Supplementary Information

Sulfuric acid-dimethylamine particle formation enhanced by functional organic acids: an integrated experimental and theoretical study

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Table S1. Particulate and gas phase concentrations (ng·m^{-3} and ppbv, respectively) of pyruvic, succinic, and malic acids in different global regions.

Organics	Location	Sampling time	Size	Concentration (ng·m^{-3})	References
Pyruvic acid	[1]China, Beijing (urban)	2017 Winter	$PM_{2.5}$	37-405	Yu et al. (2021)
	[2]China, Chengdu (urban)	2012 Winter	$PM_{2.5}$	41.3-189	Li et al. (2015)
	[3]China, Mt. Tai (Mountainous)	2006 Late spring	TSP	3.0-140	Kawamura et al. (2013)
	[4]India, Raipur (urban)	2012-2013 Winter	$PM_{2.1}$	6.6-24.1	Deshmukh et al. (2016)
	[5]Canada, Alert (arctic)	1987-1988	TSP	0.0-0.5	Kawamura et al. (1996)
	[6]USA, Colorado (semi-rural)	2014 Summer	Gas-phase	BDL-0.51	Mattila et al. (2018)
Succinic acid	China, Beijing (urban)	2017 Winter	$PM_{2.5}$	42.5-132.5	Yu et al. (2021)
	China, Chengdu (urban)	2012 Winter	$PM_{2.5}$	197-636	Li et al. (2015)
	China, Mt. Tai (Mountainous)	2006 Late spring	TSP	7.0-829	Kawamura et al. (2013)
	India, Raipur (urban)	2012-2013 Winter	$PM_{2.1}$	77.4-175	Deshmukh et al. (2016)
	Canada, Alert (arctic)	1987-1988	TSP	0.5-18	Kawamura et al. (1996)
Malic acid	China, Beijing (urban)	2017 Winter	$PM_{2.5}$	4.4-117.6	Yu et al. (2021)
	China, Chengdu (urban)	2012 Winter	$PM_{2.5}$	7.5-18.5	Li et al. (2015)
	China, Mt. Tai (Mountainous)	2006 Late spring	TSP	0.0-43.9	Kawamura et al. (2013)
	India, Raipur (urban)	2012-2013 Winter	$PM_{2.1}$	0.9-3.8	Deshmukh et al. (2016)
	Canada, Alert (arctic)	1987-1988	TSP	0.0-0.6	Kawamura et al. (1996)

TSP = total suspended particles and BDL = below detection limit

Table S2. The functional groups, solubility, acidity, saturation vapor pressures (P_s^0) and enthalpies of vaporization (ΔH_{vap}) or sublimation (ΔH_{sub}) of three organic acids. The solubility and saturation vapor pressures were measured at 298 K.

Organic Compounds	Functional groups	Solubility (g L^{-1})	pK$_a$ [c]	P_s^0 (298K, Pa)	ΔH_{sub} (kJ mol^{-1})
Pyruvic acid	=O, -COOH	2.74 x 10^7 [a]	2.5	/	51.4 (ΔH_{vap})[e]
Succinic acid	-COOH, -COOH	71[b]	4.2, 5.6	7.7 x 10^{-5} [d]	115[d]
Malic acid	-OH, -COOH	590[b]	3.4, 5.2	6.4 x 10^{-5} [d]	81[d]

[a]data are obtained from reference 7[7]
[b]data are obtained from reference 8[8]
[c]data are obtained from reference 9[9]
[d]data are obtained from reference 10[10]
[e]data are obtained from reference 11[11]

Text S1. TFT system stability

Typical experiments are depicted in Fig. S1 where total particle number concentrations are plotted as a function of time. For increasing H_2SO_4 concentration in SA-W system (Fig. S1 (A)), the particle production started to be stable rapidly in one to several minutes depending on different condition. The particle changed a little after added

pyruvic acid into SA-DMA-W system shown in Fig. S1 (B), the particle production started to be highest and then decreased to be stable in several minutes for increasing H_2SO_4 concentration, and stabilized extremely quickly for decreasing H_2SO_4 concentration. Then, the stable particle production lasts for several minutes to be assessed and subsequently averaged to obtain one experimental point.

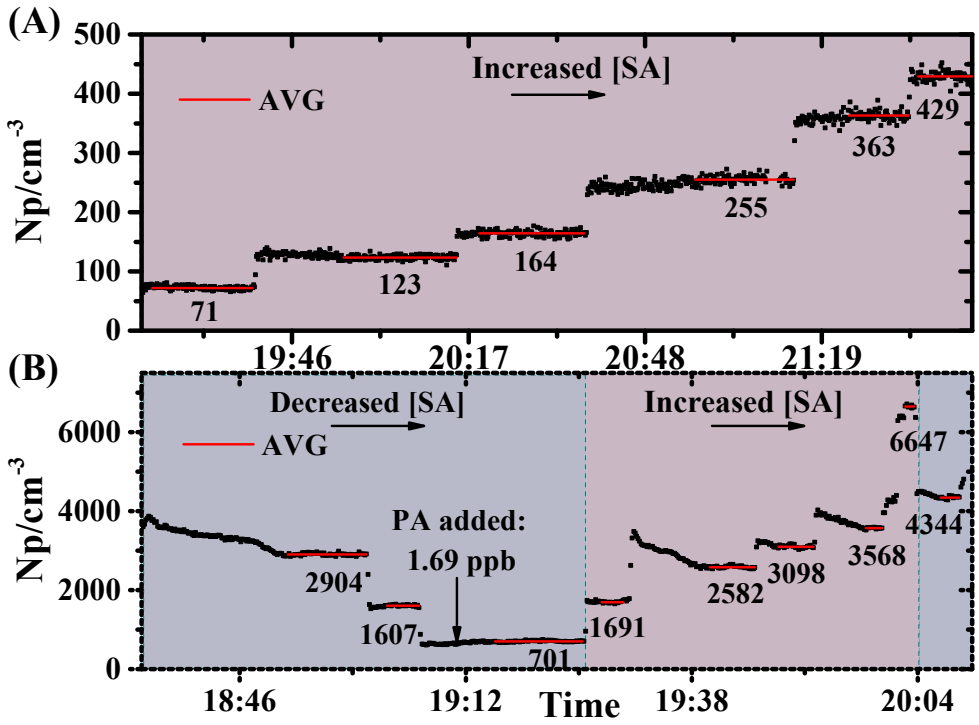

Figure S1. The particles number plotted versus time during the experiment at 283 K and 30% RH. (A) Changing sulfuric acid concentration ([SA]) to stability for sulfuric acid-water system. (B) Addition/changing acid concentration for sulfuric acid-dimethylamine-water system and pyruvic acid-added system.

