

Supplementary Information

Aliphatic Tertiary Amine Catalysed Urethane Formation – A Combined Experimental and Theoretical Study

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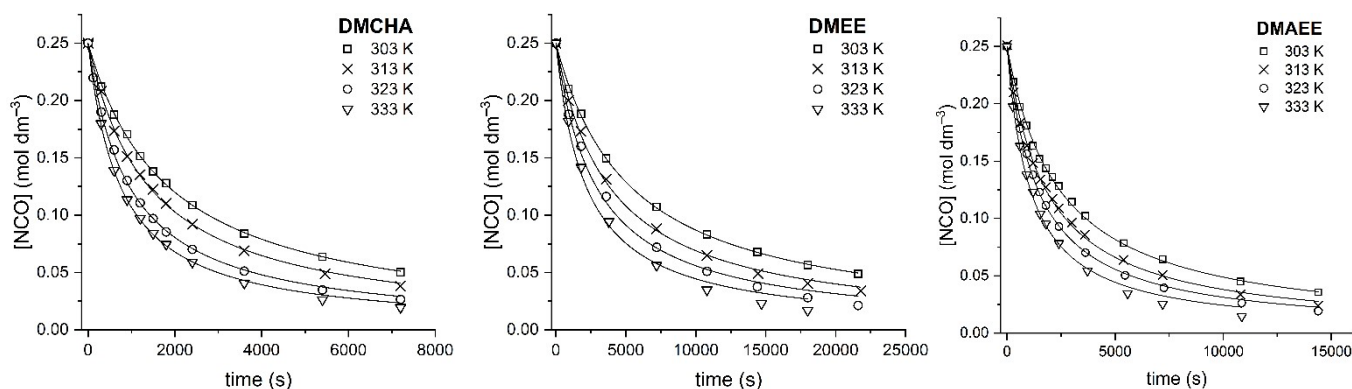
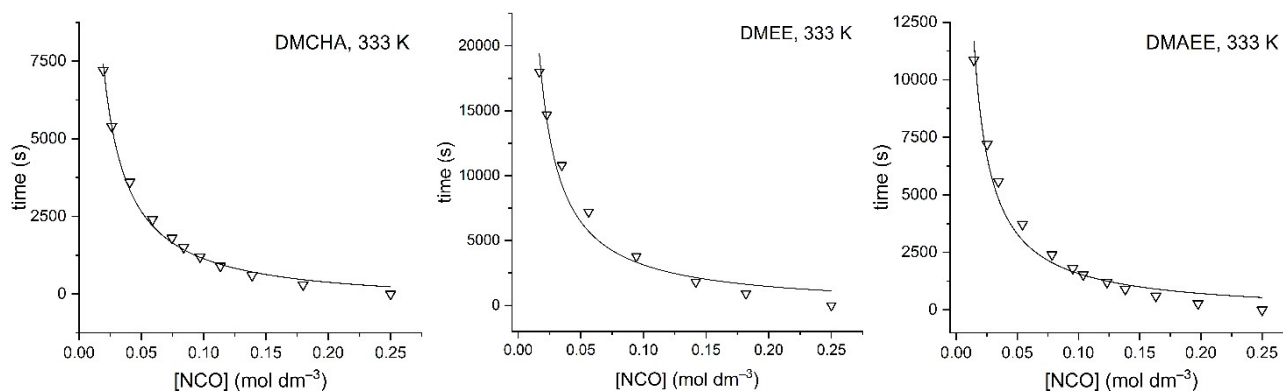


Figure S1. Second-order kinetic curves fitted using nonlinear regression.



$$\frac{d[NCO]}{dt} = k_1[NCO]^2 + k_2[NCO]^2[NCO_0 - NCO]$$

Figure S2. Experimental kinetic data points at 333 K fitted with the above rate equation (autocatalytic effect considered).

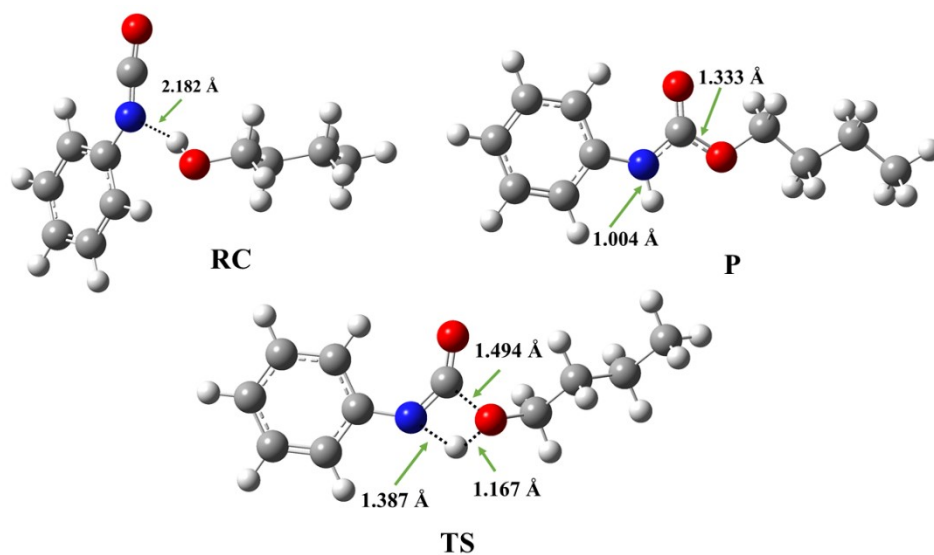


Figure S3. 3D structures of the reactant complex (**RC**), transition state (**TS**), and product (**P**) in the catalyst-free urethane formation. The structures have been optimized at the BHandHLYP/6-31G(d) level of theory in acetonitrile at 298.15 K and 1 atm.

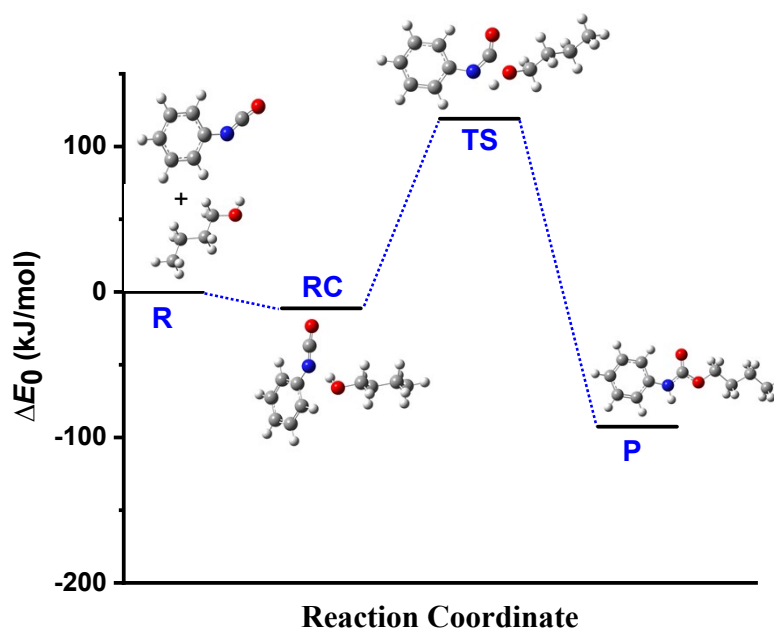


Figure S4. Energy profile (zero-point corrected) of the phenyl isocyanate (PhNCO) and butan-1-ol reaction calculated at the G3MP2BHandHLYP composite method in acetonitrile using the SMD implicit solvent model at 298.15 K and 1 atm.

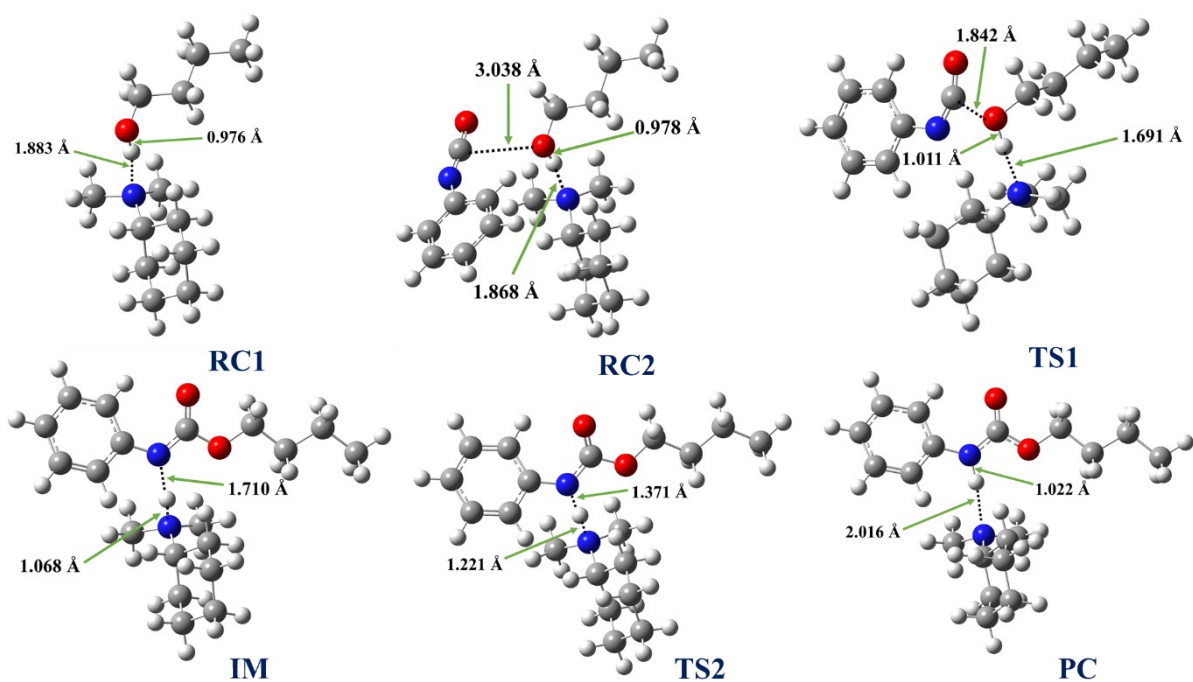


Figure S5. Optimized structures along the reaction pathway between phenyl isocyanate (PhNCO) and butan-1-ol in the presence of DMCHA calculated at the BHandHLYP/6-31G(d) level of theory in acetonitrile at 298.15 K and 1 atm. RC – reactant complex, TS – transition state, IM – intermediate, PC – product complex.

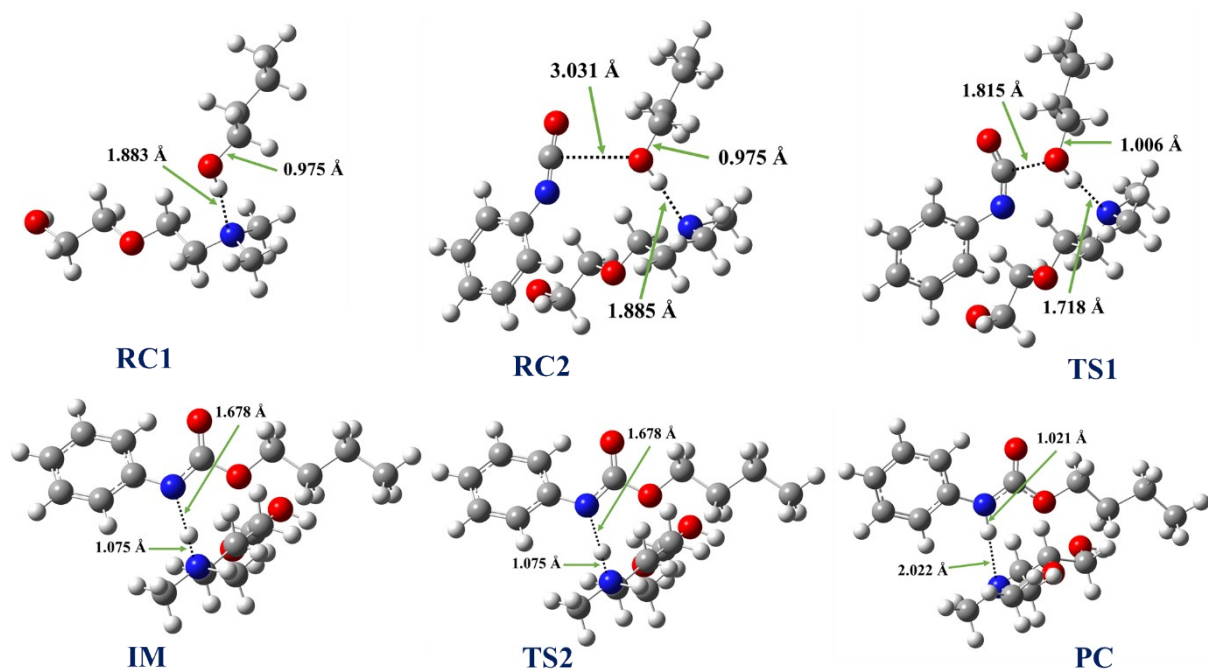


Figure S6. Optimized structures along the reaction pathway between phenyl isocyanate (PhNCO) and butan-1-ol in the presence of DMEE calculated at the BHandHLYP/6-31G(d) level of theory in acetonitrile at 298.15 K and 1 atm. RC – reactant complex, TS – transition state, IM – intermediate, PC – product complex.

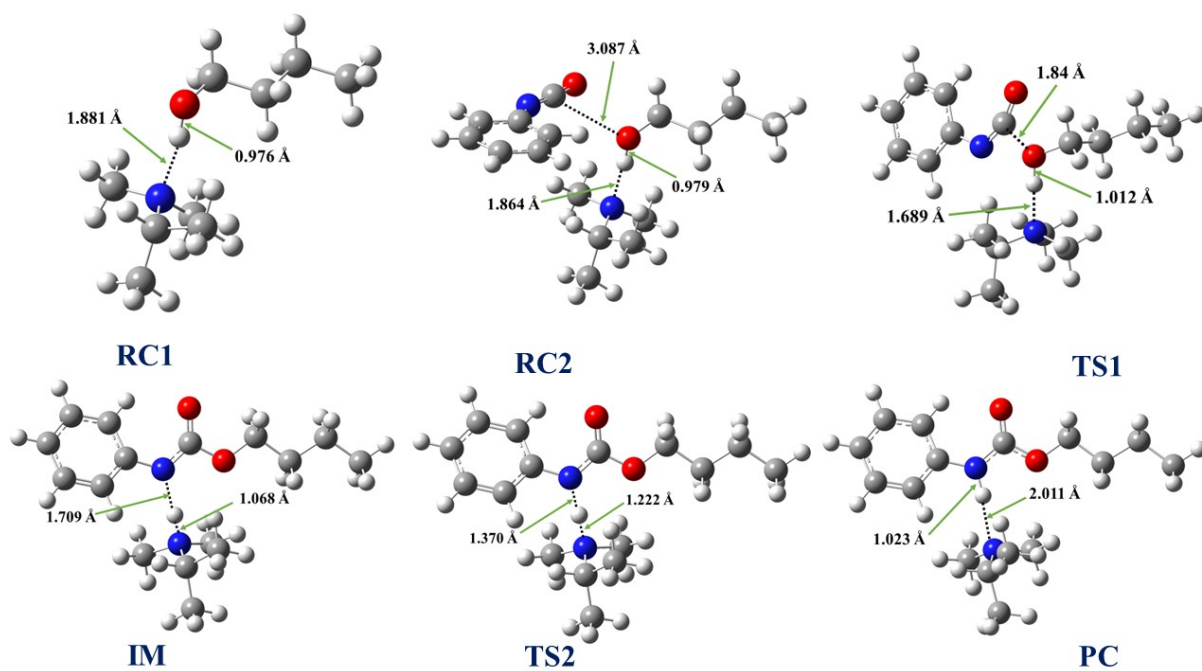


Figure S7. Optimized structures along the reaction pathway between phenyl isocyanate (PhNCO) and butan-1-ol in the presence of DMIPA calculated at the BHandHLYP/6-31G(d) level of theory in acetonitrile at 298.15 K and 1 atm. RC – reactant complex, TS – transition state, IM – intermediate, PC – product complex.

