.17486900	0.17105100
C	0.76182600	0.06996400	-0.12308700
O	0.08372200	-0.97348400	-0.15257700
O	0.24462200	1.28422200	-0.15746000
H	-0.76212400	1.24916500	-0.19181900
S	-3.20548200	0.03662600	-0.06461000
O	-4.51335400	-0.04785900	-0.64446600
O	-2.39943800	1.23716100	-0.23642100
O	-3.33527700	-0.08811900	1.54126500
H	-4.04411000	-0.72997000	1.73478400

O	-2.38736700	-1.21294700	-0.47575800
H	-1.34679900	-1.06891600	-0.31702100

BA-H₂O

O	4.11599100	0.04714200	-0.07641000
H	4.65897700	-0.01145300	0.72348200
H	3.48038100	-0.71116400	-0.03044000
C	-2.49365700	1.22491300	0.00565700
C	-1.10112700	1.20538500	0.00036400
C	-0.41902000	-0.01909800	-0.00195800
C	-1.14255200	-1.21898400	0.00018200
C	-2.53364300	-1.19500900	0.00544100
C	-3.21046400	0.02686100	0.00825600
H	-3.02207100	2.17665800	0.00715000
H	-0.53365500	2.13267300	-0.00267600
H	-0.59336100	-2.15820800	-0.00304900
H	-3.09292700	-2.12891500	0.00680900
H	-4.29930600	0.04529300	0.01202800
C	1.06509700	-0.08576400	-0.00780200
O	1.68824100	-1.14911400	-0.01011800
O	1.66541000	1.11193200	-0.00904100
H	2.65702100	0.94561800	-0.00958600

BA-NH₃

N	4.23116300	-0.15749200	0.00000200
H	4.82183400	-0.26526000	0.82387300
H	3.85002100	0.79401400	-0.00034100
H	4.82209900	-0.26574000	-0.82361500
C	-2.47836300	-1.27848600	-0.00007100
C	-1.08711500	-1.20327400	-0.00005100
C	-0.45237200	0.04586200	0.00000300
C	-1.22382000	1.21477700	0.00003600
C	-2.61342200	1.13703400	0.00001700
C	-3.24253700	-0.11011600	-0.00003700
H	-2.96886300	-2.25059100	-0.00011300
H	-0.48187700	-2.10651900	-0.00007700
H	-0.70942300	2.17373900	0.00007800
H	-3.20896000	2.04853300	0.00004400
H	-4.32994200	-0.17144400	-0.00005200
C	1.03502400	0.17395100	0.00002300
O	1.60901500	1.26015700	0.00007600
O	1.67590900	-1.00082300	0.00000600
H	2.68321300	-0.80744800	0.00000400

BA-MA

N	3.70279100	-0.00729100	-0.42787900
H	4.22396600	-0.11667100	-1.29740800
H	3.31269900	0.94004600	-0.41638500
C	4.56415200	-0.24176100	0.74063900
H	3.96890200	-0.11413400	1.65139000
H	4.93101800	-1.27383700	0.72299500
H	5.43005800	0.43425700	0.79794500
C	-2.92905100	-1.33081400	0.06574600
C	-1.54710100	-1.20476600	-0.05987200
C	-0.95603100	0.06552800	-0.06665200
C	-1.76208000	1.20464600	0.05211900
C	-3.14236300	1.07644500	0.17703800
C	-3.72771800	-0.19186300	0.18435900
H	-3.38529300	-2.31948000	0.07112100
H	-0.91462700	-2.08430600	-0.15252100
H	-1.28139400	2.18092800	0.04471900
H	-3.76487600	1.96499200	0.26924700
H	-4.80773700	-0.29266300	0.28256800
C	0.52139800	0.24690200	-0.19384400
O	1.05564400	1.35436800	-0.18775600
O	1.19852700	-0.89848900	-0.31113900
H	2.20715100	-0.66103500	-0.38454200

BA-DMA

N	3.30553700	0.04925700	0.00008400
H	2.89088600	0.98649800	0.00046000
C	4.08310600	-0.15470800	-1.22358900
H	4.40517000	-1.20188600	-1.28126400
H	3.45515600	0.05963900	-2.09527200
H	4.98220900	0.48315700	-1.27054700
C	4.08307900	-0.15565900	1.22361100
H	3.45510600	0.05800600	2.09544500
H	4.40514200	-1.20288100	1.28047100
H	4.98217900	0.48217200	1.27108900
C	-3.31640900	-1.34774800	-0.00017900
C	-1.93024300	-1.20643700	-0.00021100
C	-1.35481400	0.07100800	-0.00003400
C	-2.18073600	1.20201400	0.00018000
C	-3.56517400	1.05863400	0.00021200
C	-4.13496800	-0.21677400	0.00003400
H	-3.76033900	-2.34203400	-0.00031700
H	-1.28181700	-2.07928300	-0.00037300
H	-1.71218300	2.18420700	0.00031600
H	-4.20329700	1.94091600	0.00037800