Text S2. The concentration ratio of MA dimer to monomer

To evaluate the formation of gas-phase dicarboxylic acid dimer, the MA dimer

number concentration ([MA_2]) was computed from the monomer number concentration as $K\text{eq} \times [MA]^2$, with $K\text{eq} = (c_{ref})^{-1}\exp(-\Delta G_{dimer}/RT)$, where $c_{ref} = p^0/(k_bT)$ is the concentration of the reference vapor at which the ΔG_{dimer} is computed. Table S3 shows the concentration ratios at different MA monomer concentrations at 283 K and 1 atm.

Table S3. Concentration ratios between MA dimer and monomer at 283 K, calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6–311+G(2d,p) level of theory.

for 2MA⇔ $(MA)_2$		Percentage of $P_s^{283\,K}$ [a]	[MA] (molecule cm^{-3})	$[(MA)_2]/[MA]$
ΔG (kcal mol^{-1})	K_{eq} (cm^3 $molecule^{-1}$)			
-7.44	2.61×10^{-14}	10%	2.88×10^{8}	7.51×10^{-6}
		50%	1.44×10^{9}	3.76×10^{-5}
		100%	2.88×10^{9}	7.51×10^{-5}

[a]data are obtained from reference [10]

Table S4. Binding energies (ΔE), Gibbs free energy changes (ΔG), rate constants predicted with collision model (k), and permanent dipole moment (d) for dimers formation calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6–311+G(2d,p) level of theory and at 283 K.

X	ΔE (kcal mol^{-1})	ΔG (kcal mol^{-1})	k (10^{-10} cm^3 $molecule^{-1}$ s^{-1})	d of Product (debye)
SA + X ⇔ (SA)(X)				
SA	-17.74	-5.83	3.66	3.82
DMA	-23.83	-12.55	5.27	8.98
W	-12.68	-2.36	4.64	2.99
PA	-12.83	-1.40	4.78	2.13
MOA	-18.29	-7.29	5.14	4.90
SUA	-18.14	-6.48	6.45	4.13
MA	-23.46	-9.88	5.81	7.15
TA	-17.83	-7.56	5.45	3.96
GA	-24.04	-12.75	7.35	3.84
X + (DMA) ⇔ (X)(DMA)				
PA	-11.98	-1.70	6.71	4.27
MOA	-14.44	-3.20	7.28	3.83
SUA	-15.07	-2.47	9.12	1.80
MA	-15.89	-4.44	8.34	5.85
TA	-16.08	-5.13	7.92	4.28
GA	-20.67	-6.37	10.42	2.75

Text S3. Proton transfer and LBO analysis

According to the proton transfer parameter ρ_{PT} (Hunt et al., 2003; Kurnig and Scheiner, 1987), the degree of proton transfer in the hydrogen bond is discussed, and the degree of ionization is evaluated according to the distance between atoms. The formula is as follows:

$$\rho_{PT} = (r_{OH} - r_{OH}^{0}) - (r_{H...N} - r_{H...N}^{0}) \quad (1)$$

where, r_{OH} and r_{OH}^{0} are the O-H distance in OA or SA of cluster and in the free monomer, respectively. $r_{H...N}$ and $r_{H...N}^{0}$ are the hydrogen bond distances in the clusters and the H-N distances in fully protonated DMA, respectively. As shown in Table S5, the ρ_{PT} in $(SA)_2(DMA)$ and (OA)(SA)(DMA) clusters are positive indicting the cluster with protons completely transferred to dimethylamine. Thus, proton transfer converts the N-H hydrogen bonding to a covalent bond, leading to the formation of the dimethylamine bisulfate ion pair in the (OA)(SA)(DMA) clusters. The formation of N-H covalent bond was also confirmed by LBO values in (SA)(DMA) cluster and these with OA or SA addition, as depicted in Table S5. The LBO values of N-H covalent bond in all (OA)(SA)(DMA) clusters are higher than that of (SA)(DMA), which indicts addition of OA strengthens the preexisting covalent bonds.

Table S5. The proton-transfer parameter (ρ_{PT} in Å), the total number of proton transfers (N), and the Laplacian bond order (LBO in a.u.) of the newly formed nitrogen-hydrogen covalent bond in the clusters.

Clusters	r_{OH}	$r_{N\text{-}H}$	ρ_{PT}	LBO	N
(SA)(DMA)	**1.460**	**1.106**	**0.399**	**0.366**	**1(SA)**
$(SA)_2$(DMA)	**1.815**	**1.033**	**0.827**	**0.602**	**1(SA)**
(SA)(PA)(DMA)	**1.757**	**1.038**	**0.760**	**0.586**	**2(PA, SA)**
(SA)(MOA)(DMA)	**2.189**	**1.029**	**1.205**	**0.616**	**1 (MOA)**
(SA)(SUA)(DMA)	**1.534**	**1.078**	**0.502**	**0.445**	**1(SA)**
(SA)(MA)(DMA)	**1.694**	**1.045**	**0.694**	**0.555**	**2 (SA, MA)**
(SA)(TA)(DMA)	**1.780**	**1.035**	**0.845**	**0.592**	**2 (SA, TA)**
(SA)(GA)(DMA)	**1.859**	**1.037**	**0.867**	**0.588**	**1(SA)**

Table S6. Cartesian coordinates (in Å) of all optimized molecules and clusters.

Atmos	X	Y	Z
SA			
S	0.000029000000	0.000121000000	-0.158793000000
O	0.665675000000	-1.063976000000	-0.821141000000
O	-0.664876000000	1.065610000000	-0.819645000000
O	-1.022927000000	-0.686827000000	0.840425000000
O	1.022185000000	0.685212000000	0.842506000000
H	-1.688675000000	-0.033684000000	1.101085000000
H	1.687748000000	0.031588000000	1.102437000000
DMA			
C	-0.026944000000	-0.224033000000	1.204850000000
N	-0.026944000000	0.589628000000	0.000000000000
C	-0.026944000000	-0.224033000000	-1.204850000000
H	0.029053000000	0.416428000000	2.085079000000
H	0.798251000000	-0.950916000000	1.244120000000
H	-0.964643000000	-0.781658000000	1.257343000000
H	0.786622000000	1.193300000000	0.000000000000
H	0.029053000000	0.416428000000	-2.085079000000
H	-0.964643000000	-0.781658000000	-1.257343000000
H	0.798251000000	-0.950916000000	-1.244120000000
W			
O	0.000000000000	0.000000000000	0.116481000000
H	0.000000000000	0.763464000000	-0.465925000000
H	0.000000000000	-0.763464000000	-0.465925000000
$(SA)_2$			
S	1.976802000000	-0.002559000000	0.110418000000
O	1.061294000000	-0.203443000000	1.210679000000
O	3.364138000000	0.067395000000	0.347450000000
O	1.728382000000	-1.132276000000	-0.952924000000
O	1.555244000000	1.306897000000	-0.647537000000
H	0.775683000000	-1.180987000000	-1.158679000000
H	0.599400000000	1.276001000000	-0.843761000000
S	-1.938243000000	-0.075222000000	-0.107167000000
O	-0.885050000000	-0.072771000000	-1.094076000000
O	-3.252547000000	-0.491427000000	-0.425940000000
O	-1.465179000000	-0.870382000000	1.135265000000
O	-1.949758000000	1.426680000000	0.396294000000
H	-0.492708000000	-0.688314000000	1.281401000000
H	-2.751524000000	1.592425000000	0.915326000000
(SA)(W)			