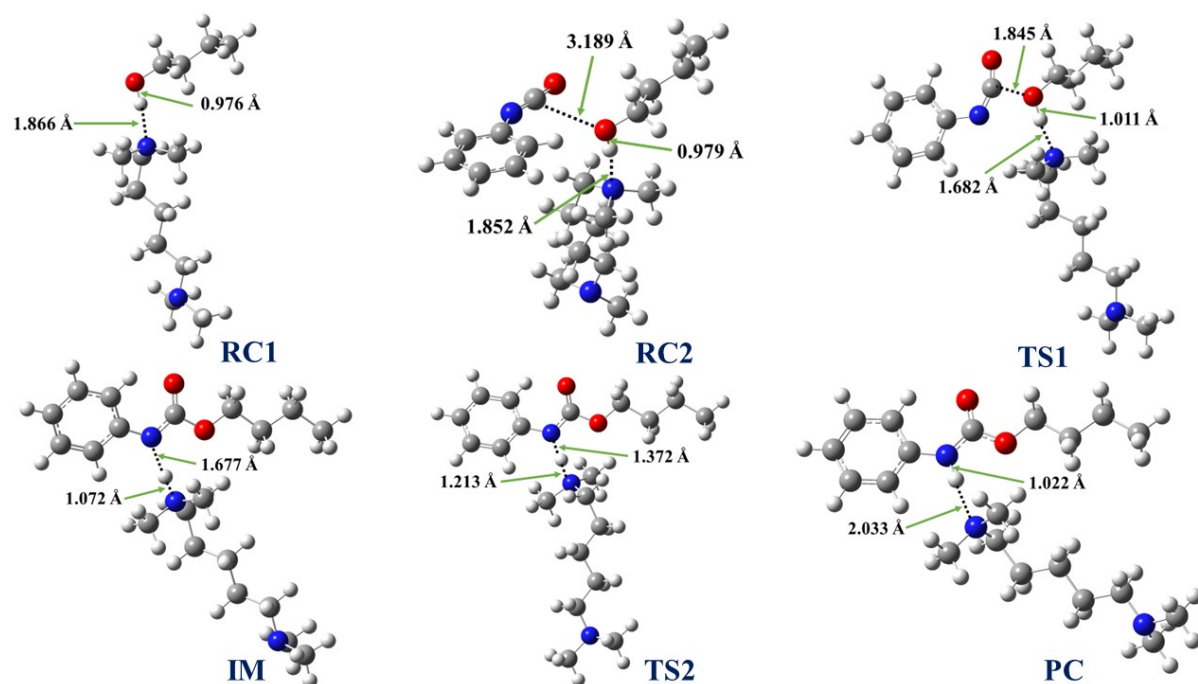


Figure S8. Optimized structures along the reaction pathway between phenyl isocyanate (PhNCO) and butan-1-ol in the presence of TMPD calculated at the BHandHLYP/6-31G(d) level of theory in acetonitrile at 298.15 K and 1 atm. RC – reactant complex, TS – transition state, IM – intermediate, PC – product complex.

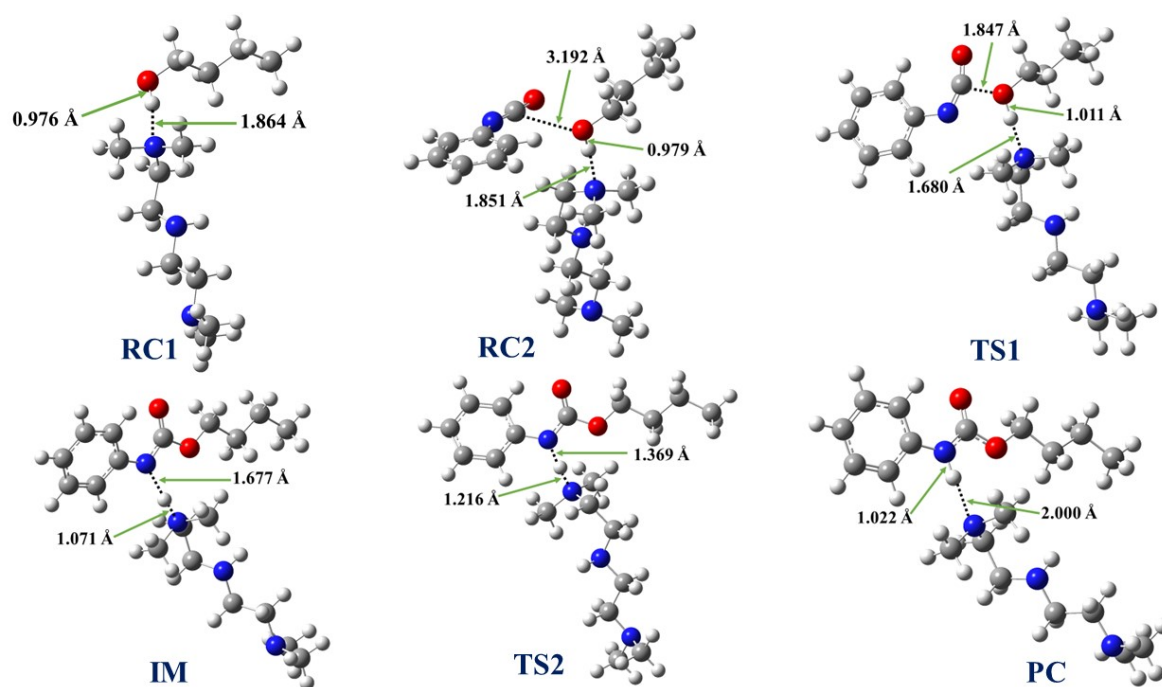


Figure S9. Optimized structures along the reaction pathway between phenyl isocyanate (PhNCO) and butan-1-ol in the presence of DMAEDMED calculated at the BHandHLYP/6-31G(d) level of theory in acetonitrile at 298.15 K and 1 atm. RC – reactant complex, TS – transition state, IM – intermediate, PC – product complex.

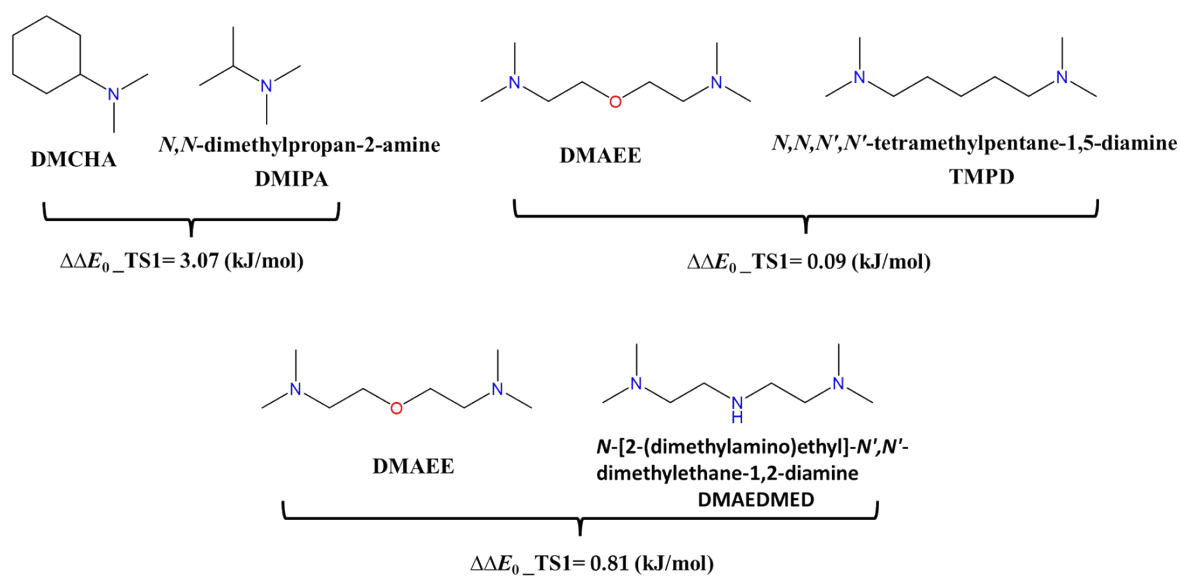


Figure S10. Tertiary amine catalysts used in this study.

Table S1. Zero-point corrected relative energies (ΔE_0), relative enthalpies (ΔH), Gibbs free energies (ΔG), and relative entropy (ΔS) of the reaction between phenyl isocyanate and butan-1-ol in presence of catalysts, calculated at the BHandHLYP/6-31G(d) level of theory in acetonitrile using the SMD implicit solvent model at 298.15 K and 1 atm. R – reactant, RC – reactant complex, TS – transition state, IM – intermediate, PC – product complex, P – product.

ΔE_0 (kJ/mol)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
DMCHA	0.00	-29.29	-51.48	-5.40	-104.97	-114.39	-130.52	-92.58
DMIPA	0.00	-27.11	-45.91	-2.33	-101.87	-110.46	-127.51	-92.58
$\Delta\Delta E_0 = 3.07$								
DMAEE	0.00	-29.04	-43.57	-3.07	-100.93	-109.33	-127.63	-92.58
TMPD	0.00	-29.61	-43.80	-3.16	-103.10	-111.06	-127.87	-92.58
DMAEDMED	0.00	-29.72	-43.79	-3.88	-103.73	-111.26	-127.48	-92.58
$\Delta\Delta E_0^* = 0.09$ $\Delta\Delta E_0 = 0.81$								
ΔH (kJ/mol)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
DMCHA	0.00	-28.14	-47.16	-5.94	-105.63	-116.14	-130.65	-94.84
DMIPA	0.00	-25.93	-41.37	-2.48	-102.78	-112.44	-127.55	-94.84
DMAEE	0.00	-27.59	-38.67	-3.20	-101.62	-111.10	-127.92	-94.84
TMPD	0.00	-27.92	-38.90	-3.53	-104.08	-112.97	-127.83	-94.84
DMAEDMED	0.00	-27.85	-38.70	-3.96	-104.44	-113.22	-127.35	-94.84
ΔG (kJ/mol)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
DMCHA	0.00	15.24	36.85	95.68	-4.69	-9.41	-30.65	-41.54
DMIPA	0.00	15.92	38.62	93.96	-0.79	-6.37	-29.69	-41.54
DMAEE	0.00	12.64	40.66	94.20	-1.46	-6.62	-26.62	-41.54
TMPD	0.00	8.59	38.23	94.85	-3.36	-7.33	-30.72	-41.54
DMAEDMED	0.00	7.08	38.39	93.25	-6.71	-6.94	-31.83	-41.54
ΔS (Cal/mol*Kelvin)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
DMCHA	0.00	-34.78	-67.34	-81.46	-80.92	-85.55	-80.16	-133.38
DMIPA	0.00	-33.55	-64.12	-77.31	-81.76	-85.03	-78.45	-133.38
DMAEE	0.00	-32.25	-63.59	-78.08	-80.29	-83.76	-81.21	-133.38
TMPD	0.00	-29.27	-61.83	-78.86	-80.74	-84.68	-77.85	-133.38
DMAEDMED	0.00	-28.00	-61.80	-77.93	-78.34	-85.20	-76.57	-133.38

* ($\Delta\Delta E_0 = TS1_{DMAEE} - TS1_{TMPD}$)

Table S2. Cartesian coordinates of the stationary points for the reaction system studied. The calculated at the BHandHLYP/6-31G(d) level of theory in acetonitrile at 298.15 K and 1 atm. Cat.- catalysts, RC – reactant complex, TS – transition state, IM – intermediate, PC – product complex.

DMCHA				DMCHA-RC1			
C	-0.43997600	-1.25038700	-0.22853300	O	-1.46222500	0.67919500	-1.68339300
H	-0.40630000	-1.30417900	-1.31818300	N	0.57381500	1.23877800	0.23712000
H	0.04152300	-2.14788400	0.14774300	C	0.78024600	2.63796200	-0.09309600
C	-0.43997500	1.25038700	-0.22853000	H	1.56707300	3.11148500	0.50076200
H	0.04152500	2.14788300	0.14775000	H	-0.14171000	3.18758100	0.08061600

H	-0.40629900	1.30418300	-1.31817900	H	1.03907200	2.73427600	-1.14387700
C	-1.89245000	1.24762000	0.24115700	C	0.14783000	1.10168900	1.61977700
H	-2.39074300	2.14471500	-0.12331600	H	-0.79135000	1.63224800	1.75508200
H	-1.91732200	1.29959700	1.33110000	H	0.86748600	1.51394200	2.33228700
C	-1.89245100	-1.24762000	0.24115300	H	-0.01853600	0.05919600	1.86862900
H	-2.39074500	-2.14471400	-0.12332300	C	1.70942800	0.38779800	-0.15363600
H	-1.91732400	-1.29960100	1.33109600	C	2.96482600	0.53143900	0.71301500
N	1.69643400	-0.00000100	-0.31886700	H	1.97013700	0.71286600	-1.16126000
C	0.32712700	-0.00000100	0.21356200	H	2.74230700	0.21128500	1.73110600
H	0.36591100	-0.00000200	1.31432500	H	3.27114200	1.57456600	0.76756100
C	-2.63496700	0.00000100	-0.21478000	C	-2.75383100	0.75765700	-1.13682500
H	-2.71054100	0.00000300	-1.30359700	H	-2.87367000	1.67015900	-0.54537400
C	2.44553400	1.18149600	0.06983600	H	-3.44539400	0.83590300	-1.97495800
H	3.46541000	1.09195900	-0.29352600	H	-0.80941300	0.81887200	-0.97066600
H	2.02487100	2.07898800	-0.36855700	C	1.29867200	-1.08059800	-0.25546100
H	2.48879800	1.32071900	1.15817400	H	1.01580200	-1.45707600	0.72757300
C	2.44553500	-1.18149500	0.06984200	H	0.42181200	-1.16181500	-0.89425500
H	2.48880000	-1.32071200	1.15818100	C	4.10899400	-0.31882900	0.16361600
H	2.02487200	-2.07899100	-0.36854500	H	4.39930500	0.06024800	-0.81779400
H	3.46541100	-1.09196000	-0.29352100	H	4.98338300	-0.22249000	0.80569400
H	-3.65314600	0.00000100	0.17219800	C	2.43984600	-1.93580300	-0.80177600
				H	2.65253400	-1.63642600	-1.82947200
				H	2.13369700	-2.98023100	-0.83856400
				C	3.70529000	-1.78411700	0.03629900
				H	3.52794000	-2.19463600	1.03197100
				H	4.51823200	-2.36242500	-0.40083100
				C	-3.12072800	-0.45023800	-0.29067800
				H	-2.41588500	-0.53130000	0.53862200
				H	-2.99479700	-1.34808600	-0.89687200
				C	-4.54223600	-0.38679100	0.25278700
				H	-5.24224100	-0.30103900	-0.57927600
				H	-4.66187500	0.52010200	0.84688000
				C	-4.90932200	-1.59681400	1.09920800
				H	-5.92874600	-1.52481100	1.47348700
				H	-4.83249000	-2.51730100	0.52237000
				H	-4.24681600	-1.69022700	1.95849000
DMCHA -RC2				DMCHA -TS1			
O	1.22283400	-1.14192400	-0.20315300	O	1.30069700	-0.48679300	-0.93392100
N	0.84097400	1.21984500	1.33286600	C	0.08291300	-1.86505400	-0.82034200
C	0.31810200	0.62084400	2.54921600	N	1.02084000	1.64566400	0.70103300
H	0.08628900	1.35469500	3.32595700	C	0.88692200	1.10577300	2.04824000
H	1.05302800	-0.06975500	2.95514100	H	0.85667800	1.88215800	2.81475400
H	-0.58649000	0.06233300	2.32576800	H	1.73477600	0.46026300	2.26005200
C	2.07721100	1.93193500	1.61158900	H	-0.01973100	0.51292300	2.11682400
H	2.80898200	1.22996100	2.00325200	C	2.26408100	2.39935800	0.58497900
H	1.95404400	2.72902300	2.34962000	H	3.09829800	1.73481000	0.79118100
H	2.48275500	2.36683500	0.70468100	H	2.31777600	3.23199900	1.28830400
C	-0.17427400	1.99418400	0.60010500	H	2.38172700	2.78777700	-0.42044300
C	-0.59127500	3.31544500	1.25464000	C	-0.18763200	2.38043000	0.26948700
H	-1.05354100	1.34996200	0.57742700	C	-0.42402200	3.71215400	0.98714800
H	0.26364600	3.99124900	1.28637200	H	-1.01656600	1.71946800	0.51928300
H	-0.90303300	3.14803800	2.28394500	H	0.38637200	4.40231500	0.75281100
C	2.53692900	-1.63827500	-0.10830800	H	-0.41985300	3.57002800	2.06575200
H	2.87700300	-1.63233100	0.92931100	C	2.66742000	-0.81172200	-1.15660200
H	2.50264400	-2.67981300	-0.42203200	H	2.67313500	-1.53824600	-1.96172000
H	1.15822900	-0.30167300	0.29499300	C	-4.49027500	-3.24362400	0.64113600
C	0.23714900	2.23077300	-0.85255000	C	-3.48374400	-3.95089700	0.00040700
H	1.11547800	2.87502100	-0.89225100	C	-4.27519700	-1.91348900	0.97360700
H	0.51589200	1.28203000	-1.30597700	C	-3.07131500	-1.30120400	0.66972200
C	-1.72256800	3.97892400	0.47103500	C	-2.05515800	-2.00692500	0.02599200
H	-2.61158900	3.34783200	0.52104700	C	-2.27564900	-3.34491600	-0.30733900
H	-1.98777400	4.92761200	0.93549900	H	-1.50624100	-3.91000700	-0.80519700
C	-0.89270900	2.88948300	-1.64091600	H	-3.63562000	-4.98542100	-0.26467800
H	-1.74021500	2.20396400	-1.69368000	H	-5.04711000	-1.34831000	1.47164500
H	-0.57213800	3.06936500	-2.66599000	H	-2.90242300	-0.26780500	0.92580500

