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SUPPLEMENTARY MATERIAL TO

The evaluation of chemoselectivity in multicomponent domino Knoevenagel/Diels–Alder reaction: A DFT study

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Table S-I. Energy of the relevant optimized transition states, intermediates, and products (**5** and **6**) compared to Gibbs free energy of starting materials in the gas phase

Gas		TS ($\Delta G^{\#}$ / kcal mol^{-1})	Int.	Product	Gas		TS ($\Delta G^{\#}$ / kcal mol^{-1})	Int.	Product
7	**8**	**9**-*SR* (TS) (Endo-y)	**9**-*SR*	**5**-*RS*	**7**	**8**	**9**-*SR* (TS) (Endo-y)	**9**-*SR*	**6**-*RS*
a	a	27.31	-17.16	-23.24	b	b	23.24	-16.61	-24.96
a	b	24.92	-15.44	-23.50	c	c	25.98	-21.05	-23.42
a	c	28.73	-19.84	-25.96					

(a = H, b = OCH_3, c = NO_2)

Table S-II. Optimized geometries (Cartesian coordinates x, y, z (in Å)) of the structures (a=H, b=OCH_3, c=NO_2) at the M062x/6-31+G(d,p) level of theory. Gibbs free energy is presented for compounds in gas phase and methanol.

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
(2a)	*G* = -345.358832 a. u. (Gas phase) *G* = -345.366162 a. u. (In methanol)			**(2b)**	*G* = -459.8130250 a. u. (Gas phase) *G* = -459.8239810 a. u. (In methanol)		
C	1.62532900	-1.21637200	0.00000000	C	-0.83956500	1.03795500	0.00020800
C	0.58745200	-2.14676000	0.00000000	C	-1.29140500	-0.28468200	0.00015800
C	-0.74422300	-1.72166900	0.00000000	C	-0.37274600	-1.34820300	0.00003500
C	-1.04023500	-0.36427000	0.00000000	C	0.98143400	-1.08825500	-0.00004100
C	0.00000000	0.57082400	0.00000000	C	1.44660400	0.23510900	-0.00001500
C	1.32951400	0.14484300	0.00000000	C	0.53099000	1.28275700	0.00013200
C	-0.29941600	2.02300000	0.00000000	C	2.89544000	0.51483400	-0.00008700
H	0.58857800	2.68838300	0.00000000	H	3.16276200	1.59342800	-0.00012300
O	-1.41628900	2.48862600	0.00000000	O	3.75627600	-0.33521000	-0.00011800
H	2.65750200	-1.55083000	0.00000000	H	-1.53564300	1.86777800	0.00041100
H	0.81482800	-3.20826900	0.00000000	H	-0.76328700	2.36015200	0.00001200
H	-1.54607200	-2.45285600	0.00000000	H	1.70950200	-1.89365300	-0.00010600
H	-2.06468900	-0.00457500	0.00000000	H	0.89132600	2.30925900	0.00014900
H	2.12964400	0.88157000	0.00000000	O	-2.59486000	-0.64374100	0.00030000
				C	-3.56315700	0.38464400	-0.00041300
				H	-3.47513300	1.01122300	-0.89557600
				H	-4.53172200	-0.11407200	0.00035300

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Atom	*x* / Å	*y* / Å	*z* / Å
(3)	*G* = -534.077618 a. u. (Gas phase)		
	G = -534.092167 a. u. (In methanol)		
O	-0.40835700	1.17791500	-0.35373900
C	0.91363100	1.27618000	-0.08696900
C	1.60005600	0.00001100	0.35178400
C	0.91366400	-1.27615300	-0.08703400
O	-0.40833800	-1.17792100	-0.35375100
C	-1.12773700	-0.00001000	0.01664600
C	-2.38585700	-0.00001200	-0.82194900
C	-1.41267300	-0.00001500	1.51133400
O	1.48525100	-2.31979600	-0.22616400
O	1.48521900	2.31980900	-0.22618900
H	2.62030800	0.00002900	-0.03244400
H	1.67468700	-0.00000900	1.44520500
H	-2.11456400	-0.00000800	-1.87883700
H	-2.97332900	-0.89239700	-0.59862700
H	-2.97333800	0.89236600	-0.59862300
H	-1.98863700	-0.89105900	1.76874600
H	-0.49318300	-0.00001100	2.10170800
H	-1.98864800	0.89102000	1.76875300
(3-Enol)	*G* = -534.0617660 a.u. (Gas phase)		
	G = -534.0826691 a.u. (In methanol)		
O	0.46638400	-1.30611300	-0.14223500
C	-0.82691200	-1.22168900	0.04158100
C	-1.57079000	-0.00492600	0.43391700
C	-0.95008300	1.22871900	-0.12032800
O	0.36086700	1.02804000	-0.53131700
C	1.15000100	-0.01491100	0.01455500
C	2.38418900	-0.11922400	-0.84960600
C	1.45347600	0.21702300	1.48383100
O	-1.44780300	2.30444300	-0.26806800
O	-1.67718500	-2.04619700	-0.28327600
H	-2.31801900	-0.82988800	-0.07926300
H	-1.78706700	0.07165700	1.50032500
H	2.08773800	-0.29139100	-1.88538900
H	2.94746300	0.81328600	-0.78575300
H	3.00582600	-0.94796800	-0.50536400
H	1.99009200	1.16207500	1.58834000
H	0.54037500	0.26729600	2.08102600
H	2.07620400	-0.59639800	1.86155600
(7a)	*G* = -786.4733010 a.u. (Gas phase)		
	G = -786.4956164 a.u. (In methanol)		
C	5.02121100	-0.39975400	0.88260200
C	2.73945600	-0.47554500	0.04502300
C	2.99520700	0.69329900	-0.68810300
C	4.23969700	1.30898800	-0.62753800
C	5.25771100	0.76674800	0.15922100
C	1.43541600	-1.15577600	0.03252300
C	0.28908400	-0.66745600	-0.46266200
C	-0.97751100	-1.42839800	-0.48354400
C	-1.01731600	-2.74234700	-0.77636100
N	-2.13380000	-0.65841400	-0.25619000
H	-3.47470600	1.01284600	0.89355200
(3-TS)	*G* = -534.0065840 a. u. (Gas phase)		
	G = -534.0308931 a. u. (In methanol)		
O	0.46638400	-1.30611300	-0.14223500
C	-0.82691200	-1.22168900	0.04158100
C	-1.57079000	-0.00492600	0.43391700
C	-0.95008300	1.22871900	-0.12032800
O	0.36086700	1.02804000	-0.53131700
C	1.15000100	-0.01491100	0.01455500
C	2.38418900	-0.11922400	0.84960600
C	1.45347600	0.21702300	1.48383100
O	-1.44780300	2.30444300	-0.26806800
O	-1.67718500	-2.04619700	-0.28327600
H	-2.31801900	-0.82988800	-0.07926300
H	-1.78706700	0.07165700	1.50032500
H	2.08773800	-0.29139100	-1.88538900
H	2.94746300	0.81328600	-0.78575300
H	3.00582600	-0.94796800	-0.50536400
H	1.99009200	1.16207500	1.58834000
H	0.54037500	0.26729600	2.08102600
H	2.07620400	-0.59639800	1.86155600
O	0.46638400	-1.30611300	-0.14223500
(4)	*G* = -400.8992150 a.u. (Gas phase)		
	G = -400.9067700 a.u. (In methanol)		
C	2.06912700	0.66642200	-0.33707300
C	1.75446600	-0.82653200	-0.36269900
N	0.82812000	-0.95428500	0.76529800
C	-0.08281600	0.17998900	0.70391500
C	0.69120500	1.29226700	-0.06521500
C	-1.38409900	-0.15536400	-0.00467200
O	-1.66181000	-1.22385500	-0.49436400
O	-2.22974400	0.89293000	-0.02227300
H	-3.03736800	0.61144500	-0.47925800
H	2.75545900	0.87808100	0.48771100
H	2.51677700	1.02714200	-1.26591000
H	1.29318200	-1.10093100	-1.32611200
H	2.63371900	-1.45648800	-0.20588900
H	0.31500600	-1.83096900	0.74154400
H	-0.35596400	0.51603500	1.71146100
H	0.18297800	1.52616000	-1.0054620
H	0.74450400	2.21622700	0.51238600
(7b)	*G* = -900.9243880 a.u. (Gas phase)		
	G = -900.9408619 a.u. (In methanol)		
C	4.25486000	-0.82968300	0.62875000
C	2.95904400	-1.34143500	0.62266200
C	1.91530600	-0.70658300	-0.05269600
C	2.21310800	0.47990500	-0.74721100
C	3.49053300	1.00284600	-0.75083300
C	4.52362000	0.35202800	-0.06106000
C	0.57372100	-1.29571400	-0.00808700
C	-0.55783200	-0.75904800	-0.48587500
C	-1.86269300	-1.44774000	-0.44249800
C	-1.98701200	-2.76582500	-0.67111300