136	S	0.578769000000	-0.068624000000	0.131227000000
137	O	-0.217148000000	0.364775000000	1.237408000000
138	O	1.756968000000	-0.846471000000	0.293285000000
139	O	-0.335934000000	-0.803571000000	-0.896046000000
140	O	0.967059000000	1.267019000000	-0.637732000000
141	H	-1.284378000000	-0.520738000000	-0.744751000000
142	H	1.716588000000	1.079572000000	-1.220927000000
143	O	-2.670846000000	0.094683000000	-0.117309000000
144	H	-2.295053000000	0.417331000000	0.714598000000
145	H	-3.398252000000	-0.489653000000	0.114596000000
146				
147	(SA)(DMA)			
148	S	-1.270827000000	-0.175350000000	0.059219000000
149	O	-0.574293000000	0.060312000000	1.311436000000
150	O	-2.501363000000	-0.908588000000	0.083311000000
151	O	-1.646239000000	1.326500000000	-0.421594000000
152	O	-0.315071000000	-0.657424000000	-0.976980000000
153	H	-2.400183000000	1.253070000000	-1.020699000000
154	H	1.015904000000	-0.428880000000	-0.422397000000
155	C	3.101826000000	-0.893366000000	-0.140133000000
156	N	1.893046000000	-0.115490000000	0.173602000000
157	C	2.036484000000	1.343056000000	-0.016366000000
158	H	2.897708000000	-1.949372000000	0.020683000000
159	H	3.928784000000	-0.573620000000	0.492727000000
160	H	3.359011000000	-0.729990000000	-1.184994000000
161	H	1.555128000000	-0.288073000000	1.123661000000
162	H	1.087641000000	1.808767000000	0.243133000000
163	H	2.267866000000	1.533239000000	-1.062749000000
164	H	2.835926000000	1.724345000000	0.617525000000
165				
166	$(SA)_2(DMA)$			
167	S	-2.233914000000	0.142064000000	0.046894000000
168	O	-1.231338000000	1.073994000000	-0.433576000000
169	O	-3.563691000000	0.585309000000	0.242929000000
170	O	-2.275451000000	-1.068536000000	-0.935564000000
171	O	-1.708527000000	-0.472004000000	1.379355000000
172	H	-1.363532000000	-1.450083000000	-1.014623000000
173	H	-0.709295000000	-0.580783000000	1.331263000000
174	S	1.320843000000	-1.307464000000	-0.121663000000
175	O	2.136531000000	-0.453845000000	-0.963999000000
176	O	0.232888000000	-2.014374000000	-0.778334000000
177	O	2.341151000000	-2.433188000000	0.357032000000
178	O	0.872953000000	-0.602870000000	1.094782000000
179	H	1.832069000000	-3.188031000000	0.683537000000
180	H	0.375858000000	1.631303000000	0.198658000000
181	C	1.133938000000	3.064510000000	-1.053858000000

182	N	1.310275000000	1.994828000000	-0.048772000000
183	C	2.055670000000	2.397152000000	1.162277000000
184	H	0.545809000000	2.664258000000	-1.875966000000
185	H	2.110996000000	3.389181000000	-1.405404000000
186	H	0.604698000000	3.897193000000	-0.595047000000
187	H	1.770693000000	1.164016000000	-0.479222000000
188	H	2.119167000000	1.533256000000	1.819253000000
189	H	1.525737000000	3.211095000000	1.653128000000
190	H	3.051232000000	2.725343000000	0.870637000000
191				
192	PA			
193	O	-0.981156000000	-1.455401000000	-0.000138000000
194	C	-0.762488000000	-0.282121000000	-0.000057000000
195	C	0.672955000000	0.290441000000	-0.000379000000
196	O	-1.700859000000	0.656315000000	0.000630000000
197	C	1.787026000000	-0.700225000000	0.000155000000
198	O	0.799395000000	1.488016000000	-0.000467000000
199	H	-1.251483000000	1.518725000000	0.000711000000
200	H	1.692453000000	-1.348109000000	0.873721000000
201	H	2.741983000000	-0.182354000000	0.000405000000
202	H	1.693049000000	-1.348281000000	-0.873351000000
203				
204	(PA)(SA)			
205	O	-1.005914000000	0.403154000000	1.610699000000
206	C	-1.486129000000	0.676222000000	0.539193000000
207	C	-2.322753000000	-0.329306000000	-0.282938000000
208	O	-1.348604000000	1.846977000000	-0.038944000000
209	C	-2.425936000000	-1.712904000000	0.254374000000
210	O	-2.817045000000	0.080939000000	-1.299843000000
211	H	-1.812655000000	1.804866000000	-0.895497000000
212	H	-1.421069000000	-2.140136000000	0.285030000000
213	H	-3.077092000000	-2.307531000000	-0.380046000000
214	H	-2.793568000000	-1.682214000000	1.281292000000
215	S	1.759457000000	-0.253000000000	-0.185414000000
216	O	2.982595000000	-0.924147000000	-0.445006000000
217	O	0.510544000000	-0.689656000000	-0.724520000000
218	O	1.643895000000	-0.116829000000	1.368753000000
219	O	1.888827000000	1.257361000000	-0.657499000000
220	H	0.727931000000	0.153188000000	1.616744000000
221	H	2.799663000000	1.553353000000	-0.51379200000037
222				
223	(PA)(DMA)			
224	O	-2.219403000000	1.607154000000	0.315401000000
225	C	-1.270789000000	0.893588000000	0.119877000000
226	C	-1.515711000000	-0.611130000000	-0.162854000000
227	O	-0.027902000000	1.293966000000	0.130454000000