C	-1.34100600	4.19420500	-0.99000000	N	-0.86786100	-1.30151300	-0.24002600
H	-0.52718700	4.91955000	-1.04427600	O	0.60878400	-2.78387800	-1.34198800
H	-2.17893700	4.62142700	-1.53929500	H	1.17302100	0.28358700	-0.29066600
C	3.51924200	-0.87450000	-0.97966300	H	3.16700100	0.08627000	-1.51371500
H	3.53011100	0.17217200	-0.67107400	H	-5.42729500	-3.72136100	0.87741800
H	3.15786100	-0.89363800	-2.00844600	C	-0.21890300	2.58126300	-1.24498300
C	4.93218700	-1.44007600	-0.91611100	H	0.59878500	3.23329700	-1.55140400
H	4.91461300	-2.48771600	-1.21898500	H	-0.07056800	1.62535000	-1.74172400
H	5.28048900	-1.42688500	0.11738600	C	-1.74864200	4.33705800	0.55238400
C	5.91660200	-0.67754800	-1.79061200	H	-2.57084800	3.69303400	0.86885000
H	6.91678100	-1.10150900	-1.72465500	H	-1.88886500	5.29224400	1.05615000
H	5.61415400	-0.70314400	-2.83645800	C	-1.54104600	3.20739900	-1.68521200
H	5.97949300	0.36764000	-1.49124500	H	-2.35432100	2.51000300	-1.47787900
C	-0.52567100	-2.90679600	1.54624200	H	-1.53201400	3.36468200	-2.76263100
C	-4.05428100	-1.26989100	-1.90871800	C	-1.80890900	4.52191100	-0.96007800
C	-2.67383900	-1.22338300	-2.04781900	H	-1.06076100	5.25713100	-1.26170300
C	-4.60916700	-1.76222500	-0.73663900	H	-2.77841500	4.92267900	-1.25278600
C	-3.79306000	-2.20779200	0.29025800	C	3.35740900	-1.37120000	0.07092600
C	-2.41220100	-2.16128500	0.14113100	H	3.30496400	-0.64276700	0.88004300
C	-1.84470500	-1.66570200	-1.02941900	H	2.81946700	-2.25787900	0.40445500
H	-0.77187500	-1.61764400	-1.11775300	C	4.81403900	-1.72445700	-0.20421300
H	-2.23546900	-0.84022500	-2.95543400	H	4.86229000	-2.44222600	-1.02351800
H	-5.67989200	-1.80126300	-0.61802800	H	5.34372500	-0.83405100	-0.54410000
H	-4.21299700	-2.59304200	1.20444700	C	5.51878900	-2.29905200	1.01553000
N	-1.62683000	-2.62163100	1.19382700	H	5.03046600	-3.21021300	1.35743000
O	0.48039700	-3.24598200	2.03186700	H	6.55621900	-2.54153300	0.79430400
H	-4.69121000	-0.92422500	-2.70660200	H	5.51273700	-1.59072700	1.84258000
DMCHA -IM				DMCHA -TS2			
O	1.03440300	-1.61394500	-0.00660000	O	1.18616000	-1.50774800	0.01810300
C	-0.25025400	-2.02665200	-0.22892400	C	-0.06151500	-1.96635900	-0.25550300
N	-0.09607800	1.23313700	1.26164600	N	-0.30438500	1.15978600	1.24176900
C	-1.16663800	1.48815900	2.25113400	C	-1.43510500	1.33874400	2.16689600
H	-0.85970600	2.26540900	2.93879800	H	-1.23480900	2.12931200	2.88234500
H	-1.34537500	0.56974000	2.79712400	H	-1.58885400	0.40885400	2.70388000
H	-2.06861000	1.78361500	1.73184700	H	-2.32962400	1.57563200	1.60423900
C	1.15430800	0.86947600	1.96280100	C	0.91718500	0.88504700	2.01384100
H	0.95730700	-0.01543300	2.55445800	H	0.76508500	-0.03390900	2.56843400
H	1.45699900	1.68177000	2.61129200	H	1.11975500	1.69146800	2.71146600
H	1.92867200	0.64853800	1.24500300	H	1.75776900	0.74979200	1.34999200
C	0.03310400	2.34368600	0.25333500	C	-0.19173100	2.28033100	0.26008900
C	0.50824200	3.66118800	0.85356000	C	0.17722100	3.62409800	0.88447000
H	-0.98157000	2.47566100	-0.11429100	H	-1.19179900	2.36521000	-0.16065100
H	1.51944300	3.54588600	1.24066900	H	1.17466000	3.56396700	1.31829800
H	-0.12631800	3.96150600	1.68316300	H	-0.50977500	3.87858300	1.68775100
C	2.04990400	-2.57975900	-0.21939300	C	2.26032100	-2.39044600	-0.27465200
H	1.90777900	-3.41992200	0.45703000	H	2.15298900	-3.30227900	0.30763300
H	1.98450400	-2.96548200	-1.23376500	H	2.22925100	-2.66639400	-1.32544800
C	-5.28435400	-1.30793900	-0.35345300	C	-5.11471800	-1.64513300	-0.40517600
C	-4.53524700	-2.46074600	-0.16788200	C	-4.30054600	-2.69718300	-0.00844000
C	-4.61649500	-0.09312600	-0.43754100	C	-4.53288900	-0.41453500	-0.67182800
C	-3.23781800	-0.04032700	-0.33887600	C	-3.16362300	-0.24300800	-0.54706300
C	-2.46016900	-1.19575700	-0.14998200	C	-2.33186600	-1.29291500	-0.14292100
C	-3.15290800	-2.41675300	-0.06783800	C	-2.93180700	-2.52975500	0.12576800
H	-2.59605600	-3.32434600	0.06713400	H	-2.31714800	-3.35606200	0.43276400
H	-5.03248200	-3.41673100	-0.09695300	H	-4.73517400	-3.66157300	0.20610300
H	-5.17159900	0.82081000	-0.58562300	H	-5.14428200	0.41699600	-0.98676700
H	-2.73064200	0.90876500	-0.41703800	H	-2.71849300	0.71283000	-0.77435500
N	-1.09194000	-1.01855700	-0.01523100	N	-0.97167300	-1.02826700	0.02774000
O	-0.45456300	-3.18009200	-0.59027000	O	-0.22286700	-3.08575000	-0.71590000
H	-0.42096600	0.37405500	0.71643200	H	-0.57840800	0.14533800	0.61907700
H	-6.35881800	-1.35409100	-0.43167100	H	-6.17934900	-1.78294200	-0.50574900
C	0.90831400	1.92328800	-0.92183300	C	0.76133200	1.93284500	-0.88010000
H	1.93508900	1.77943500	-0.59038100	H	1.77795300	1.84109400	-0.50117700
H	0.55871000	0.97564900	-1.32255700	H	0.48923900	0.97282000	-1.30974900
C	0.50012800	4.74933300	-0.22074700	C	0.15717500	4.72311700	-0.17762000

H	-0.52847400	4.93446100	-0.53277400	H	-0.86377000	4.85090600	-0.54034000
H	0.87029800	5.67901300	0.20656300	H	0.44948900	5.66947500	0.27362600
C	0.88678300	3.00790700	-1.99707200	C	0.73192700	3.02707000	-1.94528400
H	-0.12324100	3.09820000	-2.39875600	H	-0.26096400	3.06557900	-2.39566000
H	1.52824000	2.70981600	-2.82390100	H	1.42859700	2.77693900	-2.74322200
C	1.33315400	4.35384300	-1.43540000	C	1.07136700	4.39033800	-1.35178100
H	2.38327500	4.29087700	-1.14613300	H	2.10756300	4.38446800	-1.00972200
H	1.26333800	5.12326000	-2.20241200	H	0.99678300	5.16289400	-2.11548000
C	3.38966700	-1.91876000	0.01780500	C	3.55377100	-1.68226400	0.05963300
H	3.48883700	-1.06612000	-0.65405800	H	3.54643300	-1.40203400	-1.11278700
H	3.42136000	-1.52690400	1.03435500	H	3.61082300	-0.75785600	-0.51487600
C	4.55129100	-2.88096400	-0.19766900	C	4.77364700	-2.54621000	-0.23492800
H	4.50639300	-3.27972100	-1.21148500	H	4.70780000	-3.47229500	0.33671100
H	4.44269700	-3.73392100	0.47275900	H	4.76706700	-2.83336300	-1.28671200
C	5.90590200	-2.22682100	0.02958700	C	6.08258700	-1.84202100	0.08952600
H	6.71793300	-2.93343700	-0.12974400	H	6.13210000	-1.57108900	1.14305700
H	6.05631800	-1.38996900	-0.65074800	H	6.93801400	-2.47772700	-0.12983100
H	5.99258700	-1.84582800	1.04605500	H	6.19074700	-0.92787500	-0.49218300
DMCHA -PC							
O	1.47033600	-1.50607300	-0.00122500				
C	0.35010300	-2.20586600	-0.20115900				
N	-0.31677100	1.32058900	1.25760700				
C	-1.27658800	1.25069500	2.34521500				
H	-1.18643600	2.07769700	3.05576600				
H	-1.12671100	0.32505800	2.89647000				
H	-2.28807400	1.24940700	1.95029700				
C	1.03502700	1.30700900	1.79056400				
H	1.19305000	0.37564500	2.32747900				
H	1.22693900	2.13006700	2.48486600				
H	1.76411100	1.35530900	0.99058100				
C	-0.60131700	2.41473500	0.31691300				
C	-0.34812400	3.82802100	0.85472300				
H	-1.66849500	2.33517800	0.10654800				
H	0.71367700	3.95135100	1.06931000				
H	-0.88110000	3.97919300	1.79172000				
C	2.69913100	-2.19197800	-0.25563600				
H	2.76807400	-3.05187000	0.40430400				
H	2.69903500	-2.55192100	-1.27995300				
C	-4.79054000	-2.42670900	-0.31810000				
C	-3.84752700	-3.43639600	-0.20604700				
C	-4.36554700	-1.10608800	-0.30602900				
C	-3.02024100	-0.80271700	-0.18981600				
C	-2.07142200	-1.81873000	-0.07236700				
C	-2.49734500	-3.14607600	-0.07873500				
H	-1.77896200	-3.93814500	0.00970000				
H	-4.16032300	-4.46865200	-0.21052600				
H	-5.08127500	-0.30429400	-0.39497500				
H	-2.69604400	0.22499400	-0.19523500				
N	-0.73059500	-1.43847600	0.07778500				
O	0.34139500	-3.35527500	-0.58033100				
H	-0.54938800	-0.47513000	0.36959200				
H	-5.83767000	-2.66377900	-0.41379000				
C	0.12691500	2.21812500	-1.01192400				
H	1.20396000	2.28719000	-0.86044400				
H	-0.07706900	1.21843100	-1.39150800				
C	-0.77589500	4.88441400	-0.16226800				
H	-1.85593700	4.82573400	-0.30843800				
H	-0.56833600	5.87999700	0.22740500				
C	-0.29538800	3.27185700	-2.03360200				
H	-1.35190500	3.13787000	-2.27197900				
H	0.25460600	3.12731900	-2.96229000				
C	-0.07652100	4.68528700	-1.50288200				
H	0.99364700	4.85988300	-1.37803200				
H	-0.43150200	5.41832500	-2.22610200				
C	3.82969600	-1.21986000	-0.01480300				

		H	3.70339200	-0.35855000	-0.66996800				
		H	3.77420800	-0.85355500	1.00963800				
		C	5.19012000	-1.86064000	-0.26094400				
		H	5.30536400	-2.72551200	0.39256100				
		H	5.23203900	-2.23861600	-1.28261800				
		C	6.34086200	-0.89280800	-0.03039200				
		H	7.30083000	-1.37204500	-0.21098000				
		H	6.26905700	-0.03268400	-0.69417000				
		H	6.34256600	-0.52153200	0.99321000				
			DMEE			DMEE -RC1			
N	2.64711800	0.01262900	-0.30549100	O	1.63057200	-0.38043900	1.71964100		
C	3.69167600	-0.97261200	-0.11541600	C	2.90240100	0.07547300	1.33384200		
H	3.87412400	-1.20192400	0.94231700	H	3.50732800	-0.74558700	0.93801000		
H	4.62216400	-0.60732100	-0.54286200	H	1.25628100	-0.90563600	0.98776200		
H	3.42676700	-1.89799500	-0.62023800	H	3.40045500	0.42366500	2.23793100		
C	3.03372800	1.27554700	0.29195400	N	0.46266300	-2.04743800	-0.28291300		
H	3.97583900	1.60690000	-0.13715300	C	0.82797000	-3.37097800	0.19266000		
H	3.16296800	1.20402200	1.37969700	C	0.94838200	-1.84412100	-1.63813100		
H	2.29176600	2.04187500	0.09110000	C	-0.97443400	-1.83816500	-0.16920600		
C	1.37693000	-0.47403200	0.20124600	H	0.52486100	-3.48585400	1.22933900		
C	0.19423100	0.32030800	-0.31768600	H	0.36041300	-4.16801500	-0.39485300		
H	1.35157500	-0.48505500	1.29845000	H	0.75151200	-0.82996100	-1.96878200		
H	1.24913400	-1.50131900	-0.13078800	H	0.48156300	-2.53479600	-2.34866700		
H	0.21605300	0.34044200	-1.40954000	H	-1.28655900	-2.17991400	0.81390000		
H	0.21635700	1.35350500	0.03195700	H	2.02254800	-2.00307100	-1.66370500		
O	-0.97271600	-0.31209300	0.14207600	H	1.90584900	-3.49350700	0.13453200		
C	-2.14930200	0.33410900	-0.25657700	H	-1.52245500	-2.43073500	-0.90974000		
H	-2.17526800	1.36070800	0.11616100	C	-1.37155100	-0.37953500	-0.29172800		
H	-2.22098200	0.37581500	-1.34589200	H	-1.17276600	0.01143000	-1.29044900		
C	-3.31835100	-0.44082300	0.30180500	H	-0.79998200	0.21894700	0.42025600		
H	-3.28577500	-1.46477000	-0.07261600	O	-2.74607500	-0.30054200	-0.01462800		
H	-3.24000500	-0.48035500	1.38905000	C	-3.26010200	0.99971500	-0.10303900		
O	-4.49272100	0.22138200	-0.10742400	H	-3.12290600	1.40048900	-1.11198600		
H	-5.24451200	-0.26222600	0.23962700	H	-2.74769500	1.67013300	0.59048900		
						C	-4.73470200	0.94523000	0.23590900
						H	-4.86109400	0.57636500	1.24943600
						H	-5.23964800	0.25059700	-0.43607900
						O	-5.32132400	2.22486100	0.19444800
						H	-5.34020000	2.51345600	-0.72095500
						C	2.84900600	1.20513400	0.31871700
						H	2.33313800	0.85406800	-0.57674700
						H	2.24381400	2.01291900	0.73189300
						C	4.22723100	1.73146500	-0.05982800
						H	4.82701300	0.91552200	-0.46501400
						H	4.74216600	2.07121400	0.83965700
						C	4.17275100	2.86793800	-1.07019500
						H	5.17019800	3.22312700	-1.32203400
						H	3.69168200	2.54955000	-1.99392500
						H	3.60875100	3.71368000	-0.67957100
			DMEE -RC2			DMEE -TS1			
O	-2.19660300	-0.81476100	1.19272300	O	-2.04938200	-0.95369800	0.82757700		
C	0.06088200	-2.63666500	0.31382500	C	-0.74703200	-2.06857900	0.23115600		
C	-3.46652300	-1.20104600	0.73340800	C	-3.33825300	-1.03039900	0.22817800		
H	-4.25424100	-0.68889900	1.29434300	H	-4.04724700	-0.57217900	0.91386300		
C	4.94787700	-1.06481300	0.70191000	C	4.15681300	-2.95932600	-0.06254900		
C	4.39668100	-1.92428000	-0.23898700	C	3.07272000	-3.82077400	-0.14272800		
C	4.13825000	-0.51405100	1.68481200	C	3.93499300	-1.61648500	0.20999100		
C	2.78676000	-0.81681500	1.73067900	C	2.64828000	-1.14177900	0.40119700		
C	2.24180300	-1.67912400	0.78793300	C	1.55456700	-2.00395900	0.31927700		
C	3.04807600	-2.23534100	-0.20143200	C	1.78101600	-3.35398900	0.04551100		
H	2.61741600	-2.90397400	-0.92925500	H	0.95048900	-4.03643900	-0.01889900		
H	5.01780600	-2.35731200	-1.00636700	H	3.22913500	-4.86738100	-0.35201500		
H	4.55712800	0.15350000	2.42028400	H	4.76773300	-0.93390000	0.27538900		
H	2.14980900	-0.39549300	2.49043400	H	2.47153900	-0.09761400	0.60528300		
N	0.87842200	-1.96056700	0.86493400	N	0.28661900	-1.44167700	0.54854300		