Atom	*x* / Å	*y* / Å	*z* / Å
C	-3.42637100	-1.34234000	-0.14127200
C	-4.34426600	-0.27240900	0.44259600
C	-3.41465100	0.43580100	1.43247800
C	-2.08006300	0.48952100	0.66657900
C	-1.95608400	1.81985200	-0.09244200
O	-1.82857300	2.87228200	0.47666400
O	-2.01988700	1.72580500	-1.42664900
H	5.80735500	-0.83190400	1.49367400
H	3.59049700	-1.92417200	1.38886600
H	2.22193100	1.11959000	-1.31974700
H	4.41963300	2.21262300	-1.20127100
H	6.22906000	1.24894600	0.20185100
H	1.41385500	-2.14222800	0.49480800
H	0.25653900	0.34502600	-0.86447200
H	-1.93671500	-3.31362900	-0.78304600
H	-0.10652000	-3.25130000	-1.06318300
H	-3.34611500	-2.19843500	0.54694600
H	-3.74580900	-1.71891200	-1.11786100
H	-4.67161900	0.42020700	-0.34099300
H	-5.23169100	-0.69810200	0.91485900
H	-3.28949700	-0.17663400	2.33067100

Atom	*x* / Å	*y* / Å	*z* / Å
N	-2.96774600	-0.59766000	-0.22887800
C	-4.29708500	-1.19785000	-0.07912500
C	-5.13769800	-0.05764800	0.48692800
C	-4.15665100	0.59604900	1.46398200
C	-2.83146300	0.55459600	0.68402700
C	-2.63801400	1.86818900	-0.09158300
O	-2.49065600	2.92279400	0.46540100
O	-2.66602000	1.74639900	-1.42430500
H	5.03397800	-1.35546400	1.16759700
H	2.75554900	-2.26222700	1.16366500
H	1.43380600	0.99761000	-1.29823100
H	3.72649500	1.91721300	-1.28460900
H	0.50610800	-2.26687300	0.48190900
H	-0.55247400	0.23700900	-0.92776100
H	-2.93649700	-3.28429400	-0.62742500
H	-1.11566400	-3.34159100	-0.95493700
H	-4.26130700	-2.03704900	0.63274300
H	-4.65119400	-1.58254200	-1.04038800
H	-5.41065500	0.64505200	-0.30862100
H	-6.05449200	-0.41042800	0.96339000
H	-4.06797000	-0.01445200	2.36799900
H	-4.41495800	1.61521900	1.75641600
H	-1.96895200	0.44902800	1.34840900
H	-2.83273800	0.79488800	-1.60088800
O	5.74132100	0.94490500	-0.12882100
C	6.80798700	0.32232600	0.55264800
H	7.68387800	0.94679500	0.37877100
H	6.61070500	0.26197300	1.62970800
H	6.99505400	-0.68550100	0.16270200

(7c) *G* = -990.9057230 a.u. (Gas phase)
G = -990.9402728 a.u. (In methanol)

C	3.95199300	-1.12068500	0.71862700
C	2.64374800	-1.58171100	0.67782600
C	1.64510400	-0.87988100	-0.01246200
C	1.99448100	0.30603800	-0.67839100
C	3.29489800	0.78313700	-0.64656000
C	0.27868000	-1.41881100	-0.00689300
C	-0.81592600	-0.80957000	-0.48126600
C	-2.15517400	-1.43210900	-0.48570100
C	-2.33234300	-2.73288700	-0.77043300
N	-3.21828400	-0.53634400	-0.26325600
C	-4.58071200	-1.07129000	-0.17125600
C	-5.37636000	0.09456500	0.40700200
C	-4.39379900	0.66408300	1.43412900
C	-3.04547500	0.57124400	0.69808300
C	-2.74093600	1.89785600	-0.01694600
O	-2.52481500	2.91261600	0.58806100
O	-2.75099600	1.83538600	-1.35481800
H	4.73235300	-1.65200100	1.24922000
H	2.38565300	-2.50251800	1.19274800
H	1.24643400	0.86033800	-1.23527200
H	3.58065000	1.69608700	-1.15429300
H	0.16295800	-2.40183100	0.44707600
H	-0.75477900	0.20128300	-0.88349900

(8a) *G* = -803.0435920 a.u. (Gas phase)
G = -803.0671536 a.u. (In methanol)

O	2.79130600	0.97553600	-0.25201500
C	1.52373200	1.42133500	-0.41872700
C	0.44975500	0.37589700	-0.36985900
C	0.44975500	0.37589700	-0.36985900
C	0.87410000	-1.03842300	-0.52685300
O	2.18975600	-1.28124600	-0.31245900
C	2.99015100	-0.30205900	0.34594400
C	-0.80939200	0.86028600	-0.22103300
H	-0.80605100	1.94921500	-0.16823100
C	-2.15318500	0.30746300	-0.06317800
C	-3.15066400	1.25994000	0.23043100
C	-4.47213500	0.88453800	0.43119300
C	-4.82719500	-0.46042300	0.33771200
C	-3.85504400	-1.41533200	0.04043400
C	-2.52993800	-1.04518100	-0.16231200
C	2.65926100	-0.25455000	1.83122500
C	4.42789800	-0.67911000	0.07059700
O	1.32732900	2.59056700	-0.62305100
O	0.17277500	-1.94994800	-0.88482300
H	-2.87482900	2.30838100	0.30357300
H	-5.22105800	1.63626900	0.65725000
H	-5.85862200	-0.76288500	0.49011200
H	-4.13116200	-2.46152900	-0.04224600

