

Supplementary Information

Stoichiometric reaction and catalytic effect of 2-dimethylaminoethanol in urethane formation

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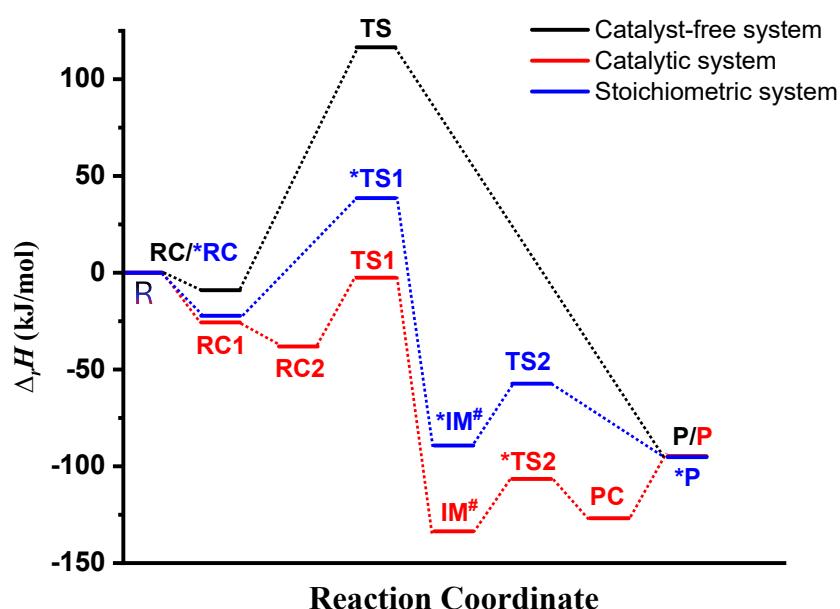


Figure S1. Relative enthalpy ($\Delta_r H$) profiles of the catalyst-free, catalytic, and stoichiometric urethane formation reactions, where the latter two involves 2-dimethylaminoethanol (DMEA) as catalyst or reactant as follows: phenyl isocyanate (PhNCO)-butan-1-ol (BuOH) (catalyst-free system) - black line; PhNCO-BuOH and DMEA (catalyst) - red line; PhNCO-DMEA (stoichiometric reaction) - blue line. The energies were calculated at the G3PMP2BHandHLYP level of theory at (298.15 K and 1 atm) in acetonitrile using the SMD implicit solvent model. #Corrected relative enthalpies of IM calculated according to Ref.47,48.

Table S1. Zero-point corrected relative energies ($\Delta_r E_0$), enthalpies ($\Delta_r H$), relative Gibbs free energies ($\Delta_r G$), and entropies ($\Delta_r S$) of the reaction between phenyl isocyanate and butan-1-ol in the presence 2-dimethylaminoethanol (DMEA) (catalytic system), and reaction between 2-dimethylaminoethanol (DMEA) and phenyl isocyanate (PhNCO) (stoichiometric), 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.

	$\Delta_r E_0$ (kJ/mol)							
	R	RC1	RC2	TS1	IM	TS2	PC	P
Catalyst-free system	0.0	-	-10.48'	122.75	-	-	-	-120.94
Catalytic system	0.0	-25.35	-37.91	13.59	-86.98	-96.11	-138.33	-120.94
Stoichiometric system	0.0	*-17.68	-	*44.49	*-46.78	*-52.21	-	*-118.02
	$\Delta_r H$ (kJ/mol)							
	R	RC1	RC2	TS1	IM	TS2	PC	P
Catalyst-free system	0.00	-	-8.23'	120.13	-	-	-	-123.20

Catalytic system	0.0	-24.04	-33.85	13.04	-88.21 (-126.31 [#])	-98.45	-138.50	-123.20
Stoichiometric system	0.0	*-15.89	-	*40.03	*-51.44 (-89.54 [#])	*-57.40	-	*-121.32
$\Delta_r G$ (kJ/mol)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
Catalyst-free system	0.0	-	29.65'	173.69	-	-	-	-69.89
Catalytic system	0.0	16.44	49.00	111.31	15.66 (-9.24 [#])	8.69	-41.55	-69.89
Stoichiometric system	0.0	*24.04	-	*100.13	*12.68 (-12.22 [#])	*7.88	-	*-64.77
$\Delta_r S$ (Cal/mol*K)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
Catalyst-free system	0.0	-	-30.4'	-97.3	-	-	-	-42.73
Catalytic system	0.0	-32.45	-66.42	-78.78	-83.28	-85.89	-77.72	-42.73
Stoichiometric system	0.0	*-32.01	-	*48.18	*51.40	*-52.34	-	*-45.33

' RC for catalysts-free reaction. * pathway for stoichiometric reaction. # Corrected values calculated according to ref. 47,48.