O	-0.79286200	-3.27736500	-0.15258900	O	-1.31205600	-2.99366100	-0.23971800
H	-2.14580500	0.15939400	1.19304500	H	-1.78230900	-0.01276400	1.06563200
H	-3.56711300	-2.26345400	0.94810700	H	-3.57139500	-2.08708100	0.16304300
H	5.99881600	-0.82821900	0.66909300	H	5.15891800	-3.32853000	-0.20957900
N	-1.94862900	2.02294700	1.40409100	N	-1.53077000	1.52299000	1.79500800
C	-2.17097800	2.18509100	2.83101300	C	-1.78748200	1.18623300	3.19040500
C	-2.91350500	2.80799200	0.65135100	C	-2.49799200	2.51173100	1.33316400
C	-0.57247300	2.34986900	1.05544800	C	-0.15305900	1.98296100	1.64295000
H	-1.49351100	1.54175500	3.38487900	H	-1.10066900	0.40847300	3.51014500
H	-2.01548900	3.21748500	3.16128700	H	-1.66548000	2.05157900	3.84694000
H	-2.80443000	2.63353000	-0.41353600	H	-2.38035500	2.69486600	0.27100600
H	-2.80203300	3.88162600	0.83767500	H	-2.38826400	3.46096900	1.86508300
H	0.08094700	1.87543100	1.78255700	H	0.49547300	1.23014700	2.08033700
H	-3.91920100	2.51475600	0.93848400	H	-3.50297900	2.13769300	1.50240300
H	-3.19067500	1.90012700	3.07439000	H	-2.80282000	0.81572800	3.29449200
H	-0.39348900	3.42903400	1.11146900	H	0.00474300	2.91544000	2.19306800
C	-0.17529900	1.84250100	-0.31732900	C	0.26372300	2.17309500	0.19797500
H	-0.75271800	2.32439300	-1.10744800	H	-0.23945200	3.02624500	-0.25788000
H	-0.35684800	0.76790200	-0.38007500	H	0.01640100	1.28511200	-0.38507600
O	1.18997200	2.12515200	-0.48617600	O	1.65277500	2.39180300	0.19858500
C	1.68393300	1.76137500	-1.74577300	C	2.17700500	2.63982000	-1.07856500
H	1.14658100	2.29282500	-2.53710900	H	1.68342300	3.50432700	-1.53183800
H	1.55634200	0.69131100	-1.92270100	H	2.01790000	1.78421600	-1.73780900
C	3.15526600	2.11460400	-1.79420400	C	3.65984000	2.91143100	-0.93795700
H	3.68966000	1.55449200	-1.03298300	H	4.15620600	2.03836900	-0.52498200
H	3.28369700	3.17587200	-1.57866800	H	3.81605400	3.74047800	-0.24710400
O	3.72837500	1.76451200	-3.03239000	O	4.25628000	3.16012000	-2.18936400
H	3.35891400	2.34190200	-3.70440100	H	3.93180800	4.00455900	-2.51061200
C	-3.66450100	-0.96431500	-0.75428200	C	-3.39569400	-0.38117300	-1.13930200
H	-3.54507000	0.10007300	-0.96486400	H	-3.10869100	0.66711700	-1.05508700
H	-2.87106100	-1.48270700	-1.29271200	H	-2.66406300	-0.86126100	-1.78866800
C	-5.02485200	-1.43282200	-1.25445100	C	-4.78357900	-0.48512400	-1.75959100
H	-5.14151100	-2.49534000	-1.03732700	H	-5.06742900	-1.53534500	-1.83154700
H	-5.81118300	-0.91987600	-0.69915300	H	-5.51099000	-0.01493300	-1.09728000
C	-5.22351900	-1.19727100	-2.74452400	C	-4.86188600	0.15728500	-3.13637800
H	-4.47100900	-1.72480600	-3.32882800	H	-4.16580000	-0.31309200	-3.82901700
H	-6.20131700	-1.54311500	-3.07446300	H	-5.86111400	0.06653300	-3.55741600
H	-5.14728600	-0.13851300	-2.98826000	H	-4.61652100	1.21714900	-3.08978800
DMEE -IM				DMEE -TS2			
N	0.38127300	0.04588200	2.30708300	N	0.53395200	0.19798600	2.19471500
C	1.45853100	-0.03175100	3.31720700	C	1.65747700	0.30717600	3.13934000
C	-0.81661400	-0.67847700	2.78280100	C	-0.52678800	-0.63579000	2.78208600
C	0.10862700	1.46335000	1.96232500	C	0.06681000	1.54824700	1.82340800
H	2.32925100	0.49189700	2.94543300	H	2.44043700	0.91125400	2.69830800
H	1.11475800	0.42436900	4.23866900	H	1.32034100	0.76688200	4.06447400
H	-1.55109900	-0.72499400	1.99362100	H	-1.31276100	-0.79768000	2.05988200
H	-1.21761700	-0.16599900	3.65038000	H	-0.92599400	-0.15389000	3.67080800
H	1.04847200	1.89221700	1.63369400	H	0.92336600	2.08487300	1.42891700
H	-0.52059900	-1.68473300	3.05177600	H	-0.09970200	-1.59490400	3.05147500
H	1.69915100	-1.07372000	3.48690100	H	2.03996300	-0.68508200	3.34748100
H	-0.21117700	1.97294700	2.86565700	H	-0.27387800	2.06086100	2.72022000
C	-0.91629800	1.63239200	0.85761300	C	-1.02785600	1.55662600	0.77411600
H	-1.91548300	1.35468400	1.19312200	H	-1.95361400	1.12586500	1.15546400
H	-0.66163700	1.00853000	0.00118400	H	-0.72603100	0.98310200	-0.10181800
O	-0.88218900	2.99091200	0.51444200	O	-1.22817500	2.90494900	0.44194100
C	-1.80207900	3.33361900	-0.48877300	C	-2.23899800	3.09933000	-0.51096300
H	-2.82399700	3.12933000	-0.15728800	H	-3.19144400	2.70527300	-0.14519100
H	-1.62336300	2.75027700	-1.39400600	H	-2.00114700	2.58001900	-1.44151600
C	-1.63919800	4.80834200	-0.78936400	C	-2.35880100	4.58617900	-0.76973900
H	-0.63241200	4.99713400	-1.14969700	H	-1.41948400	4.96418700	-1.16208600
H	-1.77994700	5.38662300	0.12423400	H	-2.56120100	5.10577100	0.16728600
O	-2.51941400	5.22359100	-1.80683800	O	-3.34337800	4.86143600	-1.73812900
H	-3.41292900	5.19543400	-1.45692800	H	-4.20060200	4.65922300	-1.35620400
O	-0.74381000	-1.69924200	-0.25933500	O	-0.58236300	-1.73627400	-0.19001500
C	0.48621100	-1.61125800	-0.85247100	C	0.63534800	-1.58420000	-0.77548300

C	-1.77071600	-2.30296700	-1.02913400	C	-1.54479200	-2.47891900	-0.92642600
H	-1.92166200	-1.74120400	-1.94789400	H	-1.73319700	-1.98866100	-1.87816100
H	-1.47470100	-3.31109900	-1.30937900	H	-1.15386600	-3.47031200	-1.13979800
C	5.31994400	-0.12567600	-1.09677400	C	5.32420400	0.24269200	-1.18080400
C	4.31232800	-0.07240600	-2.05051000	C	4.27347800	0.28997300	-2.08762500
C	4.99154300	-0.51883000	0.19296900	C	5.07604500	-0.20783000	0.10686000
C	3.68659400	-0.85054900	0.51733400	C	3.80149500	-0.60712000	0.47892000
C	2.65486500	-0.80132800	-0.43158400	C	2.73338300	-0.55902000	-0.42141900
C	3.00498100	-0.40224700	-1.73207400	C	2.99715200	-0.10040600	-1.71826300
H	2.24259900	-0.35986900	-2.48818200	H	2.19467300	-0.05850000	-2.43297400
H	4.54456600	0.23376900	-3.05953000	H	4.44653000	0.64050000	-3.09363500
H	5.75593400	-0.57351200	0.95318500	H	5.87828700	-0.25871400	0.82676700
H	3.44681300	-1.16679200	1.51995500	H	3.62339400	-0.97380000	1.47676700
N	1.36266400	-1.08004500	-0.00432700	N	1.45636500	-0.90483500	0.03082000
O	0.63220600	-2.02056400	-1.99803700	O	0.85275900	-2.05886200	-1.87931900
H	0.74542200	-0.43937700	1.41845500	H	0.95125000	-0.34307700	1.20091400
H	6.33516400	0.13186100	-1.35311600	H	6.31538500	0.55000300	-1.47361000
C	-3.03415100	-2.32669800	-0.19778400	C	-2.80876300	-2.56333900	-0.10088200
H	-2.84007100	-2.86611000	0.72922400	H	-2.57897700	-3.03208500	0.85576800
H	-3.30005300	-1.30615600	0.07844300	H	-3.16340300	-1.55563700	0.11536900
C	-4.19708000	-2.97701100	-0.93664200	C	-3.90371500	-3.35071600	-0.80999400
H	-3.92298000	-3.99454600	-1.21642300	H	-3.54048500	-4.35439900	-1.03214400
H	-4.37889600	-2.44086700	-1.86849700	H	-4.12070200	-2.88281500	-1.77057200
C	-5.47458100	-3.00547500	-0.11097400	C	-5.18262200	-3.44413600	0.00854500
H	-5.79171100	-1.99861500	0.15655200	H	-5.94818500	-4.01015700	-0.51825500
H	-6.28907900	-3.47479800	-0.65902300	H	-5.00300900	-3.93737800	0.96258000
H	-5.33206200	-3.56330100	0.81333600	H	-5.58723500	-2.45525400	0.21884900
DMEE -PC							
	N	-0.55226200	-1.56440400	1.73128600			
	C	-0.86790200	-0.91932900	2.99450700			
	H	-0.40000400	-1.42156400	3.84823600			
	H	-1.94380900	-0.92346700	3.14658900			
	H	-0.52851800	0.11216900	2.97519400			
	C	-1.07725700	-2.92001400	1.71770100			
	H	-2.14296300	-2.89891100	1.92500300			
	H	-0.59577500	-3.55337700	2.47113800			
	H	-0.93406800	-3.37912600	0.74510100			
	C	0.88333400	-1.53228500	1.48764100			
	C	1.24698100	-1.84652500	0.05016600			
	H	1.41369700	-2.22097800	2.15496500			
	H	1.23704200	-0.53016500	1.70385100			
	H	0.71101400	-1.17663200	-0.62373200			
	H	0.98441300	-2.87075800	-0.21857500			
	O	2.63533100	-1.66543000	-0.07748300			
	C	3.11916700	-1.96733300	-1.35745300			
	H	2.89500700	-3.00314300	-1.62185700			
	H	2.65650900	-1.32537100	-2.11019500			
	C	4.61392100	-1.75637000	-1.35397600			
	H	4.83488400	-0.72127000	-1.09000200			
	H	5.06763800	-2.39780800	-0.59743300			
	O	5.08207400	-2.06990300	-2.64524600			
	H	6.03264100	-1.94351100	-2.65719000			
	O	0.07491000	1.47148800	0.23304200			
	C	-1.14285200	1.61248600	-0.29976400			
	C	1.00655800	2.52596900	-0.02568500			
	H	1.13273200	2.62913300	-1.09943700			
	H	0.60299400	3.45806700	0.35803100			
	C	-5.85907000	-0.30999700	-1.12176000			
	C	-5.37149400	0.98104300	-1.24815300			
	C	-5.01606700	-1.30090600	-0.63921900			
	C	-3.70983400	-1.00430700	-0.29365300			
	C	-3.21945000	0.29625500	-0.41874200			
	C	-4.06587100	1.29448600	-0.89992400			
	H	-3.70368400	2.29883600	-1.00317300			
	H	-6.01264300	1.76490400	-1.61966700			

H	-5.37220500	-2.31335900	-0.53364000				
H	-3.05869600	-1.78143600	0.07107500				
N	-1.89526400	0.52081000	-0.02270400				
O	-1.48358500	2.58582300	-0.93287000				
H	-1.43177100	-0.23144000	0.48955600				
H	-6.87602700	-0.54080700	-1.39431700				
C	2.30955100	2.16845200	0.64927100				
H	2.13941300	2.06836500	1.72099000				
H	2.64385100	1.19678100	0.28775900				
C	3.38378200	3.21886500	0.39456400				
H	3.03097600	4.18955500	0.74371300				
H	3.54469900	3.31781000	-0.67910700				
C	4.70155600	2.88302600	1.07611500				
H	5.45255300	3.64532700	0.87929100				
H	4.57799800	2.80957800	2.15543100				
H	5.09462800	1.93084500	0.72296500				
DMAEE				DMAEE -RC1			
O	-0.34201800	-0.37008200	-0.33056700	O	-3.90249300	-1.56314100	-0.10865300
N	3.20551300	0.19720400	0.38571500	C	-4.52060000	-0.45112100	0.48469900
N	-3.36204400	0.31896000	-0.23894700	H	-5.58872400	-0.66337500	0.51560500
C	4.01640600	1.37470000	0.15347200	H	-2.93758800	-1.48537000	0.02050100
C	3.91360900	-0.99225100	-0.04447300	H	-4.19510200	-0.32756700	1.52212800
C	-3.82133800	0.27726300	1.13011300	O	1.65411700	-0.29141800	-0.43672300
C	-2.68602700	1.56121900	-0.54370100	N	5.13827000	0.57409700	0.29170500
C	1.90703500	0.32950400	-0.24998500	N	-1.08467300	-1.52818200	0.25311500
C	-2.66377400	-0.88112700	-0.66204900	C	5.69484000	1.27824700	1.42843900
C	0.89145700	-0.67011300	0.26860500	C	5.71395600	1.07511600	-0.94057200
C	-1.36891700	-1.25422800	0.04149900	C	-0.86388400	-2.94620500	0.46243200
H	3.50972500	2.25687200	0.53605800	C	-0.70923700	-0.74948400	1.42013900
H	4.23236700	1.54064800	-0.90977700	C	3.68848300	0.64732200	0.29759400
H	4.11076300	-0.99670700	-1.12437500	C	-0.55469900	-1.03249600	-1.01087200
H	3.34986800	-1.88736900	0.19847700	C	3.04334700	-0.36445700	-0.62941400
H	-4.35996600	-0.65003800	1.31228800	C	0.93533900	-1.16725600	-1.26687100
H	-3.01711200	0.35250900	1.87123600	H	5.30565300	0.85890800	2.35260200
H	-2.36807700	1.56171800	-1.58311700	H	5.46611600	2.35166400	1.41892300
H	-1.80483600	1.74675100	0.07596200	H	5.46762800	2.12936700	-1.12195800
H	1.97579100	0.23983500	-1.34175700	H	5.36892800	0.49723700	-1.79208100
H	1.52411800	1.32418600	-0.03567800	H	-1.17812300	-3.50099600	-0.41791400
H	-2.45517300	-0.79386300	-1.72719000	H	0.18017200	-3.19486700	0.67151300
H	-3.34808900	-1.71961300	-0.53634900	H	-0.89920600	0.30366700	1.23372700
H	0.82237000	-0.59293300	1.35625900	H	0.34145200	-0.86286500	1.68950400
H	1.17748400	-1.69595400	0.02970600	H	3.32845000	1.65222800	0.04194400
H	-1.10113900	-2.27539600	-0.24491100	H	3.34294300	0.43201800	1.30567800
H	-1.49624600	-1.24973200	1.12628200	H	-0.82537100	0.01758500	-1.09693000
H	4.96506500	1.27516100	0.67511600	H	-1.06822000	-1.56576100	-1.80934700
H	4.86833500	-1.05250200	0.47155000	H	3.41301300	-1.36537700	-0.39491900
H	-4.50545600	1.10478700	1.30793200	H	3.28087700	-0.16222900	-1.67507100
H	-3.37863600	2.38934900	-0.40144400	H	1.12433800	-0.92621500	-2.31662800
				H	1.26858100	-2.19518300	-1.11064100
				H	6.77634700	1.16760200	1.43458500
				H	6.79637300	0.98585600	-0.89738900
				H	-1.46145900	-3.28052500	1.30698300
				H	-1.31709900	-1.06332100	2.26585900
				C	-4.28397100	0.84103900	-0.27990100
				H	-3.21116600	1.03943000	-0.31838900
				H	-4.61211600	0.69839600	-1.31014700
				C	-5.00123800	2.03703700	0.33237900
				H	-6.07202400	1.83309000	0.37166300
				H	-4.67639500	2.16276500	1.36599300
				C	-4.76112700	3.33007500	-0.43298800
				H	-5.10749900	3.24729300	-1.46214700
				H	-5.28503100	4.16618100	0.02630700
				H	-3.70118300	3.57853600	-0.46105700
DMAEE-RC2				DMAEE -TS1			