Atom	*x* / Å	*y* / Å	*z* / Å
H	-3.30677200	-3.20479600	-0.77600600
H	-1.48202500	-3.33900900	-1.05499000
H	-4.60941600	-1.93337200	0.51299600
H	-4.92439400	-1.40527100	-1.15490400
H	-5.5825900	0.83468400	-0.37319400
H	-6.32457200	-0.22282500	0.84493200
H	-4.36947000	0.02459400	2.32182300
H	-4.60607900	1.68704500	1.74934800
H	-2.21771500	0.38794500	1.38965800
H	-2.98728700	0.90972200	-1.57913300
N	5.63511700	0.55709100	0.08559800
O	6.45369700	-0.09595100	0.70671600
O	5.87422800	1.59059600	-0.51120400
(8b)	*G* = -917.4706408 a. u. (Gas phase)		
	G = -917.4974766 a. u. (In methanol)		
O	3.60150500	0.95892600	-0.16938400
C	2.33921300	1.43550000	-0.30628200
C	1.25053000	0.40991900	-0.32238800
C	1.64145900	-1.00161300	-0.54365700
O	2.95679500	-1.28127100	-0.35950700
C	3.77513600	-0.35483100	0.34558100
C	-0.00737900	0.91428900	-0.21161100
H	0.01433800	2.00162200	-0.13465500
C	-1.35782900	0.38651200	-0.13416300
C	-2.36979600	1.35261200	0.00794200
C	-3.71070300	1.01546600	0.11745500
C	-4.07131500	-0.33512400	0.09437000
C	-3.07941700	-1.31868400	-0.04101000
C	-1.75042400	-0.97072700	-0.15781700
C	3.45235100	-0.38887600	1.83321700
C	5.20508300	-0.74176800	0.04087300
O	2.16641000	2.61867400	-0.43401300
O	0.91922500	-1.88427000	-0.92949800
H	-2.09340500	2.40329700	0.03398200
H	-4.45373700	1.79654600	0.22150200
H	-3.39050200	-2.35754800	-0.05979900
H	-1.00550700	-1.74300500	-0.28271600
H	2.41155600	-0.10684000	2.01633900
H	3.61495500	-1.39791400	2.21859100
H	4.10301300	0.31026700	2.36320900
H	5.39354200	-1.75811800	0.39260800
H	5.36656900	-0.69625900	-1.03766300
H	5.88692700	-0.04929800	0.53867000
O	-5.33742600	-0.78759500	0.19394500
C	-6.37367600	0.16591900	0.32034900
H	-7.30019800	-0.40375600	0.37919800
H	-6.25230700	0.76288600	1.23140800
H	-6.40670600	0.83084500	-0.55017000
(10a-TS)	*G* = -879.361834 a. u. (Gas phase)		
	G = -879.3959555 a. u. (In methanol)		
O	-2.3554190	-1.12801500	-0.15867200
C	-1.0909470	-1.04577400	-0.63925500
C	-0.4604510	0.24751800	-0.59450900
C	-1.1229270	1.38330200	0.02779600

Atom	*x* / Å	*y* / Å	*z* / Å
H	-1.79201100	-1.79259000	-0.41410000
H	1.61315300	0.01566600	1.99892000
H	2.84216000	-1.23607200	2.27339200
H	3.29496600	0.48706000	2.31930400
H	4.63071200	-1.66966900	0.48191400
H	4.59701900	-0.69270200	-1.00733500
H	5.09232300	0.05330400	0.53278700
(8c)	*G* = -1007.408441 a. u. (Gas phase)		
	G = -100.4483290 a. u. (In methanol)		
O	3.88722600	0.77810500	-0.24977100
C	2.68700600	1.32737500	-0.54357000
C	1.50806300	0.39969600	-0.46385500
C	1.78931600	-1.06207000	-0.44843700
O	3.05245500	-1.40430600	-0.10718900
C	3.91295200	-0.43769800	0.49125500
C	0.30423400	1.01182500	-0.40927500
H	0.39892200	2.09794400	-0.41799900
C	-1.08726600	0.56627200	-0.27353000
C	-1.97082800	1.52900100	0.25107800
C	-3.31354000	1.24760700	0.44444400
C	-3.77251700	-0.00906000	0.07506000
C	-2.94411800	-0.97553300	-0.47573400
C	-1.59601000	-0.68801200	-0.64869300
C	3.50361100	-0.18889600	1.93543400
C	5.31555000	-0.98466600	0.35491800
O	2.61513900	2.47944900	-0.87269700
O	1.01812100	-1.93033800	-0.76007100
H	-1.59044700	2.51053400	0.51796000
H	-4.00107800	1.97416100	0.85879300
H	-3.35803500	-1.93417500	-0.76295900
H	-0.93829500	-1.42736200	-1.08084900
H	2.48283300	0.19971600	1.99612200
H	3.55417300	-1.12566800	2.49459000
H	4.18227300	0.53857000	2.38600800
H	5.39037900	-1.93758700	0.88243500
H	5.54083000	-1.13714800	-0.70208900
H	6.02834400	-0.27444600	0.77858000
N	-5.20102000	-0.32150200	0.26401200
O	-5.90326100	0.54618400	0.74781200
O	-5.58236400	-1.42522700	-0.07473900
(10b-TS)	*G* = -993.812271 a. u. (Gas phase)		
	G = -993.849333 a. u. (In methanol)		
O	-3.0365400	0.93794500	0.54821000
C	-1.7175630	0.86862800	0.85168000
C	-1.0164660	-0.31923200	0.43987500
C	-1.6800290	-1.34593200	-0.34861400

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
O	-2.3710970	1.12578900	0.52529500	O	-2.9963540	-1.10118900	-0.62992700
C	-3.1228840	0.07840100	-0.08265900	C	-3.7282230	-0.28747000	0.28333200
O	-0.5084310	-2.08340100	-0.93260000	O	-1.169687	1.86518200	1.30858100
O	-0.6158790	2.46449000	0.22781000	O	-1.1349450	-2.30497100	-0.84781000
C	-4.2742630	-0.21617400	0.85179300	C	-5.0081320	0.09852600	-0.42270600
C	-3.5756840	0.49378500	-1.47599800	C	-3.9678670	-1.03976600	1.58547900
C	0.91899900	-0.41747700	1.18935600	C	0.07303000	0.84693500	-1.28648800
H	0.51440300	0.32472900	1.87513500	H	-0.3689650	0.24016600	-2.07473400
C	2.20024900	-0.13609500	0.54234700	C	1.44310900	0.54909700	-0.86986500
C	2.61177600	1.20140700	0.43138900	C	1.95070300	-0.73620000	-1.11672100
C	3.82441300	1.50105200	-0.17394700	C	3.24863900	-1.04890600	-0.73687200
C	4.63268100	0.47335500	-0.66744200	C	4.0466010	-0.0853250	-0.11416300
C	4.22565000	-0.85551400	-0.55570200	C	3.54390800	1.19217500	0.12944400
C	3.01067200	-1.16473100	0.04831400	C	2.24321300	1.51366900	-0.24666300
O	0.52373900	-1.64342400	1.45553500	O	-0.4315350	2.05963400	-1.21717900
H	0.37276200	0.43583500	-1.25564900	H	-0.0938060	-0.57109900	0.94194500
H	-3.8814600	-0.50927600	1.82689700	H	-4.7654630	0.63433500	-1.34197300
H	-4.8916130	0.67717000	0.96339100	H	-5.5760510	-0.80121000	-0.66679800
H	-4.8771880	-1.03044000	0.44528100	H	-5.6039970	0.74401100	0.22544000
H	-4.1820550	1.39908800	-1.40402400	H	-4.5189900	-1.95884000	1.37570200
H	-2.7197700	0.69634100	-2.12554600	H	-3.0233430	-1.30081300	2.07051400
H	-4.1697030	-0.30811400	-1.91936000	H	-4.5493220	-0.41359500	2.26539700
H	1.95724900	1.99282800	0.78930700	H	1.30733800	-1.48607900	-1.57127700
H	4.14119500	2.53466300	-0.26461800	H	3.64031600	-2.04337300	-0.92274200
H	5.58163500	0.71007300	-1.13794900	H	4.16622700	1.94017200	0.60922800
H	4.85634400	-1.65226700	-0.93567800	H	1.86146500	2.51394900	-0.06672500
H	2.70491600	-2.20198300	0.14470600	H	-0.3406960	2.43478200	-0.31079800
H	0.54628600	-2.21048300	0.65027100	O	5.38451200	-0.40967100	0.27273800
				C	5.37379800	-1.01059800	1.57030200
				H	4.83248900	-1.93277100	1.53182600
				H	6.37910900	-1.19995400	1.88397800
				H	4.90177800	-0.34871200	2.26600600