Table S2. Zero-point corrected relative energies ($\Delta_r E_0$), enthalpies ($\Delta_r H$), and entropies ($\Delta_r S$) of the reaction between phenyl isocyanate (PhNCO) and butan-1-ol in the presence 2-dimethylaminoethanol (DMEA) (catalytic system), and DMEA with PhNCO (stoichiometric system), calculated at the G3MP2BHandHLYP level of theory at (298.15 K and 1 atm) in acetonitrile using the SMD implicit solvent model. R—reactant; RC—reactant complex; TS—transition state; IM—intermediate; PC—product complex; P—product.

$\Delta_r E_0$ (kJ/mol)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
Catalyst-free system	0.0	-	-11.22'	119.11	-	-	-	-92.58
Catalytic system	0.0	-26.96	-42.13	-2.00	-94.27	-104.16	-126.62	-92.58
Stoichiometric system	0.0	*-23.98	-	*43.09	*-46.53	*-52.07	-	*-91.93
$\Delta_r H$ (kJ/mol)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
Catalyst-free system	0.0	-	-8.97'	116.49	-	-	-	-94.84
Catalytic system	0.0	-25.66	-38.08	-2.56	-95.51 (-133.61 [#])	-106.51	-126.79	-94.84
Stoichiometric system	0.0	*-22.19	-	*38.63	*-51.19 (-89.29 [#])	*-57.27	-	*-95.23
$\Delta_r S$ (Cal/mol*K)								
	R	RC1	RC2	TS1	IM	TS2	PC	P
Catalyst-free system	-	-	-30.36'	-42.94	-	-	-	-42.73
Catalytic system	0.0	-32.45	-66.42	-78.78	-83.28	-85.89	-77.72	-42.73
Stoichiometric system	0.0	*-32.01	-	*-101.64	*-141.43	*-122.97	-	*-111.81

' RC for catalysts-free reaction. * pathway for stoichiometric reaction. # Corrected values calculated according to ref. 47,48..

Table S3. Cartesian coordinates of the stationary points for the studied species. The structures 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, P – product. * Pathway for autocatalysis.

Keywords included in the input files to carry out the calculations on the studied structures:

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# bhandhlyp/6-31g(d) opt=(tight) freq scrf=(smd,solvent=acetonitrile)
# bhandhlyp/6-31g(d) opt=(calcfc,tight,ts,noeigentest) freq scrf=(smd,solvent=acetonitrile)
# MP2/GTMP2large scrf=(smd,solvent=acetonitrile)
# QCISD(T)/6-31G(d) scrf=(smd,solvent=acetonitrile)
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DMEA				DMEA-RC1		
N	0.98199200	-0.00776600	-0.32318300	N	-1.54343300	-0.89098700 0.37213700