228	C	-2.950482000000	-1.034470000000	-0.200581000000
229	O	-0.586614000000	-1.358606000000	-0.332849000000
230	H	0.701552000000	0.580811000000	-0.060577000000
231	H	-3.430668000000	-0.774274000000	0.743833000000
232	H	-3.012552000000	-2.102476000000	-0.391541000000
233	H	-3.473785000000	-0.467951000000	-0.972771000000
234	C	3.159155000000	0.604523000000	-0.673671000000
235	N	2.043719000000	-0.235963000000	-0.244526000000
236	C	2.302587000000	-0.903276000000	1.030525000000
237	H	2.933832000000	1.048053000000	-1.642677000000
238	H	4.100971000000	0.048830000000	-0.742353000000
239	H	3.286725000000	1.411978000000	0.048770000000
240	H	1.831704000000	-0.935734000000	-0.948180000000
241	H	1.457854000000	-1.546264000000	1.273045000000
242	H	2.401012000000	-0.145357000000	1.809595000000
243	H	3.220109000000	-1.501397000000	1.010712000000
244				
245	(PA)(SA)(DMA)			
246	O	1.486909000000	-1.099349000000	0.513036000000
247	C	2.051918000000	0.017289000000	0.155646000000
248	C	3.580391000000	-0.124543000000	-0.068395000000
249	O	1.500663000000	1.085335000000	-0.000941000000
250	C	4.174775000000	-1.490680000000	0.106115000000
251	O	4.200126000000	0.854570000000	-0.367140000000
252	H	-0.191819000000	1.551671000000	0.070740000000
253	H	3.981393000000	-1.850904000000	1.118046000000
254	H	5.242872000000	-1.444572000000	-0.088478000000
255	H	3.687481000000	-2.193807000000	-0.571791000000
256	S	-2.050258000000	-1.153576000000	-0.039337000000
257	O	-2.951852000000	-2.112751000000	0.525310000000
258	O	-2.671473000000	-0.033526000000	-0.747800000000
259	O	-0.997376000000	-0.645255000000	0.864408000000
260	O	-1.186706000000	-1.945264000000	-1.151594000000
261	H	0.485180000000	-0.978725000000	0.644110000000
262	H	-1.653238000000	-2.769701000000	-1.339546000000
263	C	-1.584338000000	2.441227000000	1.308045000000
264	N	-1.105756000000	2.032662000000	-0.029324000000
265	C	-0.960473000000	3.147273000000	-0.984728000000
266	H	-1.639612000000	1.550391000000	1.928887000000
267	H	-2.570033000000	2.891910000000	1.208391000000
268	H	-0.885646000000	3.159781000000	1.733093000000
269	H	-1.758900000000	1.296902000000	-0.402332000000
270	H	-0.598035000000	2.752441000000	-1.930758000000
271	H	-0.243255000000	3.864703000000	-0.590296000000
272	H	-1.927938000000	3.625013000000	-1.127734000000
273				

MOA

O	-1.590718000000	0.750797000000	0.887325000000
O	2.383996000000	-0.412451000000	0.268755000000
O	-1.966424000000	-0.551894000000	-0.893166000000
O	1.057428000000	1.113283000000	-0.690410000000
C	0.070631000000	-0.827405000000	0.346073000000
C	-1.268253000000	-0.218772000000	0.018734000000
C	1.190085000000	0.087102000000	-0.092305000000
H	0.166355000000	-1.002849000000	1.418453000000
H	0.171748000000	-1.778092000000	-0.175778000000
H	-2.428253000000	1.136242000000	0.592935000000
H	3.061111000000	0.201276000000	-0.050661000000

(MOA)(SA)

O	0.826071000000	-0.713930000000	1.222963000000
O	4.724225000000	0.316657000000	-0.065885000000
O	0.533749000000	-0.762892000000	-0.997858000000
O	2.802486000000	1.462622000000	0.019628000000
C	2.738665000000	-0.941236000000	-0.120652000000
C	1.245943000000	-0.797856000000	-0.010574000000
C	3.387549000000	0.422469000000	-0.043267000000
H	3.129064000000	-1.562161000000	0.685727000000
H	2.993967000000	-1.394732000000	-1.077680000000
H	-0.153542000000	-0.587379000000	1.253539000000
H	5.086876000000	1.213511000000	-0.025434000000
S	-2.605209000000	0.071637000000	0.057601000000
O	-4.013943000000	-0.077268000000	-0.017688000000
O	-1.860268000000	-0.445348000000	1.174529000000
O	-1.988649000000	-0.449690000000	-1.258412000000
O	-2.243896000000	1.617299000000	0.045391000000
H	-0.984138000000	-0.575882000000	-1.151493000000
H	-2.860022000000	2.080577000000	-0.540661000000

(MOA)(DMA)

O	-0.584620000000	0.907456000000	0.919104000000
O	3.077377000000	0.592306000000	-1.114014000000
O	0.192694000000	-0.490678000000	-0.644323000000
O	3.388120000000	-1.086706000000	0.328814000000
C	1.746999000000	0.593154000000	0.832829000000
C	0.372829000000	0.272756000000	0.275361000000
C	2.819573000000	-0.079298000000	0.020710000000
H	1.877220000000	1.675614000000	0.831525000000
H	1.796505000000	0.233331000000	1.859543000000
H	-1.484502000000	0.634370000000	0.492031000000
H	3.728576000000	0.075268000000	-1.608526000000
C	-2.868242000000	-1.357204000000	0.271463000000

320	N	-2.719026000000	-0.017231000000	-0.298865000000
321	C	-3.993159000000	0.685590000000	-0.424065000000
322	H	-1.892438000000	-1.841583000000	0.291417000000
323	H	-3.566809000000	-1.977386000000	-0.300479000000
324	H	-3.241572000000	-1.267696000000	1.292881000000
325	H	-2.272161000000	-0.105798000000	-1.207999000000
326	H	-3.834090000000	1.658754000000	-0.886944000000
327	H	-4.410933000000	0.843520000000	0.571185000000
328	H	-4.723181000000	0.123202000000	-1.017016000000
329				
330	(MOA)(SA)(DMA)			
331	O	4.553317000000	-0.611393000000	-0.151992000000
332	O	0.538190000000	-0.582781000000	1.111113000000
333	O	2.770425000000	0.701604000000	-0.334145000000
334	O	0.301696000000	-2.089006000000	-0.530086000000
335	C	2.480392000000	-1.631977000000	0.264428000000
336	C	3.238139000000	-0.386632000000	-0.098484000000
337	C	0.974030000000	-1.422765000000	0.274981000000
338	H	2.756869000000	-2.419802000000	-0.435489000000
339	H	2.810928000000	-1.934265000000	1.261151000000
340	H	4.985158000000	0.218620000000	-0.400928000000
341	H	1.009944000000	1.327952000000	0.152951000000
342	S	-2.531746000000	-0.367792000000	-0.157896000000
343	O	-3.940431000000	-0.218097000000	-0.079030000000
344	O	-1.797205000000	0.549844000000	-1.031220000000
345	O	-1.922179000000	-0.216217000000	1.265741000000
346	O	-2.179858000000	-1.805412000000	-0.573471000000
347	H	-0.894972000000	-0.430535000000	1.228925000000
348	H	-1.137291000000	-1.935580000000	-0.583849000000
349	C	-0.206313000000	2.591589000000	1.253003000000
350	N	0.217948000000	1.963231000000	-0.015936000000
351	C	0.576877000000	2.926118000000	-1.075732000000
352	H	-0.373335000000	1.808341000000	1.987418000000
353	H	-1.133600000000	3.134177000000	1.079199000000
354	H	0.571401000000	3.273097000000	1.593479000000
355	H	-0.568157000000	1.355977000000	-0.373356000000
356	H	0.864690000000	2.369365000000	-1.964040000000
357	H	1.409509000000	3.540322000000	-0.738291000000
358	H	-0.289246000000	3.548062000000	-1.293723000000
359				
360	SUA			
361	O	2.887412000000	-0.822922000000	0.001614000000
362	O	-2.887410000000	0.822922000000	0.001835000000
363	O	2.140057000000	1.282335000000	-0.002368000000
364	O	-2.140056000000	-1.282334000000	-0.002890000000
365	C	0.547525000000	-0.523651000000	0.000751000000