(10c-TS)	*G* = -1083.781166 a. u. (Gas phase) *G* = -1083.834224 a. u. (In methanol)			**(11a-TS)**	*G* = -879.389220 a. u. (Gas phase) *G* = -879.422796 a. u. (In methanol)		
C	1.94624000	1.38501700	-0.14274200	O	-2.75586700	0.85649500	0.10262600
O	3.31947000	-1.00079700	0.38890500	C	-1.52970400	1.27075800	-0.09974000
C	2.00774500	-0.97786000	0.72870400	C	-0.38050600	0.29434600	-0.08007300
C	2.00774500	-0.97786000	0.72870400	C	-0.83625200	-1.06521100	-0.57553500
C	1.29918200	0.25524400	0.50615900	O	-2.16009300	-1.35623500	-0.40657000
O	3.25556700	1.18528300	-0.48554400	C	-2.98833600	-0.54781000	0.40295100
C	4.00668600	0.25113300	0.28581700	O	-1.34085500	2.46963300	-0.31513600
O	1.46892700	-2.03034900	1.05117700	O	-0.13621100	-1.85084400	-1.13943700
O	1.39137200	2.40437200	-0.48786300	C	-4.41166100	-0.81647000	-0.02753600
C	5.26985900	-0.02798300	-0.49657400	C	-2.75425600	-0.79637100	1.88351100
C	4.27658900	0.81072000	1.67613400	C	0.87822900	0.89922200	-0.85065500
C	0.16953400	-0.65514200	-1.34380600	H	0.76396200	0.59296600	-1.90714900
H	0.59451200	0.05853700	-2.04730800	C	2.15000800	0.26633700	-0.30068500
C	-1.19041800	-0.42222700	-0.85833800	C	2.72540100	-0.86667300	-0.87694800
C	-1.70168200	0.88418300	-0.90812400	C	3.88652700	-1.41822400	-0.33633500
C	-2.99031600	1.13718600	-0.45854700	C	4.48218900	-0.83984700	0.78307700
C	-3.77538100	0.09325300	0.03831600	C	3.91841900	0.30171200	1.35302300
C	-3.26907900	1.20498700	0.08610800	C	2.76138700	0.85525100	0.80919900
C	-1.97761400	-1.46721600	-0.36107900	O	0.87257000	2.26219300	-0.67669900
O	0.67387600	-1.86441000	-1.45930100	H	-0.07530700	0.19570800	0.97198800

Atom	*x* / Å	*y* / Å	*z* / Å
H	0.38839500	0.43131600	1.05958300
H	5.00584000	-0.42783600	-1.47710600
H	5.83337100	0.89839900	-0.62270500
H	5.87927300	-0.75810400	0.03946500
H	4.82410700	1.75132400	1.58709000
H	3.34357300	0.99826300	2.21450000
H	4.87233800	0.09516300	2.24668800
H	-1.06768300	1.69235500	-1.26556000
H	-3.38471800	2.14726100	-0.49201600
H	-3.88146700	-2.01485000	0.46830500
H	-1.59328000	-2.48221700	-0.33408500
H	0.60293800	-2.36500800	-0.61379300
N	-5.14096500	0.36406900	0.51026900
O	-5.79097700	-0.55169100	0.93132400
O	-5.55054700	1.48996500	0.45541400

(11b-TS) *G* = -993.8632130 a. u. (Gas phase)
G = -993.9000156 a. u. (In methanol)

O	-3.50017200	0.70297600	0.26798300
C	-2.32087500	1.22365800	0.03519600
C	-1.10647900	0.33840200	-0.09125600
C	-1.49420900	-1.00696000	-0.67542000
O	-2.78149300	-1.40982400	-0.46001400
C	-3.61419400	-0.73459900	0.45952000
O	-2.23061900	2.44688300	-0.08701400
O	-0.77587600	-1.68914600	-1.34166400
C	-5.03844700	-1.07408800	0.08589000
C	-3.27381800	-1.08413400	1.89847900
C	0.05733500	1.09710200	-0.87483500
H	-0.09883600	0.86986100	-1.94581600
C	1.40165000	0.51946500	-0.45105900
C	2.01967400	-0.51636200	-1.15246900
C	3.24750200	-1.02075800	-0.72502500
C	3.86756300	-0.49184700	0.40554700
C	3.26012400	0.55386700	1.10076900
C	2.03603700	1.06080800	0.67007800
O	-0.03406600	2.43712800	-0.58508100
H	-0.73186300	0.17801400	0.93033400
H	-5.22216400	-0.78356700	-0.94962100
H	-5.18821700	-2.14998700	0.19037700
H	-5.72905700	-0.5424400	0.74294100
H	-3.41327200	-2.1578720	2.03800700
H	-2.24153800	-0.8356110	2.15182900
H	-3.94137400	-0.5440450	2.57258900
H	1.53525500	-0.93397800	-2.02948900
H	3.72129800	-1.82498700	-1.27962200
H	3.74843600	0.98500900	1.96968500
H	1.57134500	1.90580000	1.16965300
H	-1.16877000	2.61352200	-0.34867300
O	5.12850900	-1.00750100	0.84030600
C	6.18518300	-0.26312800	0.22854800
H	6.12337900	0.76057400	0.53369500
H	7.12824400	-0.66886700	0.53006300
H	6.09458400	-0.32411300	-0.83586400

Atom	*x* / Å	*y* / Å	*z* / Å
H	-4.51620800	-0.60317900	-1.09243700
H	-4.64768000	-1.86623400	0.15466300
H	-5.09495900	-0.18319100	0.54111900
H	-2.98175100	-1.84172400	2.10102000
H	-1.72151100	-0.60069000	2.17795900
H	-3.41489300	-0.15487500	2.46984900
H	2.25937100	-1.32237400	-1.74492400
H	4.32779500	-2.29833500	-0.79408100
H	5.38788900	-1.26842300	1.20129400
H	4.38978700	0.76988900	2.21207400
H	2.33525800	1.77053200	1.20945000
H	-0.25677800	2.53786900	-0.52460800

(11c-TS) *G* = -1083.733342 a. u. (Gas phase)
G = -1083.787786 a. u. (In methanol)

O	-3.72206200	0.56085700	0.37985200
C	-2.59169300	1.16578300	0.11083000
C	-1.33053200	0.36741200	-0.10481000
C	-1.65918500	-0.98049900	-0.71857400
O	-2.90563100	-1.47448900	-0.45753100
C	-3.73365000	-0.88667600	0.52416300
O	-2.58656100	2.39568000	0.02905300
O	-0.93219500	-1.59122100	-1.44229100
C	-5.14979500	-1.30696300	0.20597300
C	-3.30079900	-1.26052900	1.93182300
C	-0.25813500	1.22696600	-0.91426400
H	-0.45206200	1.02558100	-1.98424900
C	1.13988400	0.72569100	-0.57559200
C	1.78793700	-0.24316700	-1.34254100
C	3.06531700	-0.67922200	-0.99205500
C	3.70511500	-0.14831100	0.12651900
C	3.06667000	0.83131100	0.88715100
C	1.79269400	1.27026000	0.53334000
O	-0.42123300	2.54766200	-0.57200200
H	-0.89635400	0.19830700	0.89148400
H	-5.40277200	-0.99500300	-0.80848200
H	-5.22460900	-2.39328300	0.27822100
H	-5.83991000	-0.84422800	0.91373300
H	-3.36374100	-2.34517400	2.03864100
H	-2.27541700	-0.95287200	2.14511000
H	-3.96763800	-0.78841800	2.65583100
H	1.28869000	-0.66253900	-2.21035900
H	3.56195200	-1.43152200	-1.59723400
H	3.56852400	1.26469900	1.74718800
H	1.29978800	2.06564000	1.08464800
H	-1.55187500	2.64072900	-0.27612600
N	5.05327500	-0.60610500	0.49229100
O	5.58049100	-0.11766500	1.45244100
O	5.57213300	-1.44976300	-0.18405000