H	-5.21830000	-0.32923100	0.00006000
C	0.12643400	0.26787100	-0.00006100
O	0.64483400	1.38388900	0.00012100
O	0.82498500	-0.86893100	-0.00020500
H	1.84113000	-0.61294200	-0.00014800

BA-TMA

N	-3.14328300	0.16300500	-0.00003500
C	-3.98508000	1.36118800	-0.00062500
H	-3.76808800	1.96327200	0.88913500
H	-3.76769200	1.96267300	-0.89069300
H	-5.06151900	1.10947800	-0.00077900
C	-3.35527400	-0.64404500	-1.20757500
H	-3.16817600	-0.02917200	-2.09562700
H	-2.64807600	-1.48042200	-1.20332300
H	-4.38742700	-1.03529100	-1.26033600
C	-3.35584100	-0.64326200	1.20793300
H	-2.64855700	-1.47957000	1.20460900
H	-3.16926100	-0.02777700	2.09566800
H	-4.38799200	-1.03455400	1.26041800
C	3.56337200	1.40497200	-0.00001700
C	2.18190700	1.22165500	0.00007800
C	1.64457100	-0.07217500	0.00008400
C	2.50470500	-1.17741100	-0.00000600
C	3.88430100	-0.99242300	-0.00009900
C	4.41578700	0.29938600	-0.00010600
H	3.97697800	2.41228000	-0.00002000
H	1.50763000	2.07462000	0.00014900
H	2.06579500	-2.17321900	0.00000800
H	4.54858300	-1.85522500	-0.00016500
H	5.49526500	0.44424800	-0.00017900
C	0.16901200	-0.31725600	0.00019900
O	-0.31378500	-1.44609500	0.00007100
O	-0.56254900	0.79905200	0.00017700
H	-1.57855500	0.54018700	0.00020000

PAA-SA

C	4.33628900	0.08230700	1.37058200
C	3.36653600	-0.78855400	0.87437800
C	2.75765500	-0.54266500	-0.36080000
C	3.12806300	0.59415400	-1.08812500
C	4.09632900	1.46579900	-0.59180300
C	4.70293600	1.21173100	0.63863900
H	4.80617900	-0.12367100	2.33083200

H	3.07977000	-1.66794900	1.45040900
H	2.65398500	0.79720000	-2.04790200
H	4.37850500	2.34461500	-1.16923300
H	5.46084000	1.89104200	1.02494300
C	1.68567600	-1.47767800	-0.89363600
H	1.81361700	-2.48057500	-0.47357000
H	1.73571500	-1.53095200	-1.98603100
C	0.31696100	-0.95822000	-0.52221500
O	-0.28977700	-0.16004600	-1.25113000
O	-0.13147100	-1.40527500	0.63277100
H	-1.03365000	-1.01024900	0.85187700
S	-3.32127500	0.38925500	0.29597800
O	-4.27544800	1.33556200	0.79313300
O	-2.51141700	-0.39558500	1.21653800
O	-4.09803700	-0.73984600	-0.55971300
H	-4.82679600	-0.30291800	-1.03930100
O	-2.41088400	1.09074900	-0.74486200
H	-1.53417700	0.52964900	-0.93369400

PAA-H₂O

O	3.98174200	-0.03100200	-1.28016200
H	3.89789800	0.08926500	-2.23763200
H	3.48766700	0.72079400	-0.86750700
C	-2.68844400	-1.18058300	-0.51541400
C	-1.53150900	-1.20943100	0.26298900
C	-0.91213200	-0.02003400	0.66266500
C	-1.46807500	1.20050600	0.26121800
C	-2.62412600	1.23088500	-0.51780300
C	-3.23784200	0.04009500	-0.90814100
H	-3.16240400	-2.11457500	-0.81328900
H	-1.10382200	-2.16483800	0.56577700
H	-0.98946600	2.13200300	0.56206800
H	-3.04810400	2.18796200	-0.81779900
H	-4.14273100	0.06360800	-1.51313300
C	0.35712800	-0.04792800	1.49220600
H	0.41373200	-0.98016100	2.06453000
H	0.38025900	0.80236600	2.18142000
C	1.57643400	0.05930500	0.59762800
O	2.09417000	1.12966600	0.29175400
O	2.00640000	-1.12628300	0.15448300
H	2.77987300	-0.95236300	-0.46513300

PAA-NH₃

N	4.02964600	-0.65511500	-1.20080800
H	3.95096800	-1.08456500	-2.12208000
H	5.00540700	-0.71410300	-0.91157400
H	3.77887300	0.33481400	-1.28634700
C	-2.64480800	-1.35516600	-0.07586900
C	-1.50723500	-1.04946900	0.67085300
C	-0.94683500	0.23239400	0.62626200
C	-1.54516600	1.20131200	-0.18877400
C	-2.68195800	0.89749400	-0.93699900
C	-3.23607400	-0.38199500	-0.88207600
H	-3.07153000	-2.35588600	-0.02544600
H	-1.04516800	-1.81336200	1.29564800
H	-1.11132200	2.19965400	-0.23726600
H	-3.13769700	1.66382700	-1.56237400
H	-4.12634500	-0.61857100	-1.46264400
C	0.30333400	0.56053300	1.41554500
H	0.38022500	-0.09615700	2.28917200
H	0.27990800	1.60365300	1.74754000
C	1.54393800	0.38578200	0.54978900
O	2.03195700	1.29382800	-0.11025800
O	2.01416000	-0.86440100	0.57097200
H	2.80904900	-0.91423000	-0.07706900