O	-2.26041200	1.40909000	0.68597500	O	-1.91294100	1.55906500	1.17189500
C	-2.64470100	-0.07574300	-2.10459300	C	-3.37737900	0.74052900	0.39774100
C	-2.32542100	2.79168700	0.93967900	C	-1.72100700	2.94370900	0.90917000
H	-3.38133100	3.05613100	0.95940200	H	-2.69062200	3.40957000	1.04604600
C	-5.08433200	-3.36263400	1.12520000	C	-5.47891600	-3.57925300	-0.96658500
C	-4.59729900	-2.10288800	1.44502400	C	-5.94207200	-2.27390200	-1.04005500
C	-4.91548900	-3.85753400	-0.15962400	C	-4.21790600	-3.82022000	-0.43956900
C	-4.26519300	-3.10070700	-1.12051900	C	-3.43281500	-2.77081100	0.00662800
C	-3.78335200	-1.83944100	-0.79172100	C	-3.89290600	-1.45621400	-0.06404500
C	-3.94591900	-1.33303900	0.49467900	C	-5.16206400	-1.21784400	-0.59536900
H	-3.55733100	-0.35594200	0.73462400	H	-5.53876300	-0.21133700	-0.66061100
H	-4.72422900	-1.71272600	2.44224500	H	-6.92001400	-2.07031400	-1.44717600
H	-5.28953300	-4.83498700	-0.41795400	H	-3.84197900	-4.82905000	-0.37448900
H	-4.12794700	-3.47456900	-2.12147900	H	-2.45372000	-2.95598200	0.41772800
N	-3.13563100	-1.10999100	-1.78315300	N	-3.02563700	-0.45693000	0.41370200
O	-2.14172100	0.87153600	-2.56718400	O	-4.13430900	1.61777700	0.17403700
H	-1.34312300	1.09859700	0.82924200	H	-1.04729900	1.03905300	1.14182900
H	-5.59018700	-3.95351600	1.87139000	H	-1.05099700	3.33646500	1.67106600
H	-1.92352400	3.02098100	1.93051100	H	-6.09097200	-4.39571200	-1.31417100
O	3.00527800	-0.54614700	-0.06637200	O	3.08073100	-0.59380900	-0.06667600
N	6.62283300	-1.11618600	0.00977700	N	6.69239700	-1.18917200	-0.22056100
N	0.29274700	0.29744400	1.16765900	N	0.42327400	0.22851400	1.29314700
C	7.68698600	-0.22098600	0.41514600	C	7.78718900	-0.32683500	0.17458600
C	6.97008500	-1.77931500	-1.23152700	C	6.95986600	-1.77708500	-1.51836400
C	-0.04668100	-0.61671800	2.24182900	C	0.16347400	-0.72583700	2.36049400
C	1.26630500	1.28740000	1.59526500	C	1.41726400	1.21345600	1.70031100
C	5.35790900	-0.40894000	-0.07455000	C	5.43138600	-0.47068400	-0.18786500
C	0.61337000	-0.36992300	-0.08866700	C	0.69122400	-0.40039000	-0.00004200
C	4.16226400	-1.34059000	-0.11730500	C	4.22771100	-1.39253900	-0.20721200
C	1.81755400	-1.29390400	-0.12375300	C	1.88520700	-1.32952900	-0.11040000
H	7.45028100	0.22694500	1.37672800	H	7.61240600	0.06181900	1.17445100
H	7.85905400	0.58946900	-0.30467800	H	7.92354100	0.52563800	-0.50306900
H	7.07596900	-1.07683500	-2.06837700	H	7.02457400	-1.02480200	-2.31516200
H	6.21754500	-2.51339200	-1.50143600	H	6.18498500	-2.48748000	-1.78854300
H	-0.80515200	-1.31736000	1.90250700	H	-0.59461800	-1.43446600	2.04177900
H	0.80978800	-1.18728300	2.61081000	H	1.05566400	-1.27782200	2.66126300
H	1.49040100	1.95959200	0.77218600	H	1.58299900	1.91999600	0.89280900
H	2.20291300	0.84470000	1.93595300	H	2.37245700	0.76024900	1.96029300
H	5.32292300	0.26373300	-0.94119600	H	5.34873500	0.24713400	-1.01407500
H	5.25627600	0.21002100	0.81343300	H	5.39035900	0.10082700	0.73607000
H	0.74644000	0.39590300	-0.84975700	H	0.80266500	0.39224800	-0.73617900
H	-0.25635700	-0.96047400	-0.37185300	H	-0.19518100	-0.97047800	-0.26733500
H	4.19901600	-2.02442500	0.73383100	H	4.30102700	-2.11089400	0.61242800
H	4.15339100	-1.94562200	-1.02548000	H	4.16909500	-1.95954500	-1.13759100
H	1.78222600	-1.86582800	-1.05506000	H	1.80990600	-1.86208700	-1.06214800
H	1.78420600	-2.01502700	0.69543900	H	1.87397200	-2.08342800	0.67897400
H	8.61494900	-0.77775800	0.51902100	H	7.90409900	-2.31444500	-1.48578900
H	7.91483200	-2.30314400	-1.11094200	H	8.71441200	-0.89420000	0.18810900
H	-0.45425600	-0.05149900	3.07636100	H	1.04213000	1.75523000	2.56494800
H	0.84435200	1.87018700	2.41088900	H	-0.21039400	-0.19174600	3.23003800
C	-1.61043000	3.62402000	-0.11043100	C	-1.18724100	3.21756200	-0.48229900
H	-0.55798200	3.33578500	-0.13568800	H	-0.23462200	2.70347900	-0.61269000
H	-2.02458600	3.37749600	-1.08756900	H	-1.87787200	2.79900100	-1.21379500
C	-1.72207800	5.12157200	0.14407200	C	-1.00334400	4.70811100	-0.74012200
H	-2.77504700	5.40457000	0.17427200	H	-1.95621000	5.21833200	-0.59664400
H	-1.31555800	5.35250700	1.12951600	H	-0.31898300	5.12109700	0.00146700
C	-1.00481300	5.95677800	-0.90633900	C	-0.47597200	5.00267300	-2.13627600
H	-1.41261800	5.77322200	-1.89927100	H	-1.15649300	4.62878500	-2.89963600
H	-1.10096300	7.02114400	-0.70047500	H	-0.35516100	6.07238100	-2.29477600
H	0.05775800	5.72013500	-0.93765600	H	0.49258900	4.53195300	-2.29785400
DMAEE -IM				DMAEE -TS2			
O	-1.40079100	1.74848200	-0.08248500	O	2.46463900	1.38356000	-0.06421300
C	-2.70352600	1.33570900	-0.00051200	C	3.16775800	0.22266600	-0.15836500
C	0.25246900	-0.66289200	1.36356700	C	3.22421600	2.58394100	-0.11958300
C	-0.56913500	-2.69048000	0.29843700	H	3.93571600	2.60187500	0.70221500

C	-1.18282100	3.14870800	-0.01652200	C	3.65818400	-4.82104800	-0.21801400
H	-1.73396100	3.64311500	-0.81259700	C	4.44931500	-3.85385700	0.38628500
H	-1.55964300	3.53470900	0.92790400	C	2.45408900	-4.43664800	-0.78971600
C	-6.33551900	-2.21828500	0.14850500	C	2.05347200	-3.11085200	-0.75930400
C	-6.29307500	-0.93938300	0.68450800	C	2.83862000	-2.12607400	-0.14982000
C	-5.19389500	-2.71511100	-0.46636200	C	4.05115200	-2.52726600	0.42578000
C	-4.04484900	-1.94827100	-0.54076300	H	4.67788700	-1.79205200	0.89598500
C	-3.98092900	-0.65182700	-0.00387800	H	5.38816200	-4.13373500	0.83933100
C	-5.14523100	-0.16460100	0.61487900	H	1.82383200	-5.16943600	-1.26954200
H	-5.14049700	0.82504100	1.03037700	H	1.12414200	-2.81941100	-0.122198900
H	-7.16783700	-0.53251300	1.16957900	N	2.33844300	-0.82357200	-0.10294600
H	-5.19766300	-3.70540700	-0.89593400	O	4.38073800	0.24703300	-0.29440000
H	-3.16960500	-2.34151600	-1.03305400	H	1.01469500	-0.59532000	0.21423600
N	-2.76448400	0.00974600	-0.09102900	H	3.79155500	2.61287100	-1.04592000
O	-3.58998100	2.17311500	0.11731600	H	3.97449800	-5.85149400	-0.24371200
H	-1.30102700	-0.77708500	0.02442000	N	-0.12323000	-0.35861200	0.54208200
H	0.35696900	-3.18640600	0.56160000	C	-0.78002400	-1.64335900	0.83061600
H	-0.95685200	-3.09722100	-0.62690000	C	-0.02402100	0.45709500	1.76027400
H	0.37724500	0.40096800	1.21875600	C	-0.69794600	0.36649900	-0.61226700
H	1.20545900	-1.12986600	1.56671000	H	-0.84294200	-2.22585300	-0.08010600
H	-7.23398000	-2.81165200	0.20651700	H	-1.77663000	-1.48260600	1.22236300
N	-0.33723300	-1.24106700	0.13658400	H	-1.00174100	0.61436400	2.20423200
C	0.38989500	-0.89569400	-1.11634000	H	0.43169700	1.40789500	1.51756200
C	1.73081300	-1.55667900	-1.32044600	H	0.01081700	1.14913900	-0.86179200
H	0.49240900	0.18219800	-1.12545200	H	-0.17963200	-2.17858900	1.55818000
H	-0.26619600	-1.18330500	-1.93125300	H	0.60638200	-0.06845200	2.46965300
O	2.66571400	-1.06181100	-0.40095700	H	-0.73223400	-0.33364300	-1.44108800
H	2.04354200	-1.32610100	-2.34098500	C	-2.05765000	0.99745600	-0.42282100
H	1.65614400	-2.64238700	-1.24839600	O	-3.04402100	0.01012100	-0.28320700
C	3.95561000	-1.59287100	-0.59084100	H	-2.25626900	1.60777500	-1.30680100
C	4.87292700	-0.94616000	0.42813600	C	-4.34063600	0.54183100	-0.16075100
H	3.94891600	-2.67508000	-0.44750700	C	-5.30212100	-0.62216200	-0.02272900
H	4.28352100	-1.39576500	-1.61199800	H	-4.41058800	1.18309900	0.72021600
N	6.22071900	-1.48391600	0.38445300	H	-4.56864600	1.15396000	-1.03435100
H	4.86084600	0.14178900	0.28590900	N	-6.66873500	-0.19346900	0.21378500
H	4.45985900	-1.14394100	1.41406000	H	-5.22220300	-1.26479300	-0.90866100
C	6.94647100	-1.16288200	1.59629900	H	-4.97896400	-1.21325400	0.83052700
C	6.95956500	-1.03106200	-0.77780900	C	-7.47031500	-1.28200100	0.73444700
H	6.42153900	-1.56029600	2.46103000	C	-7.28744800	0.36211200	-0.97362400
H	7.07535300	-0.08286900	1.74275500	H	-7.03733400	-1.65385500	1.65936500
H	7.08366300	0.05927900	-0.79804500	H	-7.55309600	-2.12347600	0.03470800
H	6.46081500	-1.33016000	-1.69430600	H	-8.47515600	-0.92672600	0.94892800
H	-1.29253500	-2.83168200	1.09195800	H	-7.34677800	-0.36348700	-1.79509100
H	-0.43844300	-0.84107800	2.17926800	H	-6.73671500	1.22764800	-1.32792600
H	7.93453400	-1.61502600	1.56178300	H	-8.29768800	0.68668800	-0.73817600
H	7.94856300	-1.48190200	-0.77720900	H	-2.06443100	1.66938700	0.43665200
C	0.30134300	3.40780300	-0.15011700	C	2.26887000	3.75258700	-0.03396400
H	0.65303400	2.99270600	-1.09475500	H	1.55557800	3.69155700	-0.85582900
H	0.83104400	2.88216300	0.64448900	H	1.69599700	3.68086400	0.89054400
C	0.63003300	4.89433100	-0.08827800	C	2.99712200	5.09010700	-0.08372400
H	0.26564400	5.30543900	0.85358200	H	3.57857900	5.15039600	-1.00405000
H	0.09161700	5.41633200	-0.87974800	H	3.71370100	5.14163300	0.73636000
C	2.11972400	5.17338800	-0.21959800	C	2.04929600	6.27734600	-0.00441400
H	2.50683700	4.80347200	-1.16782200	H	2.59269800	7.21931800	-0.04127100
H	2.32726900	6.24044300	-0.17085300	H	1.34133700	6.27015700	-0.83173400
H	2.68164300	4.68954900	0.57787000	H	1.47599100	6.26116600	0.92126300
DMAEE-PC							
	O	-1.10737300	1.66427800	0.04530300			
	C	-2.43468000	1.59303500	-0.09904400			
	C	-0.51711200	2.95510600	-0.13686400			
	H	-0.68907200	3.27888300	-1.15948100			
	C	-6.73398600	-1.27233400	-0.08291900			
	C	-6.54246500	0.08267900	-0.29844000			
	C	-5.62947800	-2.07072200	0.17864200			
	C	-4.36084400	-1.52218800	0.22267300			

C	-4.16717200	-0.15668600	0.00469800					
C	-5.27589200	0.64778400	-0.25820600					
H	-5.14565500	1.69842600	-0.42789900					
H	-7.38817900	0.72020200	-0.50323800					
H	-5.75193100	-3.12829600	0.35089000					
H	-3.51018800	-2.15013700	0.42858500					
N	-2.85020400	0.31457100	0.06780700					
O	-3.12735300	2.55516100	-0.34208800					
H	-2.12339600	-0.38298900	0.23841600					
H	-7.72322000	-1.69889600	-0.11723500					
H	-1.00131800	3.66317900	0.52797200					
O	2.40178500	-1.28677700	-0.39188000					
N	6.02524000	-1.22139200	0.14276400					
N	-0.59511300	-1.70016000	0.43731800					
C	6.79538600	-0.52339300	1.15160300					
C	6.63622300	-1.05348500	-1.16090200					
C	-0.94692600	-3.08801900	0.66795800					
C	0.11386000	-1.14526400	1.57722900					
C	4.63793600	-0.79474800	0.16443100					
C	0.05768800	-1.48141500	-0.84849500					
C	3.71658500	-1.74176000	-0.57971700					
C	1.44375400	-2.06600200	-1.06338600					
H	6.36999200	-0.70402500	2.13531800					
H	6.82707800	0.56153900	0.98863500					
H	6.63938000	-0.00699500	-1.49241700					
H	6.11754000	-1.64272000	-1.91040100					
H	-1.51077100	-3.47336900	-0.17741500					
H	-0.07693900	-3.73374100	0.82134800					
H	0.36028500	-0.10731800	1.38449100					
H	1.03659500	-1.68041200	1.80964100					
H	4.51575700	0.21862200	-0.23985800					
H	4.30777200	-0.76600900	1.19981300					
H	0.11526200	-0.40922500	-1.01755300					
H	-0.59735800	-1.89493700	-1.61278900					
H	3.83567200	-2.75420600	-0.18685300					
H	3.94593900	-1.77362400	-1.64615600					
H	1.65496600	-2.06581300	-2.13618100					
H	1.49664100	-3.10363300	-0.72707700					
H	7.81850300	-0.89098900	1.15133300					
H	7.66660600	-1.39764600	-1.12534300					
H	-0.53414400	-1.18871100	2.45020200					
H	-1.56964300	-3.15971800	1.55629400					
C	0.95848600	2.83880900	0.16461200					
H	1.39915600	2.07743400	-0.47797400					
H	1.08589800	2.50111300	1.19258800					
C	1.68211700	4.16494300	-0.03511700					
H	1.54754500	4.49850000	-1.06415700					
H	1.22455700	4.92551400	0.59785400					
C	3.16763400	4.07065300	0.27847200					
H	3.65774100	3.33645400	-0.35919100					
H	3.66420300	5.02667300	0.12586500					
H	3.33210100	3.77247800	1.31269600					
DMIPA				DMIPA -RC1				
N	-0.66850200	-0.00002900	-0.31671700	O	-0.54887100	1.26770800	-1.25207500	
C	0.65599800	-0.00002800	0.31450400	N	1.58264400	0.34853600	0.40607700	
H	0.53698300	-0.00009300	1.40795900	C	2.08030100	1.63677400	0.85417700	
C	-1.44037100	-1.18237400	0.01828100	H	2.95833900	1.56062000	1.50179800	
H	-2.42594800	-1.10545800	-0.43253400	H	1.30056500	2.14834600	1.41307600	
H	-0.97360800	-2.07972400	-0.37180900	H	2.33994000	2.24987300	-0.00443600	
H	-1.57605200	-1.31058500	1.10043200	C	1.16748400	-0.45963800	1.53956300	
C	-1.44032700	1.18238600	0.01813700	H	0.37794600	0.06071100	2.07569700	
H	-1.57593800	1.31078000	1.10027400	H	1.97862100	-0.65210800	2.24724900	
H	-0.97357400	2.07966200	-0.37213600	H	0.77263300	-1.41328700	1.20594200	
H	-2.42593300	1.10540900	-0.43260200	C	2.50317400	-0.32383200	-0.52756400	
C	1.45301900	-1.24181000	-0.07180700	H	2.78699600	0.44788000	-1.24087900	