Atom	*x* / Å	*y* / Å	*z* / Å
(11a-Int)	*G* = -879.410214 a. u. (Gas phase)		
	G = -879.443057 a. u. (In methanol)		
O	2.12096300	-0.83853300	-0.74734700
C	0.86833400	-1.00111400	-0.14989200
C	0.29671700	0.28653500	0.43313700
C	1.17898300	1.51053000	0.38510300
O	2.47121300	1.32795200	0.05176800
C	3.01250200	-0.00912800	-0.02802900
O	0.84514000	-2.08208400	0.70336800
H	1.13428500	-2.86098500	0.20645900
O	0.74514900	2.61622400	0.57128000
C	4.25996100	0.10716600	-0.87494600
C	3.29755500	-0.50682500	1.38343300
C	-0.7091410	0.18110800	-0.75075800
H	-0.5458290	0.95091300	-1.51220000
C	-2.1624870	0.07570700	-0.39396800
C	-2.9601800	1.22123000	-0.42988100
C	-4.2969800	1.15443800	-0.04452800
C	-4.8434750	-0.05977700	0.36961500
C	-4.0482360	-1.20460500	0.40169200
C	-2.7083450	-1.13870400	0.02469800
O	-0.1140180	-1.07408400	-1.15513000
H	-0.1674890	0.17693000	1.41388600
H	3.98819800	0.46874600	-1.86792800
H	4.95555600	0.80861300	-0.41090200
H	4.73329400	-0.87284000	-0.96303100
H	4.02796100	0.15765800	1.84960400
H	2.39558100	-0.52792800	1.99909200
H	3.70258900	-1.52034300	1.34079000
H	-2.5304860	2.16618100	-0.75319400
H	-4.9125240	2.04788900	-0.07338800
H	-5.8870210	-0.11396300	0.66333700
H	-4.4724650	-2.15187100	0.71965000
H	-2.0804270	-2.02416000	0.04226700

Atom	*x* / Å	*y* / Å	*z* / Å
(11b-Int)	*G* = -993.878406 a. u. (Gas phase)		
	G = -993.913121 a. u. (In methanol)		
O	2.88989300	-0.76751700	-0.75440600
C	1.59981800	-0.94376300	-0.25109400
C	1.00996100	0.30026300	0.40056100
C	1.89997100	1.51968600	0.44761700
O	3.21505700	1.33319700	0.21384000
C	3.73758700	-0.00339700	0.07777500
O	1.50630100	-2.08436000	0.51728200
H	1.82651700	-2.82052600	-0.02333700
O	1.46255600	2.62243000	0.62907900
C	5.04177100	0.14686100	-0.67364400
C	3.92033200	-0.60497200	1.46535900
C	0.03425800	0.27526900	-0.81100800
H	0.18639600	1.11953800	-1.49132900
C	-1.4197600	0.07919000	-0.51213500
C	-2.3222630	1.12039100	-0.68650200
C	-3.6707400	0.96818500	-0.36363400
C	-4.1185700	-0.25473800	0.13559300
C	-3.2150210	-1.31135600	0.31114000
C	-1.8800980	-1.14316500	-0.00738800
O	0.68104600	-0.92016300	-1.31445400
H	0.52716200	0.12858300	1.36308300
H	4.83988100	0.57935300	-1.65435500
H	5.71393900	0.80308900	-0.11884400
H	5.50720600	-0.83243800	-0.79859700
H	4.63025400	0.00624100	2.02563300
H	2.97866800	-0.64817000	2.01609300
H	4.30784600	-1.62188200	1.37670300
H	-1.9740860	2.07333000	-1.07617000
H	-4.3513790	1.79745600	0.51077000
H	-3.5944680	-2.25103300	0.69718500
H	-1.1750820	-1.95901700	0.12470300
O	-5.4057860	-0.51996000	0.47655800
C	-6.3489590	0.51658500	0.31530000
H	-7.3058400	0.11072300	0.64139900
H	-6.0946330	1.38744900	0.93109600
H	-6.4246500	0.82804900	-0.73331600

Atom	*x* / Å	*y* / Å	*z* / Å
(11c-Int)	*G* = -1083.786748 a. u. (Gas phase)		
	G = -1083.840682 a. u. (In methanol)		
O	3.10100700	-0.95626600	-0.53196300
C	1.80700900	-1.01745900	-0.01502600
C	1.22288900	0.34898200	0.32462500
C	2.12310200	1.54424300	0.12540100
O	3.43588400	1.30651800	-0.04012700
C	3.94879700	-0.03384000	0.12426700
O	1.69229800	-1.95057700	0.98363800
H	2.05717700	-2.78256700	0.64995000
O	1.68085900	2.65867600	0.05203000
C	5.26013400	-0.05894200	-0.62818800
C	4.11113100	-0.31692700	1.61157400
C	0.29689000	0.06764600	-0.88593500
H	0.49939200	0.72688000	-1.73757000
C	-1.1737030	0.02413300	-0.58863000

Atom	*x* / Å	*y* / Å	*z* / Å
(11a)	*G* = -879.4310770 a. u. (Gas phase)		
	G = -879.4598882 a. u. (In methanol)		
O	2.15989300	-1.33705300	0.15353300
C	0.88760400	-1.11211400	-0.24378000
C	0.39222600	0.32707600	-0.18075800
C	1.51078500	1.32994800	-0.47693600
O	2.76880900	0.94015200	-0.13267900
C	3.00502600	-0.26140100	0.62034400
O	0.21783100	-2.04127100	-0.63621500
O	1.33763800	2.41397900	-0.97041700
C	4.42728700	-0.68504600	0.29523600
C	2.78092000	-0.01983300	2.11173800
C	-0.8811700	0.57954500	-1.05785300
H	-0.8738910	1.64994300	-1.27637500
C	-2.1667920	0.26563300	-0.29160300
C	-2.6137070	1.18237900	0.67273600

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	-1.8337250	1.23161200	-0.33897500	C	-3.7791670	0.94502400	1.40436900
C	-3.1883100	1.23621000	-0.04237300	C	-4.5235370	-0.21566300	1.17371500
C	-3.8568120	0.01754100	-0.00513800	C	-4.0936290	-1.12657200	0.2061990
C	-3.2244530	-1.19300500	-0.24483500	C	-2.9242160	-0.88727200	-0.52198000
C	-1.8640730	-1.18397700	-0.53616800	O	-0.7737210	-0.04686200	-2.32025800
O	0.89985300	-1.22503000	-1.07892300	H	0.11165300	0.50577800	0.86802400
H	0.70494300	0.39904800	1.28277500	H	4.52889000	-0.84315300	-0.78158400
H	5.07135300	0.14992400	-1.68187800	H	5.12633200	0.09514400	0.60917500
H	5.93237500	0.69847300	-0.22263200	H	4.66586600	-1.61576900	0.81762200
H	5.71856600	-1.04453700	-0.53074300	H	3.45343600	0.77062400	2.45743600
H	4.81942700	0.39896300	2.03232400	H	1.75342000	0.28206700	2.33318800
H	3.16356000	-0.23379100	2.14756300	H	2.99550800	-0.93770400	2.66678500
H	4.49325300	-1.32985600	1.75319600	H	-2.0545890	2.10220900	0.84163200
H	-1.2731510	2.16298600	-0.36610500	H	-4.1117580	1.67137800	2.14181600
H	-3.7317400	2.15072100	0.15860900	H	-5.4345420	-0.40266500	1.73635500
H	-3.7962910	-2.11124800	-0.19863400	H	-4.6691510	-2.02843300	0.01334400
H	-1.3278960	-2.10716800	-0.72237700	H	-2.6116260	-1.60515400	-1.27325700
N	-5.2952540	0.01246400	0.30635800	H	-0.6929100	-1.00604700	-2.17441600
O	-5.8292890	1.08646600	0.51287100				
O	-5.8602910	-1.06508300	0.33840100				

(11b) *G* = -993.8798972 a. u. (Gas phase)
G = -993.9112178 a. u. (In methanol)