C	2.02600000	-0.97351300	-0.04972200	C	-1.99075600	-2.24419600	0.08954700
H	2.21312600	-1.10703600	1.02355100	H	-2.84261200	-2.53945400	0.71116200
H	2.95512900	-0.65067400	-0.51282900	H	-1.17834400	-2.94178000	0.27302400
H	1.75690900	-1.94029800	-0.46728800	H	-2.28307700	-2.32481900	-0.95340800
C	1.37127500	1.30307000	0.15733200	C	-1.05946900	-0.79382600	1.73951600
H	2.31932200	1.58708000	-0.29218600	H	-0.26819500	-1.52152200	1.89476500
H	1.49065100	1.33337000	1.24820000	H	-1.85279800	-0.98729800	2.46965800
H	0.63638800	2.05146100	-0.12199900	H	-0.65105000	0.19209000	1.93304200
C	-0.28587900	-0.44737000	0.22990300	C	-2.59892300	0.07136700	0.08575000
C	-1.47204300	0.32111300	-0.31720100	C	-2.09605800	1.49938300	0.00657000
H	-0.29532600	-0.39051500	1.32639000	H	-3.40572900	0.00850100	0.82429800
H	-0.42763600	-1.49245400	-0.03546500	H	-3.02667000	-0.17777300	-0.88194000
H	-1.44742500	0.28951600	-1.40773200	H	-1.27165100	1.55088600	-0.70553900
H	-1.43952800	1.36717300	-0.01433500	H	-1.72561400	1.84290800	0.97187100
O	-2.63464600	-0.30203300	0.18765400	O	-3.18734400	2.29094600	-0.41320900
H	-3.39449500	0.20319100	-0.10713600	O	0.39907300	-0.50231900	-1.68402800
				C	1.69643100	-0.80013300	-1.23469400
				H	1.71645600	-1.75932500	-0.70886100
				H	2.31838000	-0.91588700	-2.12145100
				H	-0.21798400	-0.60617000	-0.93548300
				H	-2.90142400	3.20621700	-0.42983100
				C	2.28235400	0.28198700	-0.34296700
				H	1.64396800	0.40326300	0.53391300
				H	2.25424800	1.22871200	-0.88374300
				C	3.70767200	-0.01937700	0.10157700
				H	4.34041100	-0.14345600	-0.77814300
				H	3.72761500	-0.97396500	0.62891600
				C	4.29294600	1.06353900	0.99604900
				H	3.70100100	1.18698300	1.90180500
				H	5.31095000	0.82270100	1.29630500
				H	4.31713000	2.02461400	0.48448100
DMEA-RC2				DMEA-TS1			
N	1.27623500	2.30394600	0.80649200	O	0.92628100	-0.59321000	-1.29183700
C	1.34091000	2.11250600	2.24560500	C	-0.65890800	-1.31349400	-0.73151700
H	1.36544400	3.06245100	2.78956400	C	2.09500000	-1.40167200	-1.20288700
H	2.23592100	1.55168700	2.49951400	H	1.79964800	-2.38520700	-1.55003100
H	0.47519900	1.54815100	2.58025700	C	-5.40041100	-0.40624600	0.55850200
C	2.46862300	2.98769900	0.33185400	C	-4.67660700	-1.58862100	0.51423700
H	3.34931200	2.43367900	0.64312500	C	-4.77280800	0.78346600	0.21652400