H	1.97070200	2.81253600	-1.80023800	H	0.15244600	4.98446600	-0.08702700
H	1.01297400	1.33543200	-1.90862100	H	0.79327500	4.33197300	1.40983400
C	0.30682700	4.16861400	-0.04790800	C	0.80574500	2.91460300	-1.75758800
H	1.29541200	4.62110000	-0.08809400	H	0.66573200	1.91842800	-2.16786900
H	-0.31102600	4.66299100	-0.79450500	H	0.04513100	3.56557600	-2.18220800
H	-0.12424500	4.37994700	0.92763100	H	1.77310400	3.28890800	-2.08455800
DMIPA -IM				DMIPA -TS2			
O	1.27060500	-0.89456400	-0.01863700	O	1.35140900	-0.81395100	-0.01449000
C	0.04242000	-1.49134900	-0.09589000	C	0.14484500	-1.42537600	-0.12562600
N	-0.16282100	2.02084900	0.60758700	N	-0.34394300	1.93404800	0.61078900
C	-1.22906600	2.40136000	1.55961700	C	-1.47133900	2.24435500	1.50380000
H	-0.98448600	3.34148900	2.03709300	H	-1.31930400	3.19096300	2.01197100
H	-1.30280000	1.62258900	2.30921900	H	-1.54802100	1.45568700	2.24472200
H	-2.16847400	2.48541200	1.02903200	H	-2.38926700	2.28304600	0.93021500
C	1.13982900	1.97004500	1.30453200	C	0.90935000	1.95466000	1.37923300
H	1.06069400	1.24554800	2.10512200	H	0.84188100	1.20004000	2.15469700
H	1.37060400	2.94433100	1.71644800	H	1.06022500	2.92534000	1.84110400
H	1.91032900	1.65556900	0.61797600	H	1.74437400	1.71527800	0.73784100
C	-0.17731800	2.85585900	-0.64776900	C	-0.33553800	2.78822600	-0.61680600
H	-1.19950100	2.76410400	-1.00133100	H	-1.33089700	2.66052500	-1.03319500
C	2.39382400	-1.75691200	-0.08108100	C	2.49436600	-1.65076800	-0.12543300
H	2.35117400	-2.47796900	0.73207100	H	2.46086700	-2.41772000	0.64422900
H	2.37649500	-2.31728900	-1.01298900	H	2.48657700	-2.15267100	-1.08960200
C	-5.04193700	-1.41387300	-0.10351900	C	-4.91980700	-1.56791100	-0.12610100
C	-4.14837300	-2.39930700	0.29050000	C	-4.00205200	-2.43309700	0.45366100
C	-4.53582700	-0.17902700	-0.48770300	C	-4.46057200	-0.38311100	-0.68222300
C	-3.17281800	0.05701400	-0.47672800	C	-3.11013500	-0.07395000	-0.66130100
C	-2.25078200	-0.92687400	-0.08073500	C	-2.17453900	-0.93410300	-0.07611100
C	-2.78083900	-2.17113900	0.30411500	C	-2.65141900	-2.12595500	0.48470500
H	-2.10992200	-2.95317300	0.60484900	H	-1.95586500	-2.80888000	0.93680900
H	-4.51830600	-3.36679100	0.59591900	H	-4.34016900	-3.35850300	0.89439200
H	-5.20607100	0.60635800	-0.80280000	H	-5.15377400	0.30359100	-1.14299800
H	-2.79268800	1.01777800	-0.78721200	H	-2.76232500	0.84182800	-1.11220600
N	-0.91253300	-0.56561800	-0.05787900	N	-0.84023300	-0.52542900	-0.03158500
O	-0.02510000	-2.71058800	-0.20402500	O	0.07623900	-2.63079800	-0.30780000
H	-0.40234200	1.02595900	0.30164100	H	-0.54037800	0.78077100	0.25708100
H	-6.10354000	-1.60264200	-0.11243700	H	-5.96956300	-1.81320400	-0.14495500
C	3.64498100	-0.91205000	0.01349700	C	3.72562100	-0.78607500	0.02416900
H	3.64363200	-0.18227700	-0.79627100	H	3.69041200	-0.27847700	0.98790400
H	3.62707400	-0.34989400	0.94709800	H	3.71289100	-0.01239000	-0.74340600
C	4.91366700	-1.75289700	-0.05494500	C	5.01130000	-1.59648700	-0.08333000
H	4.92101500	-2.32054400	-0.98584300	H	5.01290000	-2.37406000	0.68096200
H	4.90465300	-2.48647100	0.75169500	H	5.03504500	-2.11060500	-1.04450700
C	6.17970300	-0.91437000	0.03710400	C	6.25909900	-0.73880000	0.06365400
H	7.07079100	-1.53690900	-0.01263800	H	6.27840400	-0.23586500	1.02930100
H	6.23312900	-0.19339600	-0.77726500	H	7.16287600	-1.33960700	-0.01511100
H	6.21545900	-0.35861000	0.97291300	H	6.30197300	0.02755900	-0.70875900
C	0.74861600	2.25690400	-1.69253200	C	0.67002000	2.26832500	-1.63226400
H	0.54535200	2.73476500	-2.64699500	H	0.50013300	2.77077900	-2.58102600
H	1.79502300	2.42722300	-1.45444200	H	1.69437700	2.47270200	-1.33186300
H	0.58379500	1.18946100	-1.80243400	H	0.56196900	1.19962300	-1.78801600
C	0.12838100	4.31875100	-0.38424500	C	-0.11882700	4.26551400	-0.32617100
H	1.14575500	4.46067600	-0.02956500	H	0.87223400	4.45391400	0.07901500
H	0.02676700	4.86100200	-1.32048900	H	-0.20501300	4.82019700	-1.25714900
H	-0.55693200	4.76548400	0.32966800	H	-0.85674400	4.66513300	0.36330500
DMIPA -PC							
	O	1.34172200	-0.98845700	0.02751600			
	C	0.17553800	-1.63704700	-0.03664700			
	N	-0.22553300	2.15594100	0.59484400			
	C	-1.15825300	2.42004300	1.67584800			
	H	-0.98471300	3.37988400	2.17144400			
	H	-1.06631800	1.63933000	2.42750900			
	H	-2.17692800	2.40983200	1.29961400			
	C	1.13596500	2.16301100	1.10187400			

H	1.23773100	1.38249400	1.85070000				
H	1.41068100	3.11328000	1.56894500				
H	1.84243100	1.95234600	0.30770800				
C	-0.44918500	3.02379600	-0.57331000				
H	-1.52033600	2.96946000	-0.76024200				
C	2.51938000	-1.79476600	-0.06280900				
H	2.52449700	-2.50728900	0.75689900				
H	2.49697200	-2.35232800	-0.99422800				
C	-4.96941700	-1.53228000	-0.15127600				
C	-4.09478600	-2.55995400	0.16512700				
C	-4.45727400	-0.26705900	-0.39967500				
C	-3.09404000	-0.03694800	-0.33789500				
C	-2.21377200	-1.07020700	-0.01534300				
C	-2.72736600	-2.34087800	0.24033100				
H	-2.06281400	-3.14570500	0.48875200				
H	-4.47540300	-3.54940800	0.36406600				
H	-5.11855300	0.54709500	-0.65041000				
H	-2.70297700	0.94552800	-0.54548200				
N	-0.84967800	-0.75741100	0.06259500				
O	0.08765600	-2.83709800	-0.16812800				
H	-0.60239500	0.23195400	0.14397500				
H	-6.03064700	-1.71342400	-0.20417900				
C	3.71634800	-0.87579100	-0.00134600				
H	3.65463100	-0.15603300	-0.81695900				
H	3.68498500	-0.30925600	0.92857000				
C	5.02727000	-1.64731600	-0.09171700				
H	5.07674400	-2.37176300	0.72141100				
H	5.04522800	-2.22208200	-1.01786600				
C	6.24487200	-0.73721500	-0.03544200				
H	7.16786500	-1.30969500	-0.09981500				
H	6.23924900	-0.02289100	-0.85721200				
H	6.26939700	-0.17133200	0.89450200				
C	0.25332200	2.47230900	-1.80678300				
H	-0.06201100	3.02496800	-2.68906600				
H	1.33482400	2.56419400	-1.73599700				
H	0.00997400	1.42349800	-1.95883000				
C	-0.09093600	4.49402900	-0.35851500				
H	0.98172900	4.63147700	-0.23940300				
H	-0.40279800	5.07800900	-1.22189500				
H	-0.58558100	4.91023000	0.51579000				
TMPD				TMPD-RC1			
N	3.43307500	0.14926000	0.39315400	O	-3.97617600	-1.55200100	-0.48469100
N	-3.60667500	0.16376200	-0.16451100	C	-4.75570300	-0.59902200	0.18975300
C	4.31722300	1.28488400	0.23577200	H	-5.79735200	-0.88018400	0.03865200
C	4.04365300	-1.04017300	-0.16367800	H	-3.04403100	-1.43550100	-0.21709100
C	-3.88065800	0.21706400	1.25078600	H	-4.57452000	-0.63472100	1.26834200
C	-3.23608000	1.45283000	-0.70067500	N	5.58768900	0.43897300	0.12950400
C	2.12829700	0.42937100	-0.18763100	N	-1.23574300	-1.42576000	0.24582900
C	-2.78738300	-0.96615600	-0.57238200	C	6.37430200	0.92910800	1.24181900
C	1.05495300	-0.58370900	0.18362900	C	5.96136000	1.12794600	-1.08843400
C	-1.40907100	-1.17302800	0.06670200	C	-0.99413500	-2.84954200	0.35993800
H	3.88144900	2.16347500	0.70499700	C	-1.05943600	-0.74344300	1.51327200
H	4.51827800	1.52745400	-0.81614100	C	4.16536400	0.54965000	0.41764500
H	4.19580200	-0.96808800	-1.24906500	C	-0.59417600	-0.80619700	-0.91119000
H	3.43391600	-1.91612000	0.03296300	C	3.27575900	-0.20649300	-0.55860800
H	-4.21868400	-0.75634500	1.59987400	C	0.91720100	-0.95638100	-1.10464400
H	-3.01815300	0.51241300	1.85993800	H	6.13305800	0.37050100	2.14277000
H	-3.02280300	1.36373700	-1.76293500	H	6.20515800	1.99423500	1.44832400
H	-2.36661800	1.90995500	-0.21781800	H	5.73578600	2.20224300	-1.05185100
H	2.19498000	0.50857200	-1.28252000	H	5.44685400	0.70535200	-1.94540900
H	1.81727700	1.40769100	0.17487100	H	-1.18499500	-3.33258600	-0.59508800
H	-2.67029100	-0.90857400	-1.65400100	H	0.02649000	-3.09179600	0.66909700
H	-3.37213100	-1.86438600	-0.37054800	H	-1.22520200	0.32229800	1.38395000
H	1.04284800	-0.69724000	1.26811900	H	-0.07081500	-0.88668000	1.95440300

H	1.29407800	-1.56183900	-0.23112500	H	3.85391900	1.60362500	0.45723500
H	-1.07468200	-2.16581600	-0.24027700	H	4.00557500	0.14214000	1.41445300
H	-1.50896500	-1.21610700	1.15145200	H	-0.84913200	0.25198300	-0.89095000
H	5.27004400	1.08054100	0.71825700	H	-1.07944000	-1.22779000	-1.79088400
H	5.01371600	-1.20152600	0.29982600	H	3.63011800	-1.23539100	-0.62835900
H	-4.67492900	0.93674800	1.44147400	H	3.35567700	0.22083200	-1.55702800
H	-4.06984400	2.14424200	-0.58396300	H	1.12768300	-0.60114400	-2.11480000
C	-0.32734400	-0.16442000	-0.30598400	H	1.18756200	-2.01211500	-1.09992400
H	-0.56686300	0.81329900	0.10750200	H	7.43289300	0.79452500	1.03293400
H	-0.30477000	-0.04322600	-1.39061000	H	7.02968800	1.01613000	-1.25611200
				H	-1.67429300	-3.27200000	1.09587300
				H	-1.79305200	-1.11793600	2.22433200
				C	-4.53609900	0.81725600	-0.31623900
				H	-3.48807700	1.08705400	-0.17279700
				H	-4.71793400	0.83221900	-1.39146000
				C	-5.42524700	1.84249700	0.37513800
				H	-6.47077800	1.56672100	0.23191600
				H	-5.24568300	1.81000400	1.45050400
				C	-5.20294700	3.26012000	-0.13112500
				H	-5.40686300	3.33224700	-1.19844200
				H	-5.85175500	3.96987000	0.37858000
				H	-4.17371100	3.57762100	0.02982500
				C	1.81145200	-0.19370100	-0.13223900
				H	1.73108500	-0.61790800	0.86662500
				H	1.46570300	0.83887700	-0.05793500
TMPD-RC2				TMPD-TS1			
O	2.56487200	1.17687000	-0.65006800	O	-2.23041800	1.49745400	1.10585400
C	2.57152200	-0.41776500	2.11209000	C	-3.52232100	0.40105100	0.37497400
C	2.97231800	2.50779800	-0.85624200	C	-2.30667700	2.88773000	0.81589100
H	4.06092500	2.50622800	-0.84152200	H	-3.34766000	3.16210700	0.94614500
C	4.36574600	-4.06638700	-1.15496100	C	-4.79697900	-4.27156900	-0.84470600
C	4.13235800	-2.73223200	-1.45845100	C	-5.52635900	-3.09191000	-0.86040800
C	4.10208300	-4.53532000	0.12360300	C	-3.47743300	-4.24463400	-0.41559000
C	3.60900700	-3.67895800	1.09439700	C	-2.89724500	-3.05535100	-0.00870600
C	3.37986400	-2.34451300	0.78160400	C	-3.62460200	-1.86556100	-0.02403100
C	3.64045300	-1.86278300	-0.49814600	C	-4.95223200	-1.89693900	-0.45558200
H	3.44964100	-0.82571600	-0.72512300	H	-5.53417500	-0.99131700	-0.47454100
H	4.33435400	-2.36152500	-2.45070800	H	-6.55328500	-3.09668200	-1.19039900
H	4.27948600	-5.56983100	0.36925400	H	-2.89560900	-5.15259300	-0.39633800
H	3.40020600	-4.03161200	2.09065000	H	-1.87294400	-3.03249000	0.32616300
N	2.88305800	-1.51672000	1.78255000	N	-2.95213300	-0.70880400	0.40970500
O	2.23459400	0.59701500	2.58262500	O	-4.43334400	1.11468800	0.14319200
H	1.60278900	1.10346100	-0.81639400	H	-1.28054800	1.15024100	1.08862600
H	4.74910600	-4.73466500	-1.90878700	H	-1.72510200	3.41655600	1.56794500
H	2.67020500	2.85463400	-1.84838000	H	-5.24978900	-5.19716600	-1.16134400
N	-6.96659200	-0.81735100	0.05626600	N	6.98568600	-1.14951400	-0.23549300
N	-0.16263400	0.71611000	-1.22273000	N	0.31103700	0.63574700	1.26963600
C	-8.12347600	-0.01830600	-0.28906800	C	8.18906100	-0.51630600	0.26168000
C	-7.16527200	-1.45481100	1.34145900	C	7.16268300	-1.54362200	-1.61787600
C	0.01000700	-0.14122700	-2.37836100	C	0.20276500	-0.36160500	2.32215700
C	-0.87328700	1.93571300	-1.55754600	C	1.06565900	1.79727200	1.71734700
C	-5.75464600	-0.01250500	0.01621400	C	5.83214700	-0.28238800	-0.04730200
C	-0.62941300	0.01264200	-0.02969800	C	0.71834200	0.08286400	-0.02677500
C	-4.47020400	-0.82692900	0.07146300	C	4.49595500	-0.97690200	-0.26714600
C	-1.94115100	-0.77604300	-0.08392200	C	1.97569600	-0.78407400	-0.11043600
H	-7.99629300	0.41221800	-1.27925200	H	8.07466600	-0.27525200	1.31564400
H	-8.30147700	0.80352000	0.41713100	H	8.43659300	0.41041900	-0.27278800
H	-7.25000600	-0.73075100	2.16299400	H	7.31022900	-0.68463400	-2.28624800
H	-6.34523600	-2.12787500	1.56997400	H	6.30315500	-2.10257000	-1.97355100
H	0.59092900	-1.01763900	-2.10272500	H	-0.39543800	-1.19803900	1.97440000
H	-0.93595000	-0.47795500	-2.81118400	H	1.17399200	-0.73730300	2.64920100
H	-1.02015400	2.53356800	-0.66278900	H	1.15355000	2.51272900	0.90546300
H	-1.84765800	1.76022600	-2.01788900	H	2.06586900	1.54871200	2.07153000
H	-5.75179900	0.73303900	0.82462700	H	5.89668700	0.60348400	-0.69576400