PAA-MA

N	3.59414400	-0.61396900	-0.87960100
H	3.55524600	-1.28072100	-1.65013800
H	3.28156100	0.29315400	-1.23870900
C	4.95185700	-0.52581000	-0.32175100
H	4.95272800	0.20196600	0.49702900
H	5.23975100	-1.49749100	0.09420900
H	5.71427000	-0.22115100	-1.05375300
C	-2.98871000	-1.49510500	0.13739300
C	-1.89909400	-0.94868400	0.81433300
C	-1.48000500	0.36170200	0.55410900
C	-2.17215500	1.11140500	-0.40475700
C	-3.26221800	0.56677300	-1.08332000
C	-3.67440000	-0.73855200	-0.81394900
H	-3.30464800	-2.51427700	0.35562100
H	-1.36242200	-1.54425300	1.55226600
H	-1.85043100	2.12997300	-0.62019300
H	-3.79221700	1.16574600	-1.82253200
H	-4.52764100	-1.16318200	-1.34049900
C	-0.28044400	0.94763600	1.26820200
H	-0.19437300	0.51816300	2.27291300

H	-0.37887000	2.03502300	1.34648600
C	1.00066900	0.65830000	0.49521300
O	1.47454000	1.43626600	-0.32394300
O	1.52332700	-0.53309500	0.78837000
H	2.35210600	-0.67653900	0.17625000

PAA–DMA

N	-3.35700100	0.47022500	-0.19541300
H	-3.07728100	-0.09757700	-1.00106600
C	-3.31692400	1.89027900	-0.55191100
H	-3.47389900	2.49727000	0.34834500
H	-2.33161800	2.13465500	-0.96346000
H	-4.08781800	2.16695500	-1.29102400
C	-4.66191300	0.03266300	0.30357000
H	-4.63491000	-1.04399700	0.50397200
H	-4.88513800	0.55134200	1.24416700
H	-5.48226300	0.23989700	-0.40456400
C	3.19065200	1.17456100	1.02792800
C	2.20883300	0.20876000	1.24696700
C	1.83056400	-0.67047700	0.22533300
C	2.45304300	-0.55784000	-1.02400100
C	3.43498100	0.40751100	-1.24550000
C	3.80733100	1.27682500	-0.21968800
H	3.47661300	1.84738800	1.83518500
H	1.72561900	0.13502600	2.22078400
H	2.16133700	-1.23275700	-1.82819300
H	3.91234400	0.47829500	-2.22184000
H	4.57687300	2.02796200	-0.39063700
C	0.74370300	-1.70018700	0.45084900
H	0.71420100	-1.99023900	1.50734600
H	0.92677700	-2.58768700	-0.16332200
C	-0.61696600	-1.13975800	0.05316400
O	-1.10681200	-1.30864000	-1.05799800
O	-1.19078500	-0.43163900	1.02443400
H	-2.08087000	-0.02988600	0.64044000

PAA–TMA

N	3.19457400	0.49488500	0.13706800
C	3.84500300	1.62345500	-0.53239200
H	4.04752000	1.36470600	-1.57813300
H	3.18146800	2.49556400	-0.51141000
H	4.79979500	1.89610800	-0.04651000
C	2.84330500	0.82227200	1.52418800
H	2.20181600	1.71090600	1.53884100

H	2.28972000	-0.01791700	1.95678400
H	3.74196600	1.02454700	2.13469200
C	4.02381800	-0.71440600	0.08173500
H	3.46509800	-1.54726900	0.52205900
H	4.25024200	-0.95505100	-0.96349100
H	4.97566700	-0.58202700	0.62731900
C	-3.43356800	1.47855300	-0.61891300
C	-2.47103700	0.60865100	-1.13023700
C	-2.11696500	-0.55444600	-0.43598300
C	-2.74442500	-0.82453500	0.78654500
C	-3.70677400	0.04432000	1.30042300
C	-4.05498300	1.19904000	0.59870100
H	-3.70095700	2.37606300	-1.17501300
H	-1.98477700	0.83309100	-2.07921700
H	-2.47169100	-1.72359900	1.33863100
H	-4.18799700	-0.18366800	2.25047700
H	-4.80945900	1.87563400	0.99698700
C	-1.05180500	-1.48562600	-0.97366300
H	-1.00848800	-1.41480000	-2.06655700
H	-1.26931100	-2.51956500	-0.68718300
C	0.31602000	-1.13002300	-0.39868300
O	0.79155500	-1.68659000	0.58170100
O	0.91001200	-0.13892600	-1.06204000
H	1.81328600	0.10368600	-0.58536300