H	2.54454200	4.00507300	0.73048000	C	-3.44187900	0.78876300	-0.16411100
H	2.47322600	3.04319100	-0.75151400	C	-2.70863300	-0.39679600	-0.21202500
C	0.05085000	3.00214700	0.44098200	C	-3.34367900	-1.59165300	0.13353300
C	-0.20979300	3.00765500	-1.05248300	H	-2.79840900	-2.51954600	0.10481500
H	0.05455600	4.03195700	0.81503100	H	-5.15034400	-2.52126700	0.77763400
H	-0.77929200	2.48757000	0.91814600	H	-5.32046300	1.71221900	0.24501100
H	-0.11081900	1.99438900	-1.44121100	H	-2.95225300	1.71084900	-0.43251500
H	0.50475700	3.64054800	-1.57653400	N	-1.36395800	-0.28937500	-0.60843600
O	-1.52255400	3.50124600	-1.23527100	O	-0.48165000	-2.48076100	-0.69683400
O	0.92522200	-0.30313500	-0.28162700	H	1.09728100	0.36159700	-1.02052600
C	-0.68109800	-3.06929800	0.18697400	H	2.82514700	-1.00348300	-1.90370200
C	2.06718900	-0.72303200	-0.99036700	H	-6.43673400	-0.41177900	0.85516600
H	1.76386400	-1.57203600	-1.59841900	N	1.52271400	2.00845000	-0.81434700
C	-4.62624800	0.28566800	-0.13259700	C	0.45691300	2.77516900	-1.44988800
C	-3.29156400	0.53317700	-0.42573800	C	2.75665800	2.16030500	-1.57657100
C	-5.01203500	-0.97042800	0.31182000	C	1.73720300	2.40582600	0.57516500
C	-4.07289000	-1.97776600	0.46511400	H	-0.48274600	2.62667300	-0.93176800
C	-2.74018800	-1.72259900	0.16842500	H	0.68558800	3.84422300	-1.46360300
C	-2.34299100	-0.46603900	-0.27829600	H	3.54038400	1.55309000	-1.13433800
H	-1.30150200	-0.28828700	-0.49453200	H	3.09417500	3.19990500	-1.59922700
H	-2.97852100	1.50917900	-0.76309300	H	1.88023300	3.48792200	0.64926400
H	-6.04614500	-1.17028000	0.54167600	H	2.59452200	1.83020900	-2.59843300
H	-4.36083000	-2.95686800	0.81017400	H	0.33426500	2.43472900	-2.47369700
N	-1.82118300	-2.75657700	0.33153500	H	2.65221100	1.93328200	0.92126600
O	0.39245100	-3.51859100	0.09295200	C	0.62156900	1.98376600	1.51007200
H	1.10203700	0.57726400	0.10570900	H	0.47129800	0.90626900	1.44238700
H	2.40367500	0.05875300	-1.67663700	H	-0.31903800	2.46690400	1.24959000
H	-5.35980100	1.06707100	-0.24853500	O	1.02949600	2.36119500	2.80791800
H	-1.68770000	3.56570800	-2.17822000	H	0.32397000	2.13698100	3.41761600
C	3.20830700	-1.13262700	-0.07624200	C	2.66336100	-1.47601700	0.19942900
H	3.49019900	-0.28104800	0.54598000	H	2.91684800	-0.47252100	0.54195300
H	2.84586000	-1.90857300	0.59774400	H	1.89567300	-1.85882200	0.87122100