H	-5.76783700	0.54503700	-0.91877600	H	5.86559800	0.08160500	0.97818000
H	-0.68310500	0.74482700	0.77419500	H	0.81130000	0.92151900	-0.71364500
H	0.16052300	-0.68845400	0.23755200	H	-0.11865300	-0.51883600	-0.37510000
H	-4.51178700	-1.59586600	-0.70060500	H	4.47183700	-1.88486300	0.33626400
H	-4.38788200	-1.34516100	1.02565900	H	4.39406500	-1.28790300	-1.30573500
H	-1.95861400	-1.39217800	0.81656400	H	1.96799000	-1.21751400	-1.11170300
H	-1.91869200	-1.47476100	-0.91992500	H	1.89159500	-1.62584300	0.57618300
H	-9.01311200	-0.64340000	-0.30323600	H	8.03448600	-2.18748800	-1.70323300
H	-8.07935900	-2.04285900	1.31842900	H	9.03231700	-1.19510000	0.15904300
H	0.55483500	0.39916700	-3.14899000	H	0.53153900	2.27153000	2.53733700
H	-0.27795800	2.51485400	-2.26046800	H	-0.29468800	0.08029800	3.18171900
C	2.44954700	3.46156800	0.20382400	C	-1.83387500	3.23099600	-0.58222700
H	1.35822200	3.44483800	0.19011900	H	-0.79963000	2.90852700	-0.70454200
H	2.75449900	3.09088800	1.18192500	H	-2.42912500	2.67153500	-1.30336300
C	2.93938100	4.89052000	0.00819000	C	-1.94166000	4.72322400	-0.87135700
H	4.03005600	4.90162100	0.01575700	H	-2.97585500	5.04170600	-0.73806000
H	2.63743400	5.24513700	-0.97811700	H	-1.35309600	5.27636300	-0.13886800
C	2.41734700	5.84689000	1.07036300	C	-1.47616500	5.08538600	-2.27365500
H	2.73142300	5.53672900	2.06589600	H	-2.06862200	4.57114800	-3.02874700
H	2.78355300	6.85878900	0.90780600	H	-1.56404900	6.15473000	-2.45468400
H	1.32892800	5.88357100	1.06486000	H	-0.43427400	4.80774200	-2.42564800
C	-3.23042200	0.03835100	-0.12934400	C	3.31478900	-0.08414800	0.09877700
H	-3.31539900	0.56028400	-1.08018800	H	3.41891200	0.22970900	1.13553200
H	-3.19792700	0.80803700	0.64380900	H	3.34683900	0.82471300	-0.50454800
TMPD-IM				TMPD-TS2			
O	-1.65823200	1.73753600	-0.05733100	O	2.56008600	1.38371400	-0.12609500
C	-2.92412400	1.21683700	-0.07558500	C	3.22101000	0.21178500	-0.32294900
C	0.05429100	-0.43410900	1.61982100	C	3.30555500	2.57153900	-0.35909800
C	-0.46823300	-2.57649500	0.59163600	H	4.16765600	2.59552500	0.30263300
C	-1.56346000	3.15288100	-0.05003400	C	3.66003500	-4.83472100	-0.33111600
H	-2.07711300	3.55933100	-0.91772300	C	4.54451900	-3.86312100	0.11681600
H	-2.05624700	3.54985300	0.83457200	C	2.38298800	-4.45019100	-0.71258800
C	-6.24502700	-2.63340100	-0.06080900	C	2.00150300	-3.11978300	-0.64929500
C	-6.36238500	-1.32897700	0.39661400	C	2.88063000	-2.13100700	-0.19494800
C	-5.01087500	-3.05836500	-0.53476700	C	4.16666200	-2.53209400	0.18890600
C	-3.92787800	-2.19771400	-0.54831800	H	4.86532200	-1.79333400	0.53663400
C	-4.02544900	-0.87339000	-0.08973300	H	5.54169200	-4.14309800	0.42049400
C	-5.28197300	-0.45996700	0.38662400	H	1.67942100	-5.18644200	-1.06939100
H	-5.40091700	0.54689500	0.73876300	H	1.01240300	-2.82844300	-0.96481700
H	-7.31141100	-0.97617600	0.77205100	N	2.40528200	-0.82210500	-0.09538200
H	-4.88961000	-4.06667100	-0.90068600	O	4.38874000	0.21445600	-0.67898600
H	-2.97836200	-2.53800800	-0.92991300	H	1.15973600	-0.57460500	0.42527500
N	-2.86619400	-0.11204900	-0.10497000	H	3.67572500	2.57363500	-1.38087700
O	-3.88360300	1.97883900	-0.08181100	H	3.96102100	-5.86875000	-0.38321200
H	-1.34132500	-0.75757900	0.16339900	N	0.08522900	-0.32710400	0.93218500
H	0.47860500	-2.97298800	0.93644600	C	-0.52600900	-1.60063800	1.33314000
H	-0.75200200	-3.05314200	-0.33812500	C	0.38325500	0.49410300	2.11304600
H	0.17197500	0.62037000	1.41479700	C	-0.66792100	0.40329200	-0.11527500
H	0.97599900	-0.85541900	1.99631800	H	-0.76560400	-2.18170000	0.45126100
H	-7.09206800	-3.30057100	-0.05033700	H	-1.42782800	-1.42941400	1.91235400
N	-0.35497000	-1.12063800	0.37681600	H	-0.51733600	0.70556600	2.68058100
C	0.43662300	-0.76284900	-0.83963800	H	0.84635000	1.41849700	1.79411100
C	1.81346000	-1.38711200	-1.00365700	H	-0.06286100	1.27387700	-0.34001700
H	0.49408000	0.31905000	-0.84871100	H	0.18467800	-2.14949500	1.94146500
H	-0.18961900	-1.06687900	-1.67245900	H	1.07748100	-0.05203400	2.74310300
H	2.10251800	-1.14484300	-2.02621500	H	-0.65740700	-0.23255500	-0.99698700
H	1.74321100	-2.47255400	-0.96743800	C	-2.09981200	0.82441400	0.21765700
C	4.29487200	-1.36604300	-0.52563600	H	-2.28654500	1.75727800	-0.31241500
C	5.39739600	-0.89611800	0.41221000	C	-4.58706300	0.35650500	0.09365000
H	4.31994500	-2.45487000	-0.57585400	C	-5.66500600	-0.62569200	-0.34172500
H	4.47102100	-1.00051600	-1.53594200	H	-4.70380200	0.55318500	1.15969100
N	6.71025600	-1.43731400	0.09512400	H	-4.71170300	1.31021400	-0.41698400
H	5.41925600	0.20315700	0.43147900	N	-7.01246500	-0.22966900	0.03910200
H	5.15008500	-1.21867900	1.42206600	H	-5.59564300	-0.78922100	-1.42692800

C	7.63956100	-1.19405000	1.17848100	H	-5.46509300	-1.58652700	0.12960700
C	7.24089000	-0.91255900	-1.14618500	C	-7.93966400	-1.32605200	-0.14679000
H	7.26552700	-1.63996500	2.09676500	C	-7.47024700	0.93999700	-0.68209700
H	7.80813700	-0.12523700	1.36514300	H	-7.62505800	-2.18367500	0.44271400
H	7.35411700	0.17972100	-1.12844600	H	-8.01882600	-1.64591200	-1.19422200
H	6.59776500	-1.17051700	-1.98141600	H	-8.93153400	-1.03099000	0.18704800
H	-1.23048500	-2.75314300	1.34062800	H	-7.48769600	0.78535200	-1.76931500
H	-0.73369300	-0.57451200	2.35073100	H	-6.83540900	1.79528000	-0.47414000
H	8.60074100	-1.64753800	0.94866700	H	-8.47882400	1.19162300	-0.36376900
H	8.21916600	-1.34721800	-1.33557100	H	-2.18699600	1.06407700	1.27615500
C	-0.09950500	3.53277400	-0.06691100	C	2.39864800	3.75540100	-0.11045600
H	0.37136200	3.10021300	-0.94978200	H	1.53338100	3.68710400	-0.76971300
H	0.39491000	3.09811600	0.80203000	H	2.02398900	3.71171700	0.91215400
C	0.10064800	5.04334700	-0.06715800	C	3.11443000	5.08118900	-0.33818600
H	-0.38134500	5.47160900	0.81211100	H	3.49561800	5.11487100	-1.35909400
H	-0.40259700	5.47378100	-0.93333000	H	3.98424400	5.13899200	0.31664800
C	1.56882300	5.44146700	-0.08449700	C	2.21463800	6.28307700	-0.09312100
H	2.07021000	5.05416400	-0.97017300	H	2.74788900	7.21640500	-0.26197800
H	1.68487800	6.52339100	-0.08467100	H	1.35167600	6.26940300	-0.75711000
H	2.09159400	5.05216900	0.78785400	H	1.84367900	6.29362800	0.93062300
C	2.91626700	-0.90260400	-0.06735400	C	-3.18451900	-0.17208700	-0.18303100
H	2.74298900	-1.26391100	0.94427600	H	-3.04878000	-1.11699300	0.33941400
H	2.89620000	0.18682500	-0.01757600	H	-3.08373200	-0.39174300	-1.24690700

TMPD-PC

O	-1.39993700	1.73176800	0.03249100
C	-2.70929000	1.51477400	-0.12905600
C	-0.97031700	3.09215500	-0.08511800
H	-1.23988400	3.46362600	-1.06910600
C	-6.66777500	-1.79979900	-0.27690100
C	-6.62100900	-0.42606100	-0.44947100
C	-5.48808900	-2.48070900	-0.01193200
C	-4.28814500	-1.79907500	0.07739000
C	-4.24020500	-0.41453500	-0.09592300
C	-5.42503000	0.27192700	-0.36244200
H	-5.40753900	1.33510300	-0.49898100
H	-7.52686600	0.12189000	-0.65640800
H	-5.49715300	-3.55018800	0.12671100
H	-3.37870100	-2.33785700	0.28249900
N	-2.98422900	0.19593600	0.01185600
O	-3.50148800	2.39850300	-0.36650800
H	-2.19280300	-0.41729900	0.21723700
H	-7.60335500	-2.33035100	-0.34696500
H	-1.49016600	3.69140700	0.65625600
N	6.54538500	-1.26772500	0.01543600
N	-0.57133500	-1.57836900	0.61697200
C	7.48485900	-0.46642900	0.77162700
C	7.00807800	-1.42589800	-1.34789000
C	-0.85532700	-2.96740500	0.91949600
C	-0.02406000	-0.89906100	1.77585800
C	5.20838000	-0.69689800	0.08599800
C	0.18692100	-1.40268100	-0.62089000
C	4.11206000	-1.62563800	-0.41597600
C	1.61379800	-1.96500700	-0.70393100
H	7.16558300	-0.39804900	1.80861600
H	7.58729900	0.55461000	0.38083200
H	7.05017600	-0.47293300	-1.89233500
H	6.36145300	-2.10014000	-1.90019300
H	-1.29181500	-3.45491800	0.05176300
H	0.03178900	-3.53396300	1.21806500
H	0.20622400	0.13077800	1.52453000
H	0.87847400	-1.37489500	2.16884700
H	5.15995500	0.25699500	-0.45909200
H	5.01025200	-0.46621500	1.13131000
H	0.20769400	-0.33635500	-0.83742600

H	-0.41003800	-1.86824400	-1.40283000				
H	4.20407400	-2.58288600	0.09800400				
H	4.23970000	-1.82712700	-1.47862000				
H	1.81558900	-2.17182100	-1.75558700				
H	1.66604900	-2.92868800	-0.19796000				
H	8.46766400	-0.93116100	0.74989900				
H	8.00737800	-1.85396200	-1.34544800				
H	-0.76695100	-0.89688600	2.57118400				
H	-1.56909100	-3.02102200	1.73813700				
C	0.52428800	3.13121900	0.12659800				
H	1.00731900	2.49473700	-0.61396600				
H	0.75811600	2.71773700	1.10702900				
C	1.07174600	4.54948600	0.02161900				
H	0.82382200	4.96076300	-0.95703200				
H	0.57599700	5.18343300	0.75695100				
C	2.57712700	4.61029100	0.23150300				
H	3.10142400	4.00904500	-0.50959300				
H	2.94501400	5.63105000	0.15107800				
H	2.85166400	4.23510000	1.21609700				
C	2.71946600	-1.04864500	-0.18656500				
H	2.58670100	-0.85101400	0.87512500				
H	2.64273700	-0.08342000	-0.69030300				
DMAEDMED				DMAEDMED-RC1			
N	3.30129800	0.16699400	0.37879500	O	-3.87489200	-1.62431600	-0.31695700
N	-3.46543000	0.24120500	-0.19341300	C	-4.64361600	-0.65448400	0.34552600
C	4.12380200	1.35068900	0.23740400	H	-5.68119300	-0.98195100	0.28926700
C	3.97471000	-0.97973500	-0.19696100	H	-2.93244600	-1.46082400	-0.11827900
C	-3.75011300	0.37970000	1.21483500	H	-4.38681700	-0.60762900	1.40823100
C	-2.95211100	1.46503600	-0.76779100	N	5.41819300	0.47033700	0.16733300
C	1.98201600	0.38200700	-0.19182000	N	-1.10238600	-1.35911600	0.22586800
C	-2.73824400	-0.96875000	-0.53379500	C	6.14708400	0.83121500	1.36569300
C	0.95106800	-0.63803900	0.26445000	C	5.82639800	1.31432900	-0.93763700
C	-1.38896300	-1.23647200	0.13016300	C	-0.79642500	-2.76135600	0.42816600
H	3.64663500	2.19623300	0.72606600	C	-0.85669400	-0.57513000	1.42309600
H	4.30499500	1.62188000	-0.81085200	C	3.98381900	0.51325500	0.39842500
H	4.13630900	-0.87343100	-1.27783700	C	-0.54517400	-0.80740300	-1.00445500
H	3.40435000	-1.88768700	-0.02997800	C	3.18291500	-0.25135400	-0.64332000
H	-4.17946500	-0.54308100	1.59920300	C	0.95147200	-0.94880500	-1.25955300
H	-2.87117600	0.62242200	1.82327900	H	5.88839800	0.15546800	2.17677000
H	-2.76240800	1.32122000	-1.82894200	H	5.94038200	1.85671400	1.69858100
H	-2.02700500	1.81750500	-0.30534100	H	5.59663000	2.37391000	-0.76408400
H	2.02177200	0.39683600	-1.29077700	H	5.33723300	1.01089100	-1.85750100
H	1.63491000	1.36326400	0.12204400	H	-1.02369400	-3.32143100	-0.47547700
H	-2.60498400	-0.98027500	-1.61550500	H	0.24958100	-2.94098700	0.69064800
H	-3.38189500	-1.81422600	-0.28973500	H	-1.12315000	0.46264200	1.24092200
H	0.89434500	-0.61550500	1.35161500	H	0.18252900	-0.60857100	1.75055300
H	1.25424200	-1.65233200	-0.01500200	H	3.62052800	1.54964900	0.45356400
H	-1.11378300	-2.27384300	-0.10270200	H	3.78386500	0.05971400	1.36590400
H	-1.49058500	-1.18647400	1.21321300	H	-0.81524700	0.24694100	-1.03965900
H	5.08889200	1.18594100	0.71029600	H	-1.05778400	-1.29110900	-1.83511900
H	4.94522600	-1.10653400	0.27609500	H	3.51230100	-1.28907500	-0.64471500
H	-4.47772400	1.17579100	1.36199200	H	3.37210100	0.14113600	-1.64765600
H	-3.70020900	2.25014300	-0.66526500	H	1.13058000	-0.62332600	-2.29260800
N	-0.35538200	-0.29991100	-0.27240700	H	1.23837100	-1.99811000	-1.21907000
H	-0.29884600	-0.30247600	-1.28161300	H	7.21593700	0.74949800	1.18376500
				H	6.89939100	1.22417000	-1.08742600
				H	-1.41474100	-3.15086500	1.23331200
				H	-1.48487300	-0.95030500	2.22824000
				C	-4.51666100	0.72941900	-0.26999300
				H	-3.47284100	1.04537700	-0.22120000
				H	-4.77315600	0.66200000	-1.32785800
				C	-5.39617000	1.76892800	0.41234400
				H	-6.43703000	1.44635300	0.36484100
				H	-5.14060000	1.81947800	1.47151000