Atom	x / Å	y / Å	z / Å
O	-2.7275400	-0.95844100	1.01604600
C	-1.5087000	-0.39024300	1.01485500
C	-1.1152240	0.37806600	-0.23465000
C	-2.3158300	1.05878800	-0.88188900
O	-3.5117730	0.45301800	-0.69449200
C	-3.5862110	-0.85165800	-0.12513300
O	-0.8030460	-0.48953800	1.98473800
O	-2.2470760	2.06534700	-1.52587600
C	-4.9954280	-0.99351700	0.40668900
C	-3.2402840	-1.91600000	-1.15610000
C	0.03913500	1.37771600	0.03702100
H	0.01177900	2.09425600	-0.78882600
C	1.39031100	0.67626200	0.01497500
C	1.87231300	0.18864200	-1.20404200
C	3.10168300	-0.45973200	-1.27754000
C	3.87060400	-0.62319600	-0.12538300
C	3.40221600	-0.12863400	1.08904900
C	2.16915700	0.51939300	1.15918800
O	-0.2108290	2.13156200	1.19338500
H	-0.7603540	-0.36675500	-0.96007800
H	-5.1854610	-0.20621800	1.13781300
H	-5.7064310	-0.90281900	-0.41648200
H	-5.1091890	-1.96812200	0.88485100
H	-3.9329130	-1.83740800	-1.99638000
H	-2.2221110	-1.81001000	-1.53573300
H	-3.3373250	-2.90285700	-0.69926300
H	1.28760400	0.33487000	-2.11139300
H	3.46366200	-0.82668400	-2.23289000
H	3.99735000	-0.24536100	1.98928000
H	1.82262500	0.90545400	2.11186700
H	-0.2099800	1.53121700	1.95230200

(11c) *G* = -1083.862149 a. u. (Gas phase)
G = -1083.910219 a. u. (In methanol)

Atom	x / Å	y / Å	z / Å
O	-2.8406500	-0.79661700	1.23144300
C	-1.6714500	-0.15006300	1.07855500
C	-1.3462880	0.35100200	-0.31772100
C	-2.60045000	0.77659800	-1.07250500
O	-3.7430180	0.13647300	-0.73025300
C	-3.7099200	-1.01172300	0.11380800
O	-0.9560280	0.02258200	2.03083500
O	-2.6155580	1.61803300	-1.92360100
C	-5.1009180	-1.14120700	0.69450400
C	-3.2838780	-2.24763200	-0.66490900
C	-0.2749070	1.47234300	-0.29806500
H	-0.3632600	1.98416800	-1.26057700
C	1.12818800	-0.19471600	0.89024100
C	1.64270300	-1.28674700	0.18395000
C	2.91990300	-0.36736800	-1.24259600
C	3.70431700	-0.21189100	-0.09981600
C	3.20279500	0.50118900	0.98591700
C	1.92193200	1.05114100	0.93864700
O	-0.5798050	2.44156900	0.66918900
H	-0.9357360	-0.50601700	-0.86899500
H	-5.3505590	-0.22886100	1.23837700
H	-5.8203690	-1.29017800	-0.11269000
H	-5.1339390	-1.99173800	1.37783400
H	-3.9841130	-2.41073100	-1.48652500
H	-2.2791290	-2.14965900	-1.08073700
H	-3.2993370	-3.11349500	-0.00004500
H	1.04431800	-2.19102000	0.08013300
H	3.30619100	-0.90733800	-2.10142600
H	3.80917000	0.63292000	1.87652500
H	1.54949300	1.61029400	1.79032900
H	-0.5274980	2.02584900	1.54143300

Atom	*x* / Å	*y* / Å	*z* / Å
O	5.13653200	-1.28477400	-0.19350600
C	6.16844600	-0.31940100	-0.41283900
H	6.19877100	0.36353200	0.41031400
H	7.11131400	-0.81814700	-0.49741100
H	5.96738500	0.21875200	-1.31553800
(12a-TS)	*G* = -879.3373010 a. u. (Gas phase)		
	G = -879.3705264 a. u. (In methanol)		
O	-2.05520300	-1.16297100	0.60886600
C	-0.74576200	-0.90452000	0.46456400
C	-0.40583200	0.33187600	-0.31175900
C	-1.50288500	1.33439900	-0.54504300
O	-2.75396500	0.91971200	-0.28586400
C	-3.07952200	-0.45211300	-0.08698200
O	0.06521600	-1.62533800	0.97982400
O	-1.29328200	2.45661700	-0.90876800
C	-4.28074900	-0.46079400	0.83336300
C	-3.34554400	-1.11919600	-1.42601600
C	0.90833500	0.93376200	-0.22371400
H	0.88294500	2.00277600	-0.41535700
C	2.20565700	0.30406800	-0.18846100
C	2.42882600	-1.04244200	-0.52258900
C	3.72158300	-1.54495600	-0.52653800
C	4.79589100	-0.72453300	-0.18320400
C	4.58657500	0.61487400	0.14582500
C	3.30087600	1.13063200	0.12524800
O	-0.01186200	1.25861300	1.86211900
H	-0.36824200	-0.48902100	-2.13360000
H	-4.01469700	0.03275900	1.76904300
H	-5.10603500	0.07447100	0.36116000
H	-4.57920800	-1.49064300	1.03568800
H	-4.15739800	-0.59610700	-1.93425400
H	-2.45469500	-1.08948900	-2.05666500
H	-3.63042300	-2.15986600	-1.26159300
H	1.59232200	-1.67646400	-0.78565800
H	3.89416500	-2.58148700	-0.79419000
H	5.80301000	-1.12924800	-0.18006400
H	5.42467900	1.25166100	0.40617900
H	3.11899300	2.17187500	0.37436000
H	0.46266200	0.49938200	2.23736800

Atom	*x* / Å	*y* / Å	*z* / Å
N	5.05581700	-0.78769200	-0.04687500
O	5.70580000	-0.62658600	0.94810500
O	5.45449900	-1.39557800	-1.00078000
(12b-TS)	*G* = -993.7954150 a. u. (Gas phase)		
	G = -993.8315324 a. u. (In methanol)		
O	-2.73778500	-1.20307800	0.59498400
C	-1.43919700	-0.87434200	0.50634500
C	-1.12991200	0.35509400	-0.29348900
C	-2.26800900	1.28524800	-0.61371700
O	-3.50550500	0.80749600	-0.40230100
C	-3.76357500	-0.57401000	-0.17363900
O	-0.61641500	-1.53116500	1.08459200
O	-2.10324600	2.40594400	-1.00422500
C	-5.00761300	-0.62342500	0.68658500
C	-3.92358300	-1.29613900	-1.50093200
C	0.14240200	1.03395100	-0.16149200
H	0.06708000	2.09333800	-0.38993600
C	1.46941800	0.48125600	-0.04166300
C	1.78415400	-0.85983500	-0.31906600
C	3.10150100	-1.28708900	-0.24286400
C	4.10946900	-0.39609900	0.12489500
C	3.80920300	0.93854400	0.39812400
C	2.49939800	1.37866500	0.29734000
O	-0.89921400	1.36935000	1.86471900
H	-0.95406800	-0.51791400	-2.08271400
H	-4.81740200	-0.08685800	1.61706300
H	-5.83648000	-0.15125900	0.15684900
H	-5.25794600	-1.66201900	0.90852700
H	-4.73654600	-0.83645900	-2.06557200
H	-3.00491900	-1.23467700	-2.08786700
H	-4.15784600	-2.34591600	-1.31579700
H	0.99882000	-1.54868300	-0.60132100
H	3.34509800	-2.31972400	-0.46679200
H	4.59611500	1.63015900	0.67765500
H	2.24720500	2.41489700	0.50214700
H	-0.40267100	0.65054900	2.28802500
O	5.46213300	-0.85177000	0.21186900
C	6.24716500	-0.21212900	-0.79782600
H	6.42375800	0.80613300	-0.52059400
H	7.18261200	-0.72174100	-0.89849600
H	5.72252600	-0.24216600	-1.72989500