C	4.42876800	-1.63312500	-0.83797500	C	3.89860900	-2.36597400	0.26724300
H	4.14068100	-2.47977600	-1.46238600	H	4.65618700	-1.98521000	-0.41830400
H	4.77455900	-0.85491400	-1.51959200	H	3.64122800	-3.36572500	-0.08338300
C	5.57145200	-2.04630800	0.07784000	C	4.48208700	-2.45414600	1.66940400
H	6.42876100	-2.39960000	-0.49196000	H	3.75611200	-2.86096500	2.37159200
H	5.90365400	-1.21083500	0.69235700	H	5.36061300	-3.09578300	1.69143500
H	5.26628900	-2.84797900	0.74874800	H	4.77946300	-1.47191200	2.03342200
DMEA-IM				DMEA-TS2			
N	-0.18985000	1.94383700	1.02514000	O	1.28261800	-0.79969200	0.00988000
C	-1.25089100	2.26555400	2.00323200	C	0.06101800	-1.35996200	-0.19299600
H	-1.02571800	3.21494500	2.47589100	C	2.40551000	-1.64152100	-0.21292300
H	-1.28220000	1.47924300	2.74741200	H	2.34198700	-2.51270100	0.43404800
H	-2.20108500	2.32148700	1.48914400	C	-5.00938800	-1.33972000	-0.25102100
C	1.11307400	1.82544500	1.71324600	C	-4.12318100	-2.32380200	0.16449300
H	1.01480100	1.09038300	2.50197600	C	-4.50894200	-0.08910000	-0.58296300
H	1.37720300	2.78911300	2.13456500	C	-3.15000400	0.16758000	-0.50409700
H	1.86725600	1.49619000	1.01572000	C	-2.24473500	-0.81393700	-0.08349400
C	-0.17857300	2.93744300	-0.07554600	C	-2.76345000	-2.07164900	0.25191900
C	0.76852000	2.57419100	-1.20225000	H	-2.09319900	-2.84748600	0.57293500
H	0.07189500	3.90644100	0.34491100	H	-4.49313000	-3.30230300	0.43048500
H	-1.18680600	2.98026700	-0.47240900	H	-5.17672000	0.69155200	-0.91330000
H	0.59102100	1.54725300	-1.51924400	H	-2.77000700	1.13850100	-0.78078000
H	1.80677800	2.65783000	-0.88664000	N	-0.90046300	-0.45918700	0.03147000
O	0.48545000	3.49076600	-2.23440000	O	-0.03200700	-2.52373800	-0.55116600
O	1.24789400	-0.84073200	0.00039800	H	-0.55347800	0.79138200	0.53986700
C	0.01622300	-1.40934400	-0.17308000	H	2.39797900	-1.99476600	-1.24091200
C	2.36516400	-1.69406500	-0.18498900	H	-6.06612000	-1.54391000	-0.31553300
H	2.30123800	-2.53797900	0.49775300	N	-0.31033700	1.86210400	1.03088400
H	2.35897100	-2.09320000	-1.19669300	C	-1.42343500	2.16189800	1.94657500
C	-5.06651000	-1.29159400	-0.19370300	C	0.94339300	1.76584900	1.79542300
C	-4.18421500	-2.32856600	0.07334400	C	-0.24728900	2.86727600	-0.04905200
C	-4.54838800	-0.02115300	-0.40749800	H	-2.34702300	2.22064900	1.38481500
				H	-1.24480100	3.10551600	2.45486600
				H	1.16848100	2.72525400	2.25395700
				H	1.75243900	1.46360900	1.14791000
				H	-1.49794500	1.36498600	2.67794100
				H	0.81861400	1.01616100	2.56810600
				H	-1.23494300	2.92369100	-0.49433300
				H	-0.01558300	3.83729800	0.38942100
				C	0.74768700	2.53105900	-1.14956900
				H	1.77094400	2.53540700	-0.78081600
				H	0.54007700	1.54427300	-1.54897600
				O	0.59998100	3.44058700	-2.21605500
				H	0.94198800	4.29152300	-1.93194000
				C	3.65717300	-0.84380200	0.07534400
				H	3.67483600	0.03658600	-0.56702600
				H	3.62380600	-0.48620800	1.10431900
				C	4.92225800	-1.66438600	-0.14265000
				H	4.89338500	-2.54897900	0.49414500
				H	4.94495500	-2.02671200	-1.17070800
				C	6.19032800	-0.87458500	0.14448900
				H	6.21078600	-0.52592700	1.17591600
				H	7.07872800	-1.48151400	-0.01783400
				H	6.26316400	-0.00075100	-0.50119100
NEM-PC							
	N	-0.22023700	2.07431600	1.01886200			
	C	-1.04634100	2.16907500	2.21020100			
	H	-0.90580400	3.11814600	2.73915400			
	H	-0.79546400	1.36082700	2.89177100			
	H	-2.09487300	2.07894900	1.94331800			
	C	1.18494900	2.13727000	1.38636800			
	H	1.40450300	1.35197200	2.10300500			
	H	1.44536200	3.10048500	1.83947400			
	H	1.81692600	1.98199000	0.52007900			
	C	-0.58509900	3.10761800	0.06074400			
	C	0.01362500	2.88904100	-1.31456000			
	H	-0.30456400	4.10359700	0.42255400			
	H	-1.66655400	3.09899700	-0.04908800			
	H	-0.21929000	1.87943300	-1.65714000			
	H	1.09788000	2.99105300	-1.29513800			
	O	-0.55755100	3.86169800	-2.16398300			