PA-SA

S	3.67499400	-0.10439700	-0.03843600
O	4.99557800	-0.15055700	-0.58557400
O	2.94203600	-1.32747400	0.24930400
O	3.70421800	0.65019900	1.38225300
H	4.34829600	1.38209300	1.32948300
O	2.80213100	0.82672000	-0.94104900
H	1.80671100	0.67950900	-0.74387800
C	-3.63592900	-2.28016100	-0.07605500
C	-2.28001100	-1.99047200	-0.02533200
C	-1.80650600	-0.66351100	-0.01913200
C	-2.74321700	0.40818100	-0.01442400
C	-4.10583400	0.07973000	-0.03498400
C	-4.55589300	-1.23434800	-0.08685500
H	-3.96811200	-3.31600600	-0.10164000
H	-1.55532800	-2.79910300	-0.00556500
H	-4.80981200	0.90708900	0.00764800
H	-5.62459700	-1.43798400	-0.12250100
C	-2.51341200	1.91707400	0.09438200

O	-3.39646100	2.62568800	0.53274900
O	-1.36557900	2.44335500	-0.33733100
H	-0.71649600	1.72688700	-0.57558800
C	-0.32782500	-0.52871400	-0.04452600
O	0.27103500	0.46540500	-0.51418800
O	0.32313400	-1.56755000	0.42881400
H	1.32245400	-1.44508600	0.34875800

PA-H₂O

C	-1.75408700	-2.45785300	-0.09014400
C	-0.44567700	-1.99941900	-0.02846100
C	-0.14165600	-0.62434700	-0.01028900
C	-1.20598900	0.32092100	-0.01293300
C	-2.51648900	-0.17629900	-0.04901400
C	-2.79822700	-1.53605200	-0.10543100
H	-1.95317800	-3.52728400	-0.12186600
H	0.37542800	-2.70979000	-0.00627400
H	-3.31778500	0.55784000	-0.01714900
H	-3.83266700	-1.87228100	-0.15057000
C	-1.16921800	1.84966800	0.08503900
O	-2.16134000	2.44672500	0.45661400
O	-0.07073100	2.50746500	-0.27776900
H	0.68464000	1.87128700	-0.46429400
C	1.30995900	-0.29434900	-0.01674000
O	1.79193700	0.78430900	-0.40415000
O	2.09721500	-1.27871100	0.39830500
H	3.05410000	-0.95969500	0.32311100
O	4.41047600	-0.05961600	-0.00684300
H	3.81775400	0.68310400	-0.24857700
H	4.95955300	0.26183600	0.72421000

PA-NH₃

C	-1.62788100	-2.53063600	-0.08311600
C	-0.35062800	-1.98902500	-0.03830400
C	-0.13184100	-0.59853800	-0.01984300
C	-1.25465500	0.27585100	-0.00718400
C	-2.53223100	-0.30335200	-0.02620300
C	-2.72914200	-1.67764800	-0.08086800
H	-1.75884900	-3.61076200	-0.11440200
H	0.51549700	-2.64414300	-0.02644400
H	-3.37688400	0.38010500	0.01575800
H	-3.74087900	-2.07865500	-0.11160500
C	-1.31262000	1.80514600	0.08167800
O	-2.34510400	2.34308000	0.43808800

O	-0.25188200	2.52344500	-0.27011500
H	0.54716200	1.92744200	-0.44643200
C	1.30298100	-0.17762700	-0.04156000
O	1.70384400	0.93747100	-0.41448800
O	2.15276700	-1.11473500	0.33910200
H	3.12420200	-0.73871100	0.26421200
N	4.55729100	-0.02468700	0.11373400
H	4.24623200	0.88816600	-0.22559800
H	5.20009200	-0.41378000	-0.57592000
H	5.08148800	0.12402200	0.97599400

PA-MA

C	-1.91208100	2.58390800	0.09956500
C	-0.66831700	1.98037600	-0.02541900
C	-0.51789300	0.58099600	-0.04265300
C	-1.67966600	-0.23765400	0.03227500
C	-2.92395800	0.40290600	0.13067400
C	-3.05070800	1.78551200	0.18159700
H	-1.98885800	3.66940600	0.12661700
H	0.22604900	2.59139200	-0.10501700
H	-3.80097000	-0.23945500	0.15457800
H	-4.03758400	2.23571400	0.27571700
C	-1.81706300	-1.76360500	-0.03056800
O	-2.89873000	-2.25444200	-0.29940600
O	-0.76800300	-2.52845800	0.24855900
H	0.07082500	-1.96880000	0.35517600
C	0.89544400	0.09318800	-0.11858200
O	1.26413900	-1.04257500	0.23225300
O	1.76119900	0.98205000	-0.55954800
H	2.73416800	0.54223900	-0.55842400
N	4.08701100	-0.19857200	-0.50167400
H	3.73444500	-1.15022600	-0.37755800
H	4.61784200	-0.18046300	-1.37278900
C	4.93269500	0.19301400	0.64101200
H	5.27440200	1.22376400	0.50155600
H	4.33059800	0.15547600	1.55474000
H	5.81044600	-0.45348300	0.77486000