366	C	-0.547526000000	0.523650000000	0.001034000000
367	C	1.912757000000	0.104339000000	-0.000178000000
368	C	-1.912757000000	-0.104339000000	-0.000171000000
369	H	0.471032000000	-1.181315000000	-0.867748000000
370	H	0.471952000000	-1.181148000000	0.869435000000
371	H	-0.471047000000	1.181777000000	-0.867114000000
372	H	-0.471942000000	1.180684000000	0.870069000000
373	H	3.731880000000	-0.350637000000	0.000624000000
374	H	-3.731880000000	0.350639000000	0.000597000000
375				
376	(SUA)(SA)			
377	C	2.917273000000	-0.479860000000	-0.075836000000
378	C	2.144469000000	0.822701000000	-0.014859000000
379	C	4.395144000000	-0.242408000000	0.068676000000
380	C	0.664335000000	0.619200000000	-0.136860000000
381	H	2.743909000000	-1.006026000000	-1.016720000000
382	H	2.602148000000	-1.169908000000	0.709562000000
383	H	2.455432000000	1.510313000000	-0.804412000000
384	H	2.333850000000	1.355459000000	0.919731000000
385	H	6.027068000000	-1.163330000000	0.110382000000
386	H	-0.984671000000	1.560910000000	-0.177650000000
387	O	5.091608000000	-1.390222000000	0.010384000000
388	O	-0.017465000000	1.736458000000	-0.096762000000
389	O	4.915946000000	0.827525000000	0.219692000000
390	O	0.159781000000	-0.487679000000	-0.259647000000
391	S	-3.219813000000	-0.144083000000	-0.049407000000
392	O	-4.535618000000	-0.479857000000	-0.459670000000
393	O	-2.654423000000	1.146151000000	-0.337678000000
394	O	-3.128696000000	-0.252526000000	1.534403000000
395	O	-2.256440000000	-1.247816000000	-0.535104000000
396	H	-3.695772000000	-0.979250000000	1.831148000000
397	H	-1.289832000000	-0.936916000000	-0.433192000000
398				
399	(SUA)(DMA)			
400	C	2.737407000000	1.474606000000	-0.666647000000
401	N	3.176863000000	0.132745000000	-0.274258000000
402	C	3.461498000000	0.051982000000	1.160056000000
403	H	2.576451000000	1.505801000000	-1.743866000000
404	H	3.463268000000	2.246550000000	-0.387800000000
405	H	1.789501000000	1.680200000000	-0.168404000000
406	H	4.007316000000	-0.118695000000	-0.800227000000
407	H	3.828258000000	-0.944638000000	1.404893000000
408	H	2.529835000000	0.223914000000	1.699375000000
409	H	4.202102000000	0.794339000000	1.478242000000
410	C	-1.258461000000	-1.563934000000	-0.296965000000
411	C	-2.386063000000	-0.878516000000	0.447605000000

412	C	0.066854000000	-0.884343000000	-0.036158000000
413	C	-2.622673000000	0.512254000000	-0.078483000000
414	H	-1.431940000000	-1.561432000000	-1.373472000000
415	H	-1.162484000000	-2.607306000000	0.011478000000
416	H	-2.173753000000	-0.803721000000	1.514108000000
417	H	-3.324670000000	-1.428157000000	0.339833000000
418	H	1.901130000000	-0.822006000000	-0.596335000000
419	H	-3.528163000000	2.099575000000	0.326793000000
420	O	1.038854000000	-1.342081000000	-0.798163000000
421	O	-3.413600000000	1.231739000000	0.738840000000
422	O	0.209994000000	-0.020515000000	0.801993000000
423	O	-2.198531000000	0.947617000000	-1.112827000000
424				
425	(SUA)(SA)(DMA)			
426	C	-0.113872000000	1.922254000000	-1.740065000000
427	N	-0.106252000000	1.786573000000	-0.268478000000
428	C	0.322915000000	3.010418000000	0.434195000000
429	H	-0.478019000000	0.992074000000	-2.167953000000
430	H	0.897477000000	2.138959000000	-2.079946000000
431	H	-0.789317000000	2.732458000000	-2.008587000000
432	H	0.517343000000	1.016116000000	-0.009310000000
433	H	0.289337000000	2.828022000000	1.506099000000
434	H	-0.364885000000	3.815734000000	0.183534000000
435	H	1.334247000000	3.267247000000	0.124149000000
436	C	2.234117000000	-1.968135000000	-0.617916000000
437	C	3.226285000000	-1.392062000000	0.372140000000
438	C	0.820084000000	-1.516033000000	-0.345975000000
439	C	3.331127000000	0.105501000000	0.286829000000
440	H	2.240479000000	-3.059579000000	-0.569846000000
441	H	2.481529000000	-1.698281000000	-1.645279000000
442	H	4.225897000000	-1.803785000000	0.222399000000
443	H	2.938754000000	-1.627763000000	1.399502000000
444	H	-0.927743000000	-1.328070000000	-1.138364000000
445	H	4.315783000000	1.544615000000	0.981231000000
446	O	-0.006199000000	-1.772736000000	-1.311749000000
447	O	4.296205000000	0.582157000000	1.080043000000
448	O	0.511736000000	-0.953114000000	0.700052000000
449	O	2.649443000000	0.826754000000	-0.400940000000
450	S	-2.806863000000	-0.210913000000	0.271512000000
451	O	-2.089786000000	-0.448938000000	-1.009049000000
452	O	-2.379476000000	1.098156000000	0.804768000000
453	O	-4.211828000000	-0.435482000000	0.234705000000
454	O	-2.222776000000	-1.300845000000	1.277541000000
455	H	-1.078121000000	1.503031000000	0.100912000000
456	H	-1.251673000000	-1.191454000000	1.298402000000
457				