O	1.38824600	-0.92310600	0.00584700
C	0.23565000	-1.58245200	-0.14228700
C	2.58089000	-1.68201800	-0.21217700
H	2.60135900	-2.51653300	0.48243100
H	2.56590900	-2.08329400	-1.22109400
C	-4.91501400	-1.57838800	-0.14812400
C	-4.01167300	-2.62295200	-0.03068200
C	-4.43472700	-0.27754100	-0.19201800
C	-3.07517300	-0.02824200	-0.12484900
C	-2.16574200	-1.07946100	-0.00281000
C	-2.64713000	-2.38700900	0.04681700
H	-1.96038700	-3.20600000	0.13949200
H	-4.36682400	-3.64070800	0.00789000
H	-5.11853000	0.55110500	-0.28583500
H	-2.71019600	0.98453000	-0.17367200
N	-0.80688300	-0.75028100	0.09242700
O	0.17262200	-2.75236500	-0.44610000
H	-0.57774300	0.21986300	0.31802900
H	-5.97356200	-1.77341700	-0.20509900
H	-0.14463500	3.78319900	-3.02597500
C	3.76138200	-0.76338600	-0.00366300
H	3.68617300	0.07650000	-0.69359900
H	3.72183900	-0.35391200	1.00503400
C	5.08519800	-1.48791600	-0.21510900
H	5.14673500	-2.33468000	0.46875600
H	5.11290500	-1.90307100	-1.22273400
C	6.28744600	-0.57945100	-0.00729400
H	7.21976300	-1.11830800	-0.16294800
H	6.26977100	0.26020700	-0.70032400
H	6.30315400	-0.17410700	1.00319200
DMEA-RC			
O	2.23468800	1.23992600	-1.24078200
C	-0.35925300	2.28101600	0.14125600
C	3.23549600	0.99404600	-0.28162900
H	4.14937300	1.46591900	-0.63288500
C	-4.01345000	-1.33635000	-0.12591200
C	-4.13711000	-0.02641900	0.31655600
C	-2.78232200	-1.79903800	-0.56622500
C	-1.67845400	-0.96163600	-0.56624200
C	-1.81022300	0.34765500	-0.12296900
C	-3.04141500	0.81991200	0.32090900
H	-3.13328000	1.83803200	0.66312200
H	-5.09025600	0.34128400	0.66063500
H	-2.67704900	-2.81474700	-0.91142400
H	-0.71617000	-1.30884800	-0.90353300
N	-0.67630300	1.16238500	-0.13980700
O	0.05782400	3.34074200	0.38392700
H	2.97905300	1.45881600	0.67217000
H	-4.87032100	-1.99006600	-0.12710900
C	3.47036600	-0.49544000	-0.11303300
H	3.83271300	-0.88777600	-1.06005700
H	4.25094800	-0.66986800	0.63727800
N	2.23470000	-1.19391200	0.21251400
C	2.32929700	-2.60849800	-0.08860300
H	3.10259000	-3.11510300	0.50150700
H	1.37880300	-3.09279400	0.12001500
H	2.55982700	-2.74952200	-1.14103100
C	1.83548300	-0.99498500	1.59254800
H	0.88455200	-1.48948100	1.77130100
H	2.56956400	-1.39928400	2.30014900
H	1.70553500	0.06079600	1.80811500
H	1.53475000	0.60640200	-1.05230900
DMEA-IVM*			
O	1.71874800	1.47933500	0.72416000
C	0.38151200	1.49771200	0.30123700
C	2.67099500	1.36443400	-0.30581600
H	2.57286700	2.16765400	-1.03331100
C	-4.19510300	-0.69296300	-0.18854000
C	-3.78447000	0.61693800	-0.38351400
C	-3.25778700	-1.62584700	0.23814700
C	-1.94635500	-1.25015400	0.46144800
DMEA-TS1*			
O	-1.46177000	-0.83611100	-0.69007100
C	-0.01411500	-1.08592700	-0.26544500
C	-2.52753700	-1.55645700	-0.03301100
H	-2.76065200	-2.44287700	-0.60497800
C	4.71067000	0.59418600	0.22332500
C	4.16928300	-0.66995600	0.40135900
C	3.87483700	1.63164200	-0.16939100
C	2.52691300	1.40299800	-0.37819300
C	1.96613000	0.13224500	-0.20117100
C	2.81811400	-0.90704100	0.19555100
H	2.41831900	-1.89402600	0.34051100
H	4.80391500	-1.48826700	0.70549200
H	4.27418800	2.62352800	-0.31411400
H	1.87690300	2.20722700	-0.68456600
N	0.59795000	0.02592400	-0.44825700
O	0.16626800	-2.21871600	0.10969400
H	-2.19823900	-1.83162300	0.96006300
H	5.76205100	0.76852800	0.38673300
C	-3.67147100	-0.53714500	-0.03113200
H	-4.18950000	-0.57196700	-0.98251400
H	-4.38224100	-0.75604200	0.76140900
N	-3.05241500	0.78517200	0.10629400
C	-3.76262500	1.83795100	-0.60686400
H	-4.75547900	2.00762300	-0.18796300
H	-3.19301800	2.75903400	-0.53726700
H	-3.86158300	1.56681700	-1.65256000
C	-2.80167300	1.14596200	1.49812700
H	-2.21209600	2.05610700	1.53082000
H	-3.73510800	1.30654400	2.03888900
H	-2.24353000	0.35761900	1.99302500
H	-1.78981800	0.16196800	-0.51515200
DMEA-TS2*			
O	-1.83772200	1.58786600	-0.53819000
C	-0.47509800	1.61497300	-0.27724200
C	-2.73316600	1.20624200	0.49087800
H	-2.70913500	1.92595700	1.30717300
C	4.08302300	-0.68250900	0.14263500
C	3.70503200	0.63664500	0.33856700
C	3.11179400	-1.60698000	-0.21919600
C	1.79522200	-1.21539200	-0.37785900