PA-DMA

C	-2.29627800	-2.57359700	0.03052200
C	-1.03963100	-1.98395600	0.01804200
C	-0.87220900	-0.58718500	-0.02423300
C	-2.02659900	0.24483200	-0.01390400
C	-3.28200400	-0.38065500	0.02505900

C	-3.42869100	-1.76216300	0.03019100
H	-2.38741200	-3.65827200	0.04576800
H	-0.14815400	-2.60431600	0.03286700
H	-4.15018400	0.27293600	0.06373900
H	-4.42508300	-2.20088800	0.04383800
C	-2.13874600	1.77349500	0.01753900
O	-3.18329100	2.28788400	0.37536500
O	-1.11162300	2.51395600	-0.38207200
H	-0.29432200	1.93751300	-0.55497200
C	0.54940000	-0.11958200	-0.09798700
O	0.89235300	1.00032400	-0.52584700
O	1.44255500	-0.99963500	0.29118000
H	2.43616700	-0.56023000	0.17645100
N	3.73697400	0.13982800	-0.00188200
H	3.36197000	1.01779400	-0.36997000
C	4.59755100	-0.49260700	-1.01024000
H	4.89667200	-1.48630300	-0.65690800
H	4.03812300	-0.61112100	-1.94412000
H	5.50818100	0.09264600	-1.21188400
C	4.42189000	0.39138200	1.27331100
H	3.73730900	0.89978000	1.96019100
H	4.71402300	-0.56581000	1.72058000
H	5.32585800	1.00745900	1.14877900

PA-TMA

C	2.54358400	2.59104000	0.06433400
C	1.28888300	1.99695800	0.05219200
C	1.12647400	0.59925200	0.03917000
C	2.28373400	-0.22694500	-0.00352700
C	3.53731400	0.40337200	-0.01913300
C	3.67909800	1.78443000	0.03192100
H	2.63096800	3.67577400	0.09318700
H	-2.90690300	-1.83484600	-0.59941500
H	4.40767300	-0.24512300	-0.08491700
H	4.67382200	2.22709700	0.03594500
C	2.39827700	-1.75237400	-0.09384900
O	3.43866100	-2.25114400	-0.48460900
O	1.37767400	-2.50855400	0.29350300
H	0.56171500	-1.93913900	0.49725400
C	-0.29367300	0.12151700	0.09772800
O	-0.62853400	-1.00685000	0.50661900
O	-1.18770500	1.00295800	-0.28011800
H	-2.20335100	0.58380600	-0.18184200
N	-3.58226500	0.08474300	-0.08167900

C	-3.81197900	-0.25239700	1.33238600
H	-3.05529900	-0.97617300	1.65158900
H	-3.71646900	0.65232000	1.94303000
H	-4.81679600	-0.68001600	1.48437700
C	-4.50791800	1.12930700	-0.54127400
H	-4.38681700	2.02422300	0.07895800
H	-4.27899700	1.38894500	-1.58064000
H	-5.55744100	0.79558900	-0.48161900
C	-3.66676700	-1.11791400	-0.92627500
H	-3.47001200	-0.84518200	-1.96889600
H	0.39495800	2.61399600	0.06099100
H	-4.66412200	-1.58322800	-0.86142500

mPA-SA

C	-3.00849800	2.34445100	0.06198300
C	-3.96608800	1.33374400	0.07354400
C	-3.57470000	-0.01097500	0.02229100
C	-2.21798200	-0.33957300	-0.04044100
C	-1.25695100	0.67772600	-0.05266700
C	-1.65611000	2.02055400	-0.00124000
H	-3.31685400	3.38706100	0.10189000
H	-5.02917100	1.56125300	0.12226600
H	-1.90787400	-1.37950000	-0.08044000
H	-0.89254400	2.79514400	-0.01257100
C	0.19025000	0.36459700	-0.12316300
O	1.04382700	1.26836400	-0.12941600
O	0.47459700	-0.92221300	-0.17626900
H	1.47174600	-1.07223600	-0.20866500
C	-4.64267000	-1.04803600	0.03637300
O	-5.83310900	-0.81152900	0.09098400
O	-4.14898000	-2.31433400	-0.01931000
H	-4.92672300	-2.90378100	-0.00514400
S	4.09748800	-0.32993900	-0.06069800
O	5.39948200	-0.47944100	-0.63917000
O	3.08006100	-1.35253000	-0.25780100
O	4.23985900	-0.26211200	1.54629300
H	5.05824900	0.22671600	1.75456900
O	3.53074900	1.06128400	-0.44867000
H	2.48797500	1.10951400	-0.29394800