MA				
	O	0.358117000000	1.674494000000	-0.037114000000
	O	2.076528000000	-1.440064000000	0.346566000000
	O	-2.868724000000	-0.374513000000	-0.882334000000
	O	2.739355000000	0.542161000000	-0.453617000000
	O	-2.204875000000	0.179086000000	1.178118000000
	C	0.483263000000	0.326685000000	0.317546000000
	C	-0.551729000000	-0.506792000000	-0.427954000000
	C	1.886144000000	-0.157479000000	0.018896000000
	C	-1.938320000000	-0.177716000000	0.066668000000
	H	0.314891000000	0.204330000000	1.394144000000
	H	-0.390573000000	-1.572651000000	-0.246583000000
	H	-0.488085000000	-0.325128000000	-1.500817000000
	H	1.216963000000	1.973290000000	-0.365622000000
	H	2.995262000000	-1.664363000000	0.139309000000
	H	-3.727804000000	-0.172970000000	-0.484302000000
$(MA)_2$				
	O	-3.737435000000	-0.484269000000	-1.148023000000
	O	-1.377291000000	-1.556683000000	1.299851000000
	O	-1.651081000000	1.535801000000	-0.832320000000
	O	-1.289825000000	-1.586192000000	-0.938700000000
	O	-0.988068000000	1.870255000000	1.275167000000
	C	-3.210199000000	-0.625645000000	0.130887000000
	C	-3.054489000000	0.719202000000	0.882975000000
	C	-1.864430000000	-1.334188000000	0.098111000000
	C	-1.801487000000	1.449923000000	0.480306000000
	H	-3.902276000000	-1.245261000000	0.705474000000
	H	-3.013927000000	0.565075000000	1.958319000000
	H	-3.925959000000	1.325159000000	0.629057000000
	H	-3.025257000000	-0.205276000000	-1.738372000000
	H	-0.420697000000	-1.791503000000	1.225632000000
	H	-0.743412000000	1.867109000000	-1.037556000000
	O	3.737429000000	-0.484655000000	1.147936000000
	O	1.376960000000	-1.556575000000	-1.299836000000
	O	1.651412000000	1.535851000000	0.832352000000
	O	1.289575000000	-1.586054000000	0.938721000000
	O	0.988290000000	1.870239000000	-1.275111000000
	C	3.210100000000	-0.625905000000	-0.130947000000
	C	3.054619000000	0.719003000000	-0.882987000000
	C	1.864186000000	-1.334176000000	-0.098120000000
	C	1.801726000000	1.449881000000	-0.480276000000
	H	3.902016000000	-1.245647000000	-0.705590000000
	H	3.014024000000	0.564928000000	-1.958337000000
	H	3.926187000000	1.324802000000	-0.629036000000
	H	3.025304000000	-0.205670000000	1.738354000000

504	H	0.420326000000	-1.791257000000	-1.225585000000
505	H	0.743787000000	1.867228000000	1.037632000000
506				
507	(MA)(SA)			
508	S	2.556304000000	0.254958000000	0.029749000000
509	O	3.877986000000	0.752274000000	-0.005973000000
510	O	1.875659000000	0.059804000000	1.290030000000
511	O	1.666855000000	1.198926000000	-0.853669000000
512	O	2.542748000000	-1.098037000000	-0.752243000000
513	H	0.720879000000	1.145402000000	-0.606852000000
514	H	1.634077000000	-1.477903000000	-0.695593000000
515	O	-2.616828000000	-1.405847000000	-1.284021000000
516	O	-0.565242000000	-0.981539000000	1.593825000000
517	O	-2.981182000000	2.370404000000	-0.028227000000
518	O	-0.088248000000	-1.607675000000	-0.507744000000
519	O	-1.081044000000	1.262202000000	-0.357232000000
520	C	-2.366846000000	-1.235173000000	0.080177000000
521	C	-2.972516000000	0.081397000000	0.550943000000
522	C	-0.876902000000	-1.289681000000	0.359773000000
523	C	-2.234703000000	1.270970000000	-0.001027000000
524	H	-2.824815000000	-2.046919000000	0.659841000000
525	H	-2.937793000000	0.156805000000	1.640753000000
526	H	-4.016358000000	0.131711000000	0.243400000000
527	H	-1.785323000000	-1.658206000000	-1.708352000000
528	H	0.402755000000	-0.799281000000	1.650112000000
529	H	-2.434125000000	3.099876000000	-0.356454000000
530				
531	(MA)(DMA)			
532	O	-1.404276000000	1.704456000000	-0.697223000000
533	O	0.914338000000	-0.588440000000	0.754055000000
534	O	-4.084322000000	-1.156244000000	-0.585883000000
535	O	1.161442000000	1.074042000000	-0.722603000000
536	O	-3.672926000000	0.268360000000	1.083842000000
537	C	-1.018955000000	0.653766000000	0.145951000000
538	C	-1.819700000000	-0.598424000000	-0.183916000000
539	C	0.472334000000	0.395122000000	0.012407000000
540	C	-3.268557000000	-0.415540000000	0.187399000000
541	H	-1.213426000000	0.920968000000	1.191212000000
542	H	-1.444979000000	-1.449693000000	0.390567000000
543	H	-1.738932000000	-0.836031000000	-1.244842000000
544	H	-0.597916000000	2.022592000000	-1.127535000000
545	H	1.946099000000	-0.687364000000	0.626554000000
546	H	-4.985677000000	-1.006672000000	-0.266826000000
547	C	3.711393000000	-0.968470000000	-1.046888000000
548	N	3.492234000000	-0.742174000000	0.385219000000
549	C	4.028909000000	0.551461000000	0.820020000000

550	H	3.152545000000	-0.212201000000	-1.598419000000
551	H	3.335214000000	-1.952970000000	-1.323248000000
552	H	4.770272000000	-0.899371000000	-1.316691000000
553	H	3.932397000000	-1.486634000000	0.916650000000
554	H	3.480586000000	1.337691000000	0.300635000000
555	H	5.095703000000	0.651593000000	0.595583000000
556	H	3.875858000000	0.668422000000	1.892490000000
557				
558	(MA)(SA)(DMA)			
559	S	2.648490000000	-0.419342000000	-0.329015000000
560	O	2.338387000000	-0.204107000000	1.189527000000
561	O	4.033840000000	-0.197422000000	-0.539792000000
562	O	2.305657000000	-1.896178000000	-0.578163000000
563	O	1.696303000000	0.401382000000	-1.070383000000
564	H	1.273964000000	-2.055647000000	-0.439534000000
565	H	0.492588000000	1.233826000000	-0.217601000000
566	O	-2.432698000000	0.675475000000	1.402248000000
567	O	-3.510319000000	-0.836688000000	-1.636857000000
568	O	-0.141574000000	-0.677067000000	1.414050000000
569	O	-2.153592000000	0.903317000000	-1.299454000000
570	O	-0.136133000000	-2.235398000000	-0.194073000000
571	C	-2.928296000000	-0.371300000000	0.608055000000
572	C	-2.202144000000	-1.704127000000	0.864053000000
573	C	-2.807865000000	-0.007780000000	-0.864538000000
574	C	-0.699908000000	-1.546994000000	0.669795000000
575	H	-3.993170000000	-0.506980000000	0.815723000000
576	H	-2.584777000000	-2.474557000000	0.199176000000
577	H	-2.388121000000	-1.991211000000	1.900690000000
578	H	-1.590696000000	0.354678000000	1.776013000000
579	H	-3.347892000000	-0.597614000000	-2.561164000000
580	H	1.353861000000	-0.451054000000	1.345833000000
581	C	0.512081000000	2.509937000000	1.410966000000
582	N	-0.046163000000	2.064143000000	0.116726000000
583	C	0.053840000000	3.079066000000	-0.955975000000
584	H	1.574076000000	2.707646000000	1.279078000000
585	H	0.384001000000	1.715620000000	2.141797000000
586	H	-0.007800000000	3.410733000000	1.731634000000
587	H	-1.024397000000	1.760469000000	0.215729000000
588	H	1.107116000000	3.292717000000	-1.124858000000
589	H	-0.476384000000	3.978937000000	-0.650227000000
590	H	-0.390303000000	2.663582000000	-1.856090000000
591				
592	TA			
593	O	0.164037000000	1.468084000000	0.793542000000
594	O	-0.164215000000	-1.468158000000	0.793178000000
595	O	2.256164000000	-0.659849000000	-1.167300000000