				C	-5.26798800	3.15395800	-0.20457800
				H	-5.54968200	3.14274300	-1.25647000
				H	-5.90740800	3.87463400	0.30164700
				H	-4.24369700	3.51855200	-0.14171100
				N	1.76957500	-0.21733600	-0.30968700
				H	1.46423600	0.74620300	-0.30014000
DMAEDMED-RC2				DMAEDMED-TS1			
O	2.44033100	1.19818200	-0.68728900	O	-2.07091800	1.49475700	1.15517000
C	2.52603500	-0.40317900	2.07294700	C	-3.45731300	0.49118700	0.45860900
C	2.81928100	2.52924000	-0.94124800	C	-2.08543200	2.89521700	0.90900600
H	3.90397700	2.53253500	-1.03484500	H	-3.10040000	3.22191900	1.10672300
C	4.48197300	-3.95999400	-1.20198000	C	-5.02866800	-4.06856600	-0.84237800
C	4.14447900	-2.65027000	-1.51384400	C	-5.68741400	-2.84822200	-0.81611900
C	4.29796500	-4.42647400	0.09137000	C	-3.69898900	-4.12749300	-0.44922000
C	3.78030400	-3.59196000	1.06833800	C	-3.03922300	-2.98261600	-0.03630300
C	3.44575400	-2.28212400	0.74660200	C	-3.69579500	-1.75258700	-0.00809800
C	3.62647300	-1.80283900	-0.54769900	C	-5.03362600	-1.69738300	-0.40426100
H	3.35807100	-0.78424900	-0.78029500	H	-5.56165200	-0.75919100	-0.39011200
H	4.28479200	-2.28159200	-2.51743500	H	-6.72102600	-2.78622000	-1.11832500
H	4.55693800	-5.44198900	0.34376800	H	-3.17126200	-5.06801000	-0.46308000
H	3.63253000	-3.94293000	2.07605300	H	-2.00680100	-3.02609900	0.27050200
N	2.92630200	-1.47618400	1.75401800	N	-2.94474400	-0.64629400	0.42820500
O	2.11262400	0.58721400	2.53458900	O	-4.33949100	1.25870100	0.29952900
H	1.46848400	1.11660300	-0.77450800	H	-1.14396200	1.09758100	1.07443500
H	4.88459000	-4.61127300	-1.96063700	H	-1.43371300	3.36839100	1.64043200
H	2.41829900	2.86808300	-1.90049400	H	-5.54343200	-4.95952300	-1.16370500
N	-6.83679000	-0.81886800	0.01121100	N	6.84216100	-1.17611500	-0.18361000
N	-0.31353100	0.71276100	-1.07254600	N	0.42203600	0.49185200	1.14635000
C	-7.93164400	0.01894400	-0.43251500	C	7.96821600	-0.58619200	0.51044200
C	-7.14171100	-1.39439300	1.30571600	C	7.17062800	-1.38498600	-1.57953700
C	-0.21530200	0.00779200	-2.33565200	C	0.32408800	-0.54221200	2.16468800
C	-1.10353700	1.92570200	-1.19203500	C	1.27268000	1.58898500	1.59006400
C	-5.58449500	-0.08099500	0.01306700	C	5.64516300	-0.37064700	-0.00865100
C	-0.66291000	-0.14826300	0.05304200	C	0.73887400	-0.02774400	-0.18606500
C	-4.35765900	-0.97853800	0.03642000	C	4.36232300	-1.11673100	-0.33876300
C	-1.94084800	-0.97697500	-0.02421900	C	1.95154900	-0.93608100	-0.34480700
H	-7.73019800	0.39684800	-1.43151000	H	7.74398300	-0.48989700	1.56963100
H	-8.10619400	0.87865100	0.22748800	H	8.23276000	0.40795400	0.12725000
H	-7.26315700	-0.63174800	2.08624100	H	7.37451000	-0.44464300	-2.10850500
H	-6.35750500	-2.07516900	1.62064800	H	6.36210700	-1.89244000	-2.09562700
H	0.41329700	-0.87119400	-2.21771800	H	-0.32949700	-1.33699400	1.81873100
H	-1.18452000	-0.31152000	-2.72764100	H	1.29353800	-0.97161100	2.42285500
H	-1.14229100	2.43167600	-0.23116300	H	1.31334200	2.35245100	0.81848700
H	-2.12578300	1.73950600	-1.52096800	H	2.28815200	1.26671900	1.81161200
H	-5.53992300	0.62480800	0.85499200	H	5.69628600	0.55286100	-0.60349400
H	-5.54101400	0.51339900	-0.89600900	H	5.59121200	-0.06855100	1.03420700
H	-0.69453000	0.47722600	0.94371800	H	0.84136400	0.82892000	-0.84943800
H	0.16131900	-0.84740300	0.18911100	H	-0.13039700	-0.58801700	-0.52393700
H	-4.38318300	-1.62808500	-0.83700600	H	4.29968600	-2.00122400	0.29296800
H	-4.36765600	-1.63130300	0.91530300	H	4.37009700	-1.46837800	-1.37535400
H	-1.91523800	-1.68023300	0.81839600	H	1.91386900	-1.33467400	-1.36672100
H	-1.93631500	-1.58606000	-0.92646000	H	1.86396400	-1.79509800	0.31762000
H	-8.84874700	-0.56398600	-0.46898700	H	8.05631900	-2.01083400	-1.65479100
H	-8.06743700	-1.96099600	1.24364700	H	8.84057100	-1.22658100	0.40520700
H	0.24528700	0.65840400	-3.07515900	H	0.84195900	2.02925400	2.48618300
H	-0.62631100	2.59163200	-1.90787400	H	-0.10665500	-0.11378800	3.06589800
C	2.39984500	3.48808900	0.15942000	C	-1.67394200	3.25577300	-0.50415300
H	1.31277700	3.46636200	0.25470100	H	-0.66694200	2.88394100	-0.69469600
H	2.80253200	3.12604200	1.10502200	H	-2.33790100	2.75018400	-1.20478200
C	2.86079300	4.91772700	-0.09297700	C	-1.71763000	4.75961500	-0.74602800
H	3.94688300	4.93387200	-0.19223800	H	-2.72446900	5.12699300	-0.54591500
H	2.46195100	5.26366100	-1.04742000	H	-1.06099800	5.25921200	-0.03319200
C	2.44005600	5.87949400	1.00853800	C	-1.31128700	5.13924700	-2.16202500
H	2.85173200	5.57831600	1.97069300	H	-1.97141800	4.67994100	-2.89610700

H	2.78299500	6.89188300	0.80379100	H	-1.35102900	6.21671800	-2.30853800
H	1.35614900	5.91090800	1.10935500	H	-0.29588100	4.81208300	-2.38031100
N	-3.14984500	-0.17410400	-0.02348400	N	3.21169300	-0.27318800	-0.06510000
H	-3.12830400	0.43502600	0.78289200	H	3.27373500	0.55381900	-0.64301500
DMAEDMED-IM				DMAEDMED-TS2			
O	-1.75625400	1.76010300	-0.03825600	O	2.28798000	1.55376700	-0.05143700
C	-2.95869700	1.10928600	0.03567500	C	3.15732800	0.51134100	-0.13432100
C	0.25273500	-0.46910700	1.37175900	C	2.85978700	2.85452000	-0.09993100
C	-0.09708300	-2.45932300	0.01092600	H	3.56866100	2.97045200	0.71579000
C	-1.79879100	3.17226900	0.08714500	C	4.41009700	-4.39678400	-0.15371500
H	-2.45394300	3.58841800	-0.67411700	C	5.01574300	-3.32414000	0.48625300
H	-2.21238400	3.44366100	1.05576600	C	3.19016500	-4.19672300	-0.78293700
C	-5.84180600	-3.07763100	0.13132900	C	2.59123500	-2.94743400	-0.77317900
C	-6.01318900	-1.84212400	0.73898600	C	3.18706400	-1.85939500	-0.12683100
C	-4.66403000	-3.31385400	-0.56523000	C	4.41810700	-2.07429700	0.50590800
C	-3.68797500	-2.33683300	-0.64859000	H	4.90234600	-1.25511300	1.00516000
C	-3.84067500	-1.08099100	-0.03812400	H	5.96391500	-3.46070900	0.98349800
C	-5.04010900	-0.85765800	0.66003800	H	2.70259200	-5.01383800	-1.29180800
H	-5.19950600	0.09297500	1.13260400	H	1.65205400	-2.79747500	-1.28108000
H	-6.92004500	-1.63612300	1.28783900	N	2.49306700	-0.64797400	-0.10035100
H	-4.50417500	-4.26410600	-1.05178900	O	4.35578500	0.71520200	-0.24470500
H	-2.78211100	-2.52972200	-1.20129400	H	1.14782600	-0.62969300	0.15357300
N	-2.77572000	-0.19750100	-0.13279600	H	3.40715200	2.97625400	-1.03097100
O	-3.98145900	1.76004100	0.21401700	H	4.88053100	-5.36690300	-0.16317000
H	-1.17739000	-0.70335400	-0.06913100	N	-0.03546400	-0.57204000	0.43133000
H	0.90378000	-2.79505800	0.25092100	C	-0.50791200	-1.94641600	0.66026200
H	-0.37847800	-2.80351100	-0.97655900	C	-0.11087500	0.21438100	1.66905600
H	0.12265700	0.60468400	1.37443800	C	-0.65965200	0.09666000	-0.73387300
H	1.28365400	-0.72970200	1.56333200	H	-0.43653400	-2.50774100	-0.26364500
H	-6.60561000	-3.83587500	0.19752600	H	-1.53593500	-1.94285000	1.00043400
N	-0.14978700	-0.98456900	0.04517700	H	-1.12421500	0.23014400	2.05698000
C	0.55747700	-0.34228000	-1.10184200	H	0.22801100	1.22328500	1.47311000
C	1.94213800	-0.86785400	-1.42167100	H	0.00163700	0.91516800	-0.99857600
H	0.58080500	0.71978000	-0.88960100	H	0.12804200	-2.40904800	1.40750800
H	-0.08120500	-0.49421900	-1.96600300	H	0.54408600	-0.24282700	2.40323700
H	2.25139200	-0.35664400	-2.34032200	H	-0.64081900	-0.61932000	-1.55085700
H	1.89564900	-1.92611000	-1.66504800	C	-2.06022700	0.65337400	-0.55532100
C	4.22242400	-1.15941900	-0.68124700	H	-2.28230500	1.21813400	-1.46860000
C	5.15823900	-0.97433400	0.50235900	C	-4.40352100	0.18136200	-0.21006000
H	4.16230200	-2.22005000	-0.91783100	C	-5.39790700	-0.92858800	0.09005100
H	4.61240700	-0.65661000	-1.57107000	H	-4.43778600	0.91063300	0.59737300
N	6.49863900	-1.47844500	0.25513800	H	-4.67392700	0.71153700	-1.12833200
H	5.17831400	0.08559900	0.79372900	N	-6.76180500	-0.45161000	0.24584400
H	4.73975300	-1.52247700	1.34259600	H	-5.33277000	-1.70083400	-0.68995000
C	7.21530900	-1.67849000	1.49778200	H	-5.09573600	-1.39880200	1.02244300
C	7.25989400	-0.61593300	-0.62628300	C	-7.58032500	-1.43700900	0.92179100
H	6.67562800	-2.37795000	2.13091500	C	-7.36747900	-0.08249100	-1.01794600
H	7.35797300	-0.74827100	2.06286400	H	-7.16003200	-1.66384700	1.89815900
H	7.40784800	0.38772000	-0.20650900	H	-7.66624200	-2.37723500	0.36175200
H	6.76434800	-0.50895300	-1.58577200	H	-8.58327600	-1.04331300	1.06732300
H	-0.79645200	-2.84184000	0.74380800	H	-7.43416400	-0.92843300	-1.71467000
H	-0.39820200	-0.91393400	2.11552700	H	-6.80272600	0.70774300	-1.50185800
H	8.19753800	-2.09644500	1.29129600	H	-8.37423600	0.28884300	-0.84394100
H	8.23929100	-1.05227900	-0.80555400	H	-2.07495000	1.37543200	0.25781800
C	-0.39196300	3.70609200	-0.06635000	C	1.74152800	3.86646500	0.00597500
H	0.00271200	3.39705900	-1.03432000	H	1.03434100	3.70439600	-0.80737600
H	0.24728600	3.25865600	0.69499500	H	1.19843100	3.70417200	0.93696100
C	-0.33879200	5.22454600	0.04854200	C	2.26053100	5.29830100	-0.04217300
H	-0.74277600	5.52786600	1.01476600	H	2.80977700	5.45203300	-0.97135600
H	-0.98778700	5.66651800	-0.70790900	H	2.97588600	5.45048600	0.76641300
C	1.07019700	5.77652800	-0.10753800	C	1.14721300	6.32943400	0.06514700
H	1.48810800	5.51692400	-1.07902500	H	1.54241600	7.34251900	0.02723300
H	1.08145000	6.86116500	-0.02123600	H	0.43235500	6.22166600	-0.74918000
H	1.73568900	5.37633200	0.65589900	H	0.60085100	6.22139100	1.00087300
N	2.88965100	-0.68918700	-0.33928700	N	-3.05772700	-0.36314500	-0.28158800

H	2.94188500	0.29530000	-0.11544900	H	-3.02727600	-1.05006100	-1.02270400
DMAEDMED-PC							
O	-1.51595000	1.78934000	0.00209000				
C	-2.80682200	1.44424000	0.05758600				
C	-1.23786500	3.19283500	0.01201100				
H	-1.74221300	3.65904900	-0.82886800				
C	-6.43145100	-2.21660900	0.06104100				
C	-6.48454700	-0.89111100	0.46239600				
C	-5.21593800	-2.74562300	-0.34842600				
C	-4.07678700	-1.96030000	-0.35986100				
C	-4.12934100	-0.62674800	0.04704600				
C	-5.34891300	-0.09478300	0.46391900				
H	-5.40562000	0.92889300	0.77949600				
H	-7.42023100	-0.46353300	0.78665800				
H	-5.15064700	-3.77375500	-0.66732200				
H	-3.13934400	-2.37514400	-0.69135100				
N	-2.92883900	0.09594800	0.03736900				
O	-3.70727000	2.25103500	0.11359700				
H	-2.06410900	-0.44586600	-0.03309700				
H	-7.32018000	-2.82647000	0.06610500				
H	-1.63454600	3.62547300	0.92562200				
N	6.46044600	-1.39390400	0.25554500				
N	-0.34575200	-1.46352900	0.07782900				
C	7.22456100	-1.34569400	1.48496800				
C	7.09639000	-0.57751900	-0.75888900				
C	-0.49892100	-2.90443500	0.07276300				
C	0.09833600	-0.98436700	1.37498500				
C	5.07697600	-1.01316500	0.48737100				
C	4.08306600	-0.95666200	-1.06372900				
C	4.13676000	-1.45099500	-0.62435700				
C	1.81826300	-1.48404200	-1.31343100				
H	6.78347100	-2.00955000	2.22394600				
H	7.27272400	-0.33828900	1.91852900				
H	7.13463200	0.48394900	-0.48062800				
H	6.57154000	-0.65791600	-1.70524600				
H	-0.85312800	-3.23660600	-0.89989600				
H	0.43042000	-3.43626600	0.29697300				
H	0.19532000	0.09663900	1.34959200				
H	1.05228600	-1.41004400	1.68686900				
H	4.98348100	0.07163000	0.64126500				
H	4.74451500	-1.48907700	1.40643200				
H	0.44303400	0.12699700	-0.97367400				
H	-0.17684600	-1.17875200	-1.95539200				
H	4.18942900	-2.53425800	-0.72074900				
H	4.44851700	-1.03329500	-1.58728000				
H	2.11573100	-1.13408400	-2.31075900				
H	1.80967500	-2.57146200	-1.36505600				
H	8.24326200	-1.67614700	1.29721600				
H	8.11621500	-0.92012500	-0.91517200				
H	-0.65264800	-1.23812200	2.12092100				
H	-1.23345800	-3.19339900	0.82035800				
C	0.25900400	3.37259000	-0.07739300				
H	0.62197500	2.89609600	-0.98749300				
H	0.73184800	2.86366400	0.76198400				
C	0.65234500	4.84485300	-0.07474400				
H	0.16602500	5.35018500	-0.90931100				
H	0.27660600	5.31744400	0.83289500				
C	2.15725100	5.04679100	-0.16660200				
H	2.55654000	4.61218100	-1.08164100				
H	2.41345800	6.10418100	-0.16236500				
H	2.66831300	4.57802200	0.67285100				
N	2.77121800	-1.08310500	-0.29444300				
H	2.72456100	-0.07864000	-0.19194000				