mPA-H₂O

O	4.88237300	-0.95321400	-0.07858800
H	5.39046900	-1.19019800	0.71127100
H	4.04296700	-1.47446100	-0.03060800

C	-0.95382000	2.35998000	0.00354200
C	0.35244700	1.87281700	0.00027700
C	0.58605000	0.49094100	-0.00215900
C	-0.49328000	-0.39790700	-0.00199000
C	-1.80139800	0.09185600	0.00169400
C	-2.02814300	1.47561900	0.00442600
H	-1.13283500	3.43334300	0.00496900
H	1.19837200	2.55583300	-0.00115200
H	-0.29762900	-1.46677500	-0.00523000
H	-3.05607500	1.83279400	0.00679500
C	-2.98516600	-0.80877400	0.00229400
O	-4.14137400	-0.43342500	0.00495700
O	-2.64712800	-2.12759900	-0.00024600
H	-3.49236600	-2.61526000	-0.00052900
C	1.96383200	-0.07173400	-0.00587900
O	2.18972800	-1.28176300	-0.01093900
O	2.92829300	0.85603100	-0.00215500
H	3.80882800	0.36770300	-0.00297600
mPA-NH ₃			
N	-5.07586500	-0.79546900	0.00011600
H	-5.67383000	-0.85698600	-0.82333300
H	-5.67305500	-0.85774200	0.82407200
H	-4.44532300	-1.60304000	-0.00055900
C	0.95073700	2.35045100	0.00015700
C	-0.34742400	1.84000300	0.00019000
C	-0.55960100	0.45533200	0.00008700
C	0.53534700	-0.41316900	-0.00005200
C	1.83603600	0.09805000	-0.00008400
C	2.04039200	1.48549600	0.00002100
H	1.11120800	3.42696900	0.00023800
H	-1.20609200	2.50712100	0.00029800
H	0.35463900	-1.48484100	-0.00013000
H	3.06208100	1.86011000	-0.00000900
C	3.03340200	-0.78244600	-0.00022400
O	4.18490200	-0.39056200	-0.00023700
O	2.71888000	-2.10795700	-0.00030300
H	3.57395300	-2.57799600	-0.00037900
C	-1.93373800	-0.13498000	0.00013400
O	-2.13285300	-1.34595900	-0.00000400
O	-2.90784100	0.77973100	0.00022500
H	-3.80813000	0.28024000	0.00017300

mPA-MA

N	-4.49475900	-0.61763200	-0.42496100
H	-4.94569000	-0.90445800	-1.29348200
H	-2.89431500	-0.80783600	-0.36352800
C	-5.25648000	-1.07994800	0.74592400
H	-4.74327800	-0.74983600	1.65555700
H	-6.29006900	-0.70588200	0.77768300
H	-5.28293900	-2.17490500	0.75460700
C	1.78260200	2.33867900	0.15471500
C	0.41800100	2.07842200	0.04709500
C	-0.04451400	0.76172000	-0.06819600
C	0.86991500	-0.29550000	-0.07538500
C	2.24064100	-0.03484100	0.03258600
C	2.69389700	1.28657700	0.14799200
H	2.13647300	3.36405600	0.24412700
H	-0.31495500	2.88295500	0.04980800
H	0.51033700	-1.31620100	-0.16486700
H	3.76451800	1.46265800	0.23128600
C	3.25562100	-1.11976300	0.03062500
O	4.45663100	-0.95031400	0.12276700
O	2.70768400	-2.36247900	-0.08702300
H	3.46293100	-2.98017900	-0.07605900
C	-1.51870900	0.52913100	-0.18105100
O	-1.85390400	-0.75583800	-0.28943000
O	-2.33096200	1.45142900	-0.17252600
H	-4.42112800	0.40379400	-0.43654200

mPA-DMA

N	-4.14637300	-0.34846700	0.00035000
H	-2.58449300	-0.60245700	0.00010600
C	-4.83500500	-0.76563100	-1.22376900
H	-4.29434000	-0.38230900	-2.09588500
H	-4.84601100	-1.86102300	-1.27987900
H	-5.87769400	-0.40902600	-1.26889700
C	-4.83465500	-0.76615900	1.22448400
H	-4.29373400	-0.38322400	2.09661100
H	-5.87732800	-0.40956200	1.27007400
H	-4.84565700	-1.86157500	1.28011500
C	2.27228300	2.32047500	0.00016000
C	0.89275200	2.12433400	0.00024100
C	0.36183300	0.82858700	0.00007400
C	1.22279100	-0.27260300	-0.00017400
C	2.60843000	-0.07645400	-0.00025200
C	3.13038800	1.22453000	-0.00008300