(12c-TS)	*G* = -1083.750730 a. u. (Gas phase)		
	G = -1083.803421 a. u. (In methanol)c		
O	-2.88167500	-1.23652000	0.66499400
C	-1.60529700	-0.84821500	0.51554900
C	-1.38884200	0.37535500	-0.32285800
C	-2.58293600	1.24215900	-0.61575900
O	-3.78612600	0.71087600	-0.34297300
C	-3.96708000	-0.67560200	-0.07393900
O	-0.72881400	-1.45106300	1.07332200
O	-2.48890700	2.35990800	-1.03694600
C	-5.17153200	-0.76413000	0.83793500

(13a-TS)	*G* = -879.3465120 a. u. (Gas phase)		
	G = -879.3809645 a. u. (In methanol)		
O	2.09159800	-1.29495300	0.31129600
C	1.03845600	-0.89762400	1.05326800
C	0.44119000	0.41796600	0.70667800
C	0.90987900	1.11512400	-0.51469700
O	1.96490900	0.57185200	-1.14809600
C	2.81888500	-0.40084000	-0.53450800
O	0.57374500	-1.62623600	1.89255300
O	0.35988800	2.08475700	0.98036900
C	3.35924100	-1.24749100	-1.66561600

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	-4.14505900	-1.43574000	-1.37750800	C	3.90831300	0.29684100	0.26027200
C	-0.14686600	1.11724100	-0.25840500	C	-0.89189900	0.71211400	1.28395500
H	-0.28291700	2.16611400	-0.50643500	H	-0.95746100	0.35116200	2.30659600
C	1.20927800	0.63165900	-0.18168700	C	-1.98781500	0.14556100	0.41139000
C	1.57760800	-0.69902000	-0.44276300	C	-2.45445100	-1.14044200	0.70632300
C	2.91622600	-1.06083300	-0.41194200	C	-3.44750400	0.07984100	-1.71982800
C	3.89354500	-0.11419000	-0.10563400	C	-3.97726200	-1.16182100	-1.01941900
C	3.53980200	1.21064400	0.15081300	C	-3.51078400	-1.45632900	0.26184300
C	2.20709300	1.58508600	0.09484600	C	-2.51355600	-0.67945700	0.84405200
O	-1.12106200	1.45023200	1.80146100	O	-1.07607800	2.39272800	1.48698200
H	-1.24290800	-0.53030000	-2.09849400	H	1.90606600	1.85778100	2.29846000
H	-4.97035800	-0.19722600	1.74789300	H	2.52998700	-2.19597100	-1.7188320
H	-6.04312500	-0.34482000	0.33287400	H	3.92034100	-2.35694200	-0.61614600
H	-5.36176000	-1.80797300	1.09250500	H	4.01538400	-1.25954300	-2.0194720
H	-5.00157800	-1.91782400	-1.02896300	H	4.47707500	0.40606800	-0.9481950
H	-3.25489800	-1.34428900	-2.00317800	H	3.48475200	0.89800900	1.06724100
H	-4.32018700	-2.49085200	-1.16012800	H	4.57283500	-0.45475100	0.69076300
H	0.81606600	-1.43113500	-0.67726100	H	-2.03454200	1.54920200	-1.6826160
H	3.20067100	-0.62333800	2.08563600	H	-3.80936400	-2.71486700	0.15810700
H	4.3026740	1.94553400	0.38246400	H	-4.75434900	-1.46831400	-1.77237800
H	1.9131220	2.61261700	0.28742100	H	-3.92617800	-2.29374200	0.8131400
H	-0.57338900	0.76622300	2.21931600	H	-2.15727400	-0.90633100	1.8420660
N	5.30770900	0.06376100	-0.51329600	H	-0.73592800	0.64397800	2.73232900
O	6.12876900	0.32234200	0.19312200				
O	5.58393700	-1.65861400	-0.28815300				
(13b-TS)	*G* = -993.7834441 a. u. (Gas phase) *G* = -993.8201192 a. u. (In methanol)			**(13c-TS)**	*G* = -1083.756620 a. u. (Gas phase) *G* = -1083.804768 a. u. (In methanol)		
O	2.61487800	-1.28001000	0.67626200	O	2.70661300	-1.29641900	0.78297900
C	1.71127700	-0.49266500	1.29359000	C	1.90520400	-0.36187100	1.33240200
C	1.22513500	0.68499000	0.52911500	C	1.48082000	0.75252300	0.44603100
C	1.61447200	0.82204500	-0.89464400	C	1.80645900	0.67943300	-0.99829300
O	2.51713100	-0.06135800	-1.35749500	O	2.60682800	-0.33113900	-1.38245700
C	3.32716100	-0.86534700	-0.49184600	C	3.39007300	-1.09285200	-0.45605800
O	1.27546000	-0.79587400	2.37495900	O	1.50174900	-0.49062200	2.46017800
O	1.12207500	1.63111900	-1.64462600	O	1.34568700	1.43182000	-1.82360000
C	3.62755100	-2.13027800	-1.26510100	C	3.54311900	-2.46445200	-1.07532800
C	4.57636800	-0.09904000	-0.09492800	C	4.71791200	-0.39889300	-0.20998900
C	0.01380000	1.35972700	1.05284600	C	0.35890900	1.59191800	0.92938400
H	0.03481800	1.40206000	2.13827000	H	0.43925700	1.76428600	1.99906300
C	-1.23685900	0.68750100	0.53578700	C	-0.96867200	0.97643100	0.55243600
C	-1.80306300	-0.32398200	1.31991300	C	-1.57657900	0.12299000	1.48013500
C	-2.94308100	-0.99237600	0.88002000	C	-2.78976200	-0.48921000	1.17469200
C	-3.52098400	-0.65483300	-0.34226900	C	-3.39948300	-0.25287400	-0.05587000
C	-2.95540700	0.35245300	-1.12423200	C	-2.79244100	0.59673900	-0.98087100
C	-1.81210100	1.01951200	-0.69429600	C	-1.57661000	1.20611000	-0.68526300
O	0.04292900	3.00933400	0.63147500	O	0.50453600	3.16850800	0.30267600
H	3.02457400	2.36498900	1.36117400	H	3.45524500	2.35342300	0.98590600
H	2.69244400	-2.63183600	-1.52027900	H	2.55735400	1.22703800	-2.90756800
H	4.16584600	-1.87814100	-2.18053800	H	4.05281600	2.03636500	-2.37512600
H	4.23917700	-2.79408500	-0.65138500	H	4.12770800	-3.10055300	-0.40824000
H	5.12750100	0.17934500	-0.99521400	H	5.24336600	-0.28292300	-1.15983700
H	4.32421300	0.80639300	0.46060300	H	4.57151100	0.58647000	0.23681300
H	5.20151100	-0.73655700	0.53322100	H	5.31890100	-1.00845700	0.46754200
H	-1.34536600	-0.58481400	2.27028200	H	-1.09404700	2.43639300	-0.05991800