596	O	-2.256037000000	0.660299000000	-1.167053000000
597	O	2.610841000000	0.399912000000	0.775928000000
598	O	-2.610781000000	-0.400335000000	0.775691000000
599	C	0.468021000000	0.610280000000	-0.263993000000
600	C	-0.467975000000	-0.610191000000	-0.264220000000
601	C	1.896236000000	0.118978000000	-0.143558000000
602	C	-1.896204000000	-0.118986000000	-0.143720000000
603	H	0.357324000000	1.140218000000	-1.215308000000
604	H	-0.357266000000	-1.139932000000	-1.215646000000
605	H	0.871731000000	1.388898000000	1.448484000000
606	H	-0.872440000000	-1.389644000000	1.447612000000
607	H	3.158944000000	-0.967702000000	-1.002217000000
608	H	-3.158832000000	0.968059000000	-1.001874000000
609				
610	(TA)(SA)			
611	O	2.241924000000	1.611742000000	-0.120935000000
612	O	2.194938000000	-0.751900000000	1.568094000000
613	O	4.545224000000	-1.063301000000	-0.656774000000
614	O	-0.040895000000	-0.571563000000	-1.191062000000
615	O	4.807990000000	0.983712000000	0.219125000000
616	O	-0.318857000000	-0.067524000000	0.977743000000
617	C	2.637908000000	0.342286000000	-0.546098000000
618	C	1.842954000000	-0.728709000000	0.221015000000
619	C	4.115558000000	0.141014000000	-0.277077000000
620	C	0.369590000000	-0.426551000000	0.039592000000
621	H	2.458766000000	0.221503000000	-1.620163000000
622	H	2.052475000000	-1.708548000000	-0.213965000000
623	H	3.014490000000	2.045404000000	0.268529000000
624	H	1.648340000000	-0.104697000000	2.032301000000
625	H	5.484447000000	-1.131013000000	-0.431599000000
626	H	-1.000894000000	-0.348884000000	-1.271792000000
627	S	-3.537270000000	0.159653000000	-0.145026000000
628	O	-4.777519000000	0.838204000000	-0.253269000000
629	O	-2.663389000000	0.018952000000	-1.278502000000
630	O	-2.752178000000	0.764534000000	1.040836000000
631	O	-3.801182000000	-1.336698000000	0.317630000000
632	H	-1.791139000000	0.443229000000	1.023335000000
633	H	-4.554679000000	-1.348947000000	0.926087000000
634				
635	(TA)(DMA)			
636	O	1.113008000000	-1.492222000000	-0.444891000000
637	O	1.410419000000	1.359041000000	-1.140931000000
638	O	3.610354000000	0.541167000000	1.099711000000
639	O	-1.089464000000	0.221345000000	1.127894000000
640	O	3.728250000000	-0.947796000000	-0.569877000000
641	O	-1.184482000000	0.888393000000	-1.009231000000

642	C	1.588500000000	-0.485708000000	0.400033000000
643	C	0.933329000000	0.866461000000	0.076374000000
644	C	3.087755000000	-0.343118000000	0.242837000000
645	C	-0.571391000000	0.661233000000	0.012167000000
646	H	1.361722000000	-0.745339000000	1.437685000000
647	H	1.159290000000	1.570495000000	0.883771000000
648	H	1.790551000000	-1.650742000000	-1.116409000000
649	H	0.662103000000	1.345425000000	-1.755801000000
650	H	4.554848000000	0.616413000000	0.902572000000
651	H	-2.102281000000	-0.000027000000	0.980506000000
652	C	-4.274192000000	0.754459000000	0.095954000000
653	N	-3.556804000000	-0.413563000000	0.615697000000
654	C	-3.399861000000	-1.458182000000	-0.402986000000
655	H	-4.409521000000	1.485267000000	0.892626000000
656	H	-5.252796000000	0.485726000000	-0.315181000000
657	H	-3.666561000000	1.202853000000	-0.690137000000
658	H	-4.056986000000	-0.792397000000	1.413459000000
659	H	-2.882356000000	-2.313718000000	0.029725000000
660	H	-2.787514000000	-1.055621000000	-1.210166000000
661	H	-4.362381000000	-1.783701000000	-0.810214000000
662				
663	(TA)(SA)(DMA)			
664	O	2.333570000000	-1.297011000000	1.472544000000
665	O	2.250533000000	1.230034000000	0.040466000000
666	O	-0.089407000000	-0.661177000000	-1.055375000000
667	O	4.594345000000	-1.277412000000	-0.906843000000
668	O	-0.237308000000	-0.942701000000	1.161491000000
669	O	4.785479000000	0.598763000000	0.305221000000
670	C	1.893771000000	-1.171541000000	0.151898000000
671	C	2.629418000000	-0.010787000000	-0.519859000000
672	C	0.386582000000	-0.915268000000	0.076742000000
673	C	4.121394000000	-0.178623000000	-0.322806000000
674	H	2.103230000000	-2.083092000000	-0.419868000000
675	H	2.395736000000	-0.010870000000	-1.586456000000
676	H	1.536852000000	-1.287071000000	2.023704000000
677	H	2.980018000000	1.509322000000	0.616112000000
678	H	-1.574799000000	-0.878906000000	-1.281346000000
679	H	5.537045000000	-1.347598000000	-0.697215000000
680	S	-3.312857000000	-0.565783000000	-0.091672000000
681	O	-4.703830000000	-0.790913000000	-0.239321000000
682	O	-2.586650000000	-1.032820000000	-1.380950000000
683	O	-2.846614000000	0.777829000000	0.217781000000
684	O	-2.766984000000	-1.513440000000	1.017115000000
685	H	-1.099132000000	1.191393000000	0.263835000000
686	H	-1.787897000000	-1.305960000000	1.158660000000
687	C	-0.667105000000	2.476784000000	-1.258602000000