H	2.67927100	3.32991700	0.00029000
H	0.20005700	2.96381000	0.00043400
H	0.81011500	-1.27702600	-0.00030400
H	4.21130800	1.35025200	-0.00014800
C	3.56841500	-1.21020300	-0.00050700
O	4.77963000	-1.09778700	-0.00059100
O	2.95557400	-2.42804200	-0.00067300
H	3.67993200	-3.08175800	-0.00084000
C	-1.12627000	0.66369100	0.00017600
O	-1.52923700	-0.60437800	-0.00001200
O	-1.89154300	1.62670300	0.00042700
H	-4.01798100	0.66787700	0.00055400

mPA-TMA

N	4.11376200	-0.16666400	0.00024200
C	4.18495900	-0.99787900	1.20838000
H	4.10066100	-0.36070500	2.09622000
H	3.34800100	-1.70414200	1.20126900
H	5.13669100	-1.55587700	1.26271400
C	4.18514800	-0.99762600	-1.20805900
H	3.34818600	-1.70388700	-1.20123200
H	4.10099000	-0.36026200	-2.09577700
H	5.13688900	-1.55561300	-1.26236400
C	5.14839900	0.87118500	0.00043200
H	5.03733000	1.50115600	-0.88953500
H	5.03720000	1.50097100	0.89051500
H	6.16558700	0.43909700	0.00046100
C	-2.20153300	2.36861000	-0.00037100
C	-0.88441000	1.90867600	-0.00021800
C	-0.61736600	0.53359200	-0.00005000
C	-1.67819700	-0.37617900	-0.00003900
C	-2.99813500	0.08370900	-0.00019200
C	-3.25674100	1.46215500	-0.00035800
H	-2.40377900	3.43816500	-0.00050000
H	-0.05181900	2.60815500	-0.00022600
H	-1.45518000	-1.43988600	0.00009300
H	-4.29221000	1.79680200	-0.00047300
C	-4.16043400	-0.84198200	-0.00018400
O	-5.32656300	-0.49516000	-0.00030700
O	-3.79590600	-2.15489900	-0.00002300
H	-4.63297900	-2.65624500	-0.00003300
C	0.78122400	-0.00451800	0.00012500
O	1.02186100	-1.20764200	0.00025700
O	1.71813000	0.94211600	0.00009500

H	2.67044900	0.48513200	0.00020800
PTA-SA			
C	3.14901500	-1.18979800	-0.02190600
C	3.88710100	0.00141600	0.01951300
C	3.22502800	1.23604400	0.00584700
C	1.83854800	1.28389600	-0.04934500
C	1.10010400	0.09190100	-0.09023000
C	1.76171300	-1.14332200	-0.07655600
H	3.66674200	-2.14514400	-0.01151500
H	3.81906400	2.14669100	0.03884000
H	1.31873800	2.23824300	-0.06063200
H	1.17271700	-2.05682900	-0.10960100
C	-0.38235800	0.10702700	-0.14868800
O	-1.03646300	-0.94928900	-0.17198000
O	-0.91979700	1.31146000	-0.17065300
H	-1.92715900	1.25857100	-0.19449200
C	5.37567300	0.01249100	0.07892300
O	6.05792600	1.01652600	0.11862800
O	5.91268900	-1.23812600	0.08435300
H	6.87962600	-1.11096000	0.12356900
S	-4.34888900	0.00186700	-0.03987800
O	-3.55803700	1.20977000	-0.22795800
O	-5.66235900	-0.10186800	-0.60193800
O	-3.52133700	-1.24161300	-0.46086700
H	-2.48919300	-1.08248300	-0.31771000
O	-4.45201100	-0.12040700	1.56664000
H	-5.15214600	-0.76753000	1.77443100
PTA-H ₂ O			
O	-5.31481400	-0.05183900	-0.07591100
H	-4.70229700	0.72252200	-0.02368300
H	-5.87181500	-0.00707800	0.71533200
C	1.33493200	1.19568400	-0.00056500
C	2.01252300	-0.03203800	0.00126900
C	1.28657700	-1.23036500	0.00003300
C	-0.10217700	-1.20575500	-0.00264800
C	-0.77984700	0.02175000	-0.00356300
C	-0.05418400	1.21974800	-0.00297900
H	1.90113500	2.12338300	-0.00035300
H	1.83364900	-2.17070200	0.00082900
H	-0.67132000	-2.13171700	-0.00453100
H	-0.60015800	2.16057300	-0.00496900
C	-2.26740400	0.09380500	-0.00554000

O	-2.88207000	1.16058000	-0.00397900
O	-2.86782600	-1.10125900	-0.00805600
H	-3.86100900	-0.93435500	-0.00635300
C	3.49797200	-0.11871600	0.00414500
O	4.13289700	-1.15495300	0.00699500
O	4.09963600	1.10359700	0.00319800
H	5.05887100	0.92368000	0.00483800

PTA-NH₃

N	5.43587700	-0.22356700	0.00031500
H	6.01973100	-0.36780600	-0.82294300
H	6.01858300	-0.36756500	0.82443400
H	5.11649300	0.74970300	-0.00003000
C	0.10532300	-1.16629800	-0.00001700
C	0.75481200	0.07594200	0.00000800
C	-0.00074100	1.25479200	0.00001000
C	-1.38911800	1.19844500	-0.00001000
C	-2.03814300	-0.04498000	-0.00003400
C	-1.28273600	-1.22520500	-0.00003800
H	0.69840000	-2.07720500	-0.00001800
H	0.52522200	2.20714200	0.00002900
H	-1.97730600	2.11249800	-0.00000700
H	-1.80687500	-2.17860300	-0.00005700
C	-3.51946600	-0.16631900	-0.00005700
O	-4.13316900	-1.21602300	-0.00012500
O	-4.15182200	1.04188300	-0.00011100
H	-5.10558900	0.83559300	-0.00016500
C	2.24728600	0.18639400	0.00003500
O	2.82867600	1.26752500	-0.00004100
O	2.87032500	-0.99453600	-0.00005500
H	3.88482000	-0.81620600	-0.00017000