C	-1.51016200	0.07047500	0.26422000	C	1.39882700	0.11449600	-0.17789500
C	-2.46952400	1.00246500	-0.16555700	C	2.38677700	1.04047100	0.18285100
H	-2.17013400	2.02000400	-0.32931000	H	2.11253500	2.06632800	0.33641700
H	-4.49690600	1.35817000	-0.71357500	H	4.44497500	1.37088300	0.61863700
H	-3.55052800	-2.65211600	0.39976000	H	3.38014800	-2.63942800	-0.38158100
H	-1.22554300	-1.97857800	0.80000000	H	1.05005000	-1.93955600	-0.66762400
N	-0.17143900	0.31974900	0.53248500	N	0.04690300	0.39245900	-0.35502400
O	-0.04200700	2.53543200	-0.18595400	O	0.05001800	2.69482500	-0.08531900
H	3.64093500	1.45610000	0.16902500	H	-3.71436400	1.25376600	0.03371900
H	-5.21938400	-0.98134400	-0.36292500	H	5.11062000	-0.98460500	0.26584300
C	2.54184500	0.03141100	-1.03353600	C	-2.47405800	-0.18281600	1.06355400
H	1.74965700	0.07094000	-1.77221400	H	-1.71700700	-0.13761700	1.83900300
H	3.46859100	-0.23617600	-1.52983700	H	-3.38917300	-0.57054500	1.50475900
N	2.16974400	-1.06573100	-0.09656000	N	-1.96284600	-1.12177300	0.04580200
C	1.89501800	-2.31705700	-0.83400900	C	-1.61696200	-2.41201400	0.65464800
H	2.79906600	-2.63970500	-1.33685600	H	-2.50498600	-2.88500200	1.06548600
H	1.57227600	-3.07178800	-0.12806900	H	-1.18360000	-3.05506800	-0.10224800
H	1.11164900	-2.13024600	-1.55766000	H	-0.89411300	-2.25090900	1.44615800
C	3.15935800	-1.28323100	0.97905800	C	-2.86286400	-1.29948300	-1.09984700
H	2.81127500	-2.09713900	1.60275500	H	-2.40473600	-1.99457300	-1.79406500
H	4.11431900	-1.53840200	0.53447800	H	-3.81931700	-1.69698100	-0.76996700
H	3.24411200	-0.38395700	1.57210100	H	-3.00941200	-0.35018500	-1.59763900
H	1.26372600	-0.74477900	0.32968800	H	-0.95042100	-0.55058800	-0.27800800
DMEA-P*							
	O	-1.18494700	0.26369300	-1.16840300			
	C	-0.08900600	0.66529400	-0.52268000			
	C	-2.36698100	1.04992600	-1.00394400			
	H	-2.10847300	2.10199300	-1.03518900			
	C	4.87475000	-0.29767300	0.61191900			
	C	4.04585700	0.74777000	0.98579700			
	C	4.36890300	-1.29680900	-0.20784700			
	C	3.05743400	-1.24882800	-0.64374100			
	C	2.22493600	-0.19535700	-0.26496800			
	C	2.72787400	0.81059400	0.55709600			
	H	2.09640000	1.62535200	0.85385100			
	H	4.42265200	1.53287300	1.62212600			
	H	4.99553300	-2.12016100	-0.51140200			
	H	2.66946600	-2.02869300	-1.28066600			
	N	0.91108000	-0.22260900	-0.74714700			
	O	-0.01882600	1.67093200	0.14470500			
	H	-2.96901500	0.81684300	-1.87267200			
	H	5.89670100	-0.33465400	0.95220600			
	C	-3.08848200	0.74700300	0.29196900			
	H	-2.43774000	1.02392700	1.11599900			
	H	-3.96311400	1.41128600	0.33631100			
	N	-3.45810000	-0.64545100	0.45938900			
	C	-3.87099900	-0.90213800	1.82321800			
	H	-4.76661500	-0.33686700	2.11222700			
	H	-4.08925100	-1.95982100	1.94784700			
	H	-3.07062100	-0.63771700	2.50958200			
	C	-4.48557500	-1.06618500	-0.46991700			
	H	-4.72067000	-2.11350400	-0.29946000			
	H	-5.41339700	-0.48867400	-0.36470100			
	H	-4.14279800	-0.96948700	-1.49554300			
	H	0.66800100	-1.00486400	-1.32803700			