688	N	-0.481655000000	2.012010000000	0.135693000000
689	C	-0.869268000000	3.012446000000	1.153305000000
690	H	-0.350318000000	1.675492000000	-1.921956000000
691	H	-0.067033000000	3.370530000000	-1.418404000000
692	H	-1.724271000000	2.686513000000	-1.406776000000
693	H	0.496470000000	1.709193000000	0.260478000000
694	H	-0.702802000000	2.588400000000	2.140675000000
695	H	-1.927122000000	3.231203000000	1.024300000000
696	H	-0.272506000000	3.912616000000	1.020068000000
697				
698	GA			
699	O	3.612207000000	-0.668743000000	-0.000825000000
700	O	-3.612208000000	-0.668744000000	0.000334000000
701	O	2.575672000000	1.306993000000	0.000870000000
702	O	-2.575677000000	1.306992000000	-0.000729000000
703	C	0.000002000000	0.153787000000	-0.000166000000
704	C	1.252422000000	-0.706326000000	0.000239000000
705	C	-1.252418000000	-0.706323000000	0.000282000000
706	C	2.515502000000	0.112119000000	0.000113000000
707	C	-2.515502000000	0.112119000000	-0.000122000000
708	H	-0.000041000000	0.809823000000	-0.869194000000
709	H	0.000049000000	0.810670000000	0.868218000000
710	H	1.289024000000	-1.363740000000	0.871766000000
711	H	1.289188000000	-1.364589000000	-0.870615000000
712	H	-1.289078000000	-1.363746000000	0.871787000000
713	H	-1.289129000000	-1.364584000000	-0.870590000000
714	H	4.380929000000	-0.084042000000	-0.000629000000
715	H	-4.380933000000	-0.084045000000	-0.000035000000
716				
717	(GA)(SA)			
718	O	-0.656223000000	2.115748000000	-0.668822000000
719	O	4.286935000000	-2.002511000000	-0.769421000000
720	O	0.030471000000	0.401616000000	0.584544000000
721	O	4.820376000000	-0.661209000000	0.931928000000
722	C	2.739409000000	1.146044000000	0.404686000000
723	C	1.627796000000	2.044734000000	-0.113127000000
724	C	2.963452000000	-0.069451000000	-0.481277000000
725	C	0.257908000000	1.431032000000	-0.032794000000
726	C	4.117058000000	-0.909370000000	-0.004604000000
727	H	2.509564000000	0.817139000000	1.416827000000
728	H	3.662411000000	1.720339000000	0.464529000000
729	H	1.573734000000	2.970691000000	0.463566000000
730	H	1.792279000000	2.347850000000	-1.148206000000
731	H	3.177222000000	0.220293000000	-1.513036000000
732	H	2.079700000000	-0.707515000000	-0.516512000000
733	H	-1.541217000000	1.685318000000	-0.596137000000

734	H	5.041640000000	-2.488253000000	-0.412744000000
735	S	-3.229186000000	-0.458521000000	0.080913000000
736	O	-4.490633000000	-0.826448000000	0.598434000000
737	O	-3.013401000000	0.850348000000	-0.456010000000
738	O	-2.157331000000	-0.761459000000	1.131668000000
739	O	-2.866015000000	-1.426854000000	-1.110909000000
740	H	-1.277032000000	-0.293309000000	0.908243000000
741	H	-3.218492000000	-2.307999000000	-0.929737000000
742				
743	(GA)(DMA)			
744	O	-5.335183000000	-0.305235000000	0.103364000000
745	O	1.827838000000	-1.247086000000	0.234569000000
746	O	-4.046386000000	1.470403000000	-0.296951000000
747	O	1.038455000000	0.739468000000	-0.404405000000
748	C	-1.642703000000	-0.000368000000	-0.042846000000
749	C	-3.000641000000	-0.659273000000	0.129933000000
750	C	-0.517421000000	-0.999377000000	0.165066000000
751	C	-4.142664000000	0.303518000000	-0.049714000000
752	C	0.852630000000	-0.395910000000	-0.034032000000
753	H	-1.540682000000	0.826004000000	0.659133000000
754	H	-1.566801000000	0.442640000000	-1.034538000000
755	H	-3.145973000000	-1.473728000000	-0.583321000000
756	H	-3.108081000000	-1.109681000000	1.119454000000
757	H	-0.599796000000	-1.841353000000	-0.526685000000
758	H	-0.544831000000	-1.434726000000	1.166036000000
759	H	-6.016698000000	0.366992000000	-0.024619000000
760	H	2.712986000000	-0.779637000000	0.058231000000
761	C	4.037838000000	1.105349000000	0.947107000000
762	N	3.991680000000	0.241656000000	-0.229870000000
763	C	5.304795000000	-0.261423000000	-0.611865000000
764	H	3.041045000000	1.499070000000	1.133133000000
765	H	4.737338000000	1.938279000000	0.826043000000
766	H	4.352155000000	0.516273000000	1.808421000000
767	H	3.569801000000	0.759554000000	-0.993490000000
768	H	5.223862000000	-0.856469000000	-1.518684000000
769	H	5.684657000000	-0.901696000000	0.183452000000
770	H	6.030461000000	0.541392000000	-0.777982000000
771				
772	(GA)(SA)(DMA)			
773	C	2.497922000000	-0.573450000000	-1.499054000000
774	C	3.176320000000	-1.081179000000	-0.218490000000
775	C	2.257316000000	-1.910291000000	0.671605000000
776	C	1.729057000000	0.718960000000	-1.322624000000
777	C	1.194450000000	-1.088935000000	1.345216000000
778	O	0.434489000000	0.706220000000	-1.614685000000
779	O	2.250295000000	1.754722000000	-0.975594000000

780	O	0.271574000000	-1.820609000000	1.953445000000
781	O	1.183837000000	0.121797000000	1.347383000000
782	H	3.266687000000	-0.342171000000	-2.240008000000
783	H	1.849749000000	-1.343734000000	-1.921563000000
784	H	4.022608000000	-1.705913000000	-0.506819000000
785	H	3.573288000000	-0.229053000000	0.336233000000
786	H	1.749116000000	-2.698177000000	0.110038000000
787	H	2.823947000000	-2.409863000000	1.462991000000
788	H	0.021146000000	-0.204201000000	-1.512719000000
789	H	-0.486889000000	-1.237551000000	2.139424000000
790	S	-1.989183000000	-0.992745000000	-0.253692000000
791	O	-2.949199000000	-2.028598000000	-0.017012000000
792	O	-0.763464000000	-1.446836000000	-0.933602000000
793	O	-2.667003000000	0.055336000000	-1.295082000000
794	O	-1.694409000000	-0.108582000000	0.877395000000
795	H	-3.164374000000	-0.464125000000	-1.940765000000
796	H	-0.480930000000	1.278641000000	0.634901000000
797	C	-1.334381000000	2.905685000000	-0.267545000000
798	N	-0.260929000000	2.287256000000	0.541330000000
799	C	-0.125670000000	2.855452000000	1.898030000000
800	H	-1.336698000000	2.430936000000	-1.244608000000
801	H	-1.147929000000	3.974644000000	-0.352872000000
802	H	-2.283814000000	2.718214000000	0.229764000000
803	H	0.640831000000	2.326828000000	0.039795000000
804	H	0.677715000000	2.329937000000	2.406701000000
805	H	-1.065037000000	2.705261000000	2.426844000000
806	H	0.094955000000	3.918391000000	1.821627000000

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