PTA-MA

N	4.92753100	-0.07230800	-0.35757000
H	5.45506100	-0.21410500	-1.21872900
H	4.60102600	0.89839900	-0.35196600
C	5.75497300	-0.36104300	0.82441200
H	5.15473900	-0.19837800	1.72609500
H	6.05789900	-1.41350500	0.80893900
H	6.65893600	0.26107700	0.89448000
C	-0.35235300	-1.12323500	-0.14863100
C	0.26479800	0.13520800	-0.12949200
C	-0.51910800	1.29138000	-0.03322500
C	-1.90325300	1.19658500	0.04420600

C	-2.51973700	-0.06326400	0.02612400
C	-1.73601400	-1.22095000	-0.07064800
H	0.26321500	-2.01594400	-0.22404700
H	-0.01797300	2.25695400	-0.02012000
H	-2.51336200	2.09304500	0.11895900
H	-2.23493700	-2.18771400	-0.08318100
C	-3.99459800	-0.22568700	0.10753900
O	-4.58103500	-1.29090300	0.09599200
O	-4.65656900	0.96330800	0.19967100
H	-5.60286200	0.72978500	0.24627900
C	1.75286100	0.28554300	-0.20738400
O	2.30422900	1.38330300	-0.17931100
O	2.40499800	-0.87218600	-0.30650500
H	3.42713800	-0.65885500	-0.34990600

PTA-DMA

N	-4.51368600	0.00109000	-0.00013000
H	-4.16279900	0.96361100	-0.00072700
C	-5.27779300	-0.25147600	1.22439500
H	-5.53286700	-1.31675400	1.28128100
H	-4.66488500	0.00222400	2.09606700
H	-6.21441700	0.32892400	1.26899400
C	-5.27793900	-0.25289000	-1.22426800
H	-4.66513900	-0.00018000	-2.09630200
H	-5.53300100	-1.31823600	-1.27989300
H	-6.21457600	0.32744600	-1.26941700
C	2.32673000	1.19681800	-0.00020300
C	2.92755600	-0.07073200	0.00000100
C	2.12705700	-1.22099100	0.00021100
C	0.74236500	-1.10819600	0.00021400
C	0.14086500	0.15793000	0.00001000
C	0.94152700	1.30658200	-0.00020000
H	2.94995700	2.08736900	-0.00036600
H	2.61396600	-2.19393600	0.00036500
H	0.11330800	-1.99471100	0.00037300
H	0.45241200	2.27837700	-0.00035900
C	-1.34803600	0.32372000	0.00000300
O	-1.88350600	1.43089000	-0.00020900
O	-2.01868300	-0.82556500	0.00018700
H	-3.04901300	-0.59263900	0.00010200
C	4.40270400	-0.24912400	0.00000200
O	4.97607600	-1.32152400	0.00019600
O	5.08186500	0.93385700	-0.00018200
H	6.02663500	0.68977800	-0.00014000

PTA-TMA

N	-4.30514600	0.23355100	-0.00003100
C	-4.56618400	-0.55857200	1.20852800
H	-3.91313300	-1.43777500	1.20422500
H	-4.34035000	0.04373000	2.09602800
H	-5.62046000	-0.88389300	1.26111900
C	-5.07360700	1.48137800	-0.00025200
H	-4.82061200	2.06891000	0.88966300
H	-4.82046200	2.06868800	-0.89027200
H	-6.16274000	1.29441200	-0.00032000
C	-4.56598100	-0.55887800	-1.20843500
H	-4.34001200	0.04320600	-2.09604900
H	-3.91292000	-1.43807100	-1.20380700
H	-5.62024500	-0.88422300	-1.26111400
C	2.66173300	-1.18953200	0.00018800
C	3.23952500	0.08870700	-0.00002700
C	2.41790700	1.22397100	-0.00018700
C	1.03548900	1.08547100	-0.00013100
C	0.45667000	-0.19119100	0.00008600
C	1.27874500	-1.32462200	0.00024600
H	3.30119900	-2.06852600	0.00031100
H	2.88668600	2.20581000	-0.00035500
H	0.39035000	1.96033800	-0.00025500
H	0.80727000	-2.30513900	0.00041300
C	-1.03002400	-0.38726300	0.00015200
O	-1.54332000	-1.50222200	0.00037800
O	-1.71953500	0.75080800	-0.00000600
H	-2.75421400	0.53075700	0.00007300
C	4.71092400	0.29426900	-0.00009400
O	5.26470200	1.37705700	-0.00034000
O	5.41219500	-0.87585600	-0.00000400
H	6.35213900	-0.61381500	-0.00011400