Atom	*x* / Å	*y* / Å	*z* / Å
H	-3.38077400	-1.77140500	1.49581500
H	-3.40697200	2.07325500	0.62298400
H	-1.37822000	-1.30053000	1.80606700
H	0.31242400	2.97090300	-0.29996600
O	-4.69486800	0.79231000	-1.33627100
C	-5.85649300	-0.32425300	-0.64601600
H	-5.85523500	-0.70572000	0.35367400
H	-6.73455100	0.66220900	-1.15562300
H	-5.84887800	-0.61961600	0.74539400
(14a-TS1) *G* = -879.3471230 a. u. (Gas phase) *G* = -879.3837326 a. u. (In methanol)			
O	2.66940800	0.87745300	-0.62247300
C	1.40416800	1.28847600	-0.73474900
C	0.32251300	0.23740900	-0.68614000
C	0.71093900	-1.02371500	0.04582500
O	2.02154000	-1.31494000	0.03624500
C	3.06491300	-0.34383500	0.01105700
O	1.15445800	2.43502400	-0.99100700
O	-0.08035800	-1.85394500	0.40373700
C	3.51001100	-0.04005600	1.42752000
C	4.15822300	-0.92964900	-0.85985300
C	-2.22659400	0.33684700	-0.10756700
C	-2.57121300	-0.92218000	-0.65160200
C	-3.88906900	-1.34417100	-0.62898400
C	-4.87481300	-0.53611300	-0.05785500
C	-4.55359400	0.71054400	0.48479600
C	3.24293400	1.14851900	0.45164000
C	-0.91740900	0.87829700	-0.14656300
H	0.15294500	-0.06971500	-1.73484300
H	2.65591400	0.34970100	1.98959100
H	3.87165300	-0.96241300	1.88788700
H	4.32191600	0.68969800	1.39607800
H	4.50394900	-1.86901100	-0.42550200
H	3.77239100	-1.11620400	-1.86404200
H	4.99173200	-0.22777100	-0.91763400
H	-1.79885000	-1.55443300	-1.06904300
H	-4.15489600	-2.30738800	-1.04951600
H	-5.90430700	-0.87984100	-0.03873000
H	-5.32700700	1.33090900	0.92317100
H	-2.97200700	2.11534600	0.86486200
H	0.10087100	1.92774300	0.79763600
O	0.63364600	0.5965200	1.95774000
H	0.12380500	0.11033600	2.37775700
(14b-TS1) *G* = -993.8198403 a. u. (Gas phase) *G* = -993.8612962 a. u. (In methanol)			
O	3.40159200	0.83249300	-0.67844700
C	2.14627600	1.28246600	-0.74235900
C	1.03546500	0.26438100	-0.66060400
C	1.41133700	-1.01295100	0.04948400
O	2.71122600	-1.34372100	-0.00933200
C	3.78219900	-0.40456000	-0.06675400
O	1.92263500	2.43779600	-0.98275800
O	0.60847200	-1.82124100	0.43107200
C	4.28721100	-0.12417400	1.33435600

Atom	*x* / Å	*y* / Å	*z* / Å
H	-3.25895500	1.90102600	-1.14492400
H	-3.26798700	1.93726500	0.78884900
H	-1.11008700	1.40291300	1.87077200
H	0.72154600	0.62668000	2.99274800
N	-4.68290700	0.37709100	-0.89360600
O	-5.17862600	0.43967600	-1.61857000
O	-5.18303400	1.44310600	-0.66580200
(14a-TS2) *G* = -879.3093445 a. u. (Gas phase) *G* = -879.3407527 a. u. (In methanol)			
O	-2.15291900	-0.21440300	-1.20539900
C	-1.72514600	1.04788600	-0.94859500
C	-0.56019700	0.94768300	0.03609900
C	-0.86130400	0.11860900	1.26253500
O	-1.68054600	-0.90998600	1.07288900
C	-2.38349300	-1.20344000	-0.18526900
O	-2.06975300	2.01369600	-1.54700500
O	-0.43511400	0.46836400	2.32865000
C	-1.87216100	-2.52917800	-0.68029800
C	-3.84836200	-1.12312100	0.19159500
C	1.87190700	0.13741600	-0.38920100
C	1.95713500	-0.88297000	0.61151600
C	3.14966400	-1.54021600	0.80870800
C	4.27459600	-1.20356700	0.03528600
C	4.21699400	-0.21797000	-0.95929500
C	3.02769900	0.44126800	-1.17786100
H	-0.22326100	2.14083000	0.88041700
H	-0.79184100	0.84045700	-2.48274200
H	-2.09887500	-3.30173500	0.05583000
H	-2.36354800	1.62399600	-2.76942700
H	-4.00336800	-1.45490900	1.21504300
H	-4.00896100	-0.06584200	0.01716000
H	-4.47308300	0.50578600	-1.68210900
H	1.09293500	-1.14415600	1.21149400
H	3.22320100	-2.31671300	1.56133700
H	5.21062200	-1.72584200	0.20969700
H	5.09485700	0.01928600	-1.54904900
H	2.95524800	1.20061300	-1.95160000
C	0.71861200	0.85896500	-0.67345500
H	0.76687400	1.54922700	-1.52015500
O	0.24157000	3.55596200	1.21621000
H	0.59762400	3.61626100	0.32672100
(14b-TS2) *G* = -993.7698883 a. u. (Gas phase) *G* = -993.8092053 a. u. (In methanol)			
O	-2.83441800	-0.36470500	-1.16249400
C	-2.54108000	0.93293400	-0.89342600
C	-1.33874800	0.94684800	0.05048700
C	-1.50300300	0.06838900	1.26847900
O	-2.20881100	-1.04201200	1.08415700
C	-2.91798500	-1.39067000	-0.15629500
O	-3.01155500	1.86423300	-1.45997000
O	-1.08162900	0.44531100	2.32722400
C	-2.27982600	-2.64218700	-0.69532700

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	4.82494700	-1.01725900	-0.98013500	C	-4.36872900	-1.48123800	0.26968300
C	-1.48686600	0.43710700	0.01065600	C	1.15216800	0.42121800	-0.47066000
C	-1.88921300	-0.80711500	-0.52778100	C	1.38506500	-0.60022600	0.50519700
C	-3.21767400	-1.18908500	-0.45979300	C	2.64943200	-1.1219000	0.64965400
C	-4.15700500	-0.35544900	0.15139000	C	3.70240400	-0.6957400	-0.15279400
C	-3.77846000	0.87712800	0.68922100	C	3.50102800	0.4029000	-1.12414800
C	-2.45707900	1.27536600	0.61105600	C	2.23891000	0.86596100	-1.29002600
C	-0.16400700	0.93885400	-0.07269400	H	-1.10754600	0.90814100	2.15555500
H	0.81884800	-0.03023600	-1.70422000	H	-1.21759200	-0.8895800	-2.4724220
H	3.46626900	0.28743300	1.92929300	H	-2.39349900	0.03148300	-3.44776400
H	4.63687800	-1.06022100	1.77595900	H	-2.77388700	-1.6273340	-2.91970000
H	5.11937400	0.58081700	1.27768800	H	-4.45024800	-1.8457800	1.29047700
H	5.15725700	-1.96964200	-0.56405100	H	-4.65191200	-0.4457350	0.12271500
H	4.39759900	-1.18511200	-1.97072300	H	-4.95120700	-2.0945820	-0.41851100
H	5.67688700	-0.34060500	-1.06406900	H	0.57663300	-0.96671600	1.12741600
H	-1.15210400	0.97662100	-1.45961600	H	2.83497500	-1.89936800	1.38309000
H	-3.52782000	0.87596100	-2.14088000	H	4.32604700	0.68435800	-1.73709600
H	-4.51622600	1.51763500	1.15895100	H	2.05562100	-2.04495000	-1.48123800
H	-2.14199300	2.23066400	1.01975400	C	-0.08340700	1.01395400	-0.70204700
H	-0.00336500	1.98245700	0.17629000	H	-0.14165200	1.71969200	-1.53525400
O	1.45266000	0.59576100	1.97227500	O	-0.79166500	3.60784700	1.25812700
H	0.93694600	-0.09825100	2.40642500	H	-0.47561500	3.72284500	0.35896700
O	-5.52460000	-0.76707200	0.22316400	O	5.01104000	-1.19890200	0.02216800
C	-6.31918500	0.06680400	-0.62429400	C	5.93730600	-0.14590000	0.30166200
H	-7.28608900	-0.75246600	-0.37316000	H	6.83705900	-0.56035100	0.70610700
H	-6.42353700	1.03332800	-0.17725800	H	6.16204000	0.60226600	0.38070100
H	-5.84247700	0.16419200	-1.57727200	H	5.50589900	0.52986000	1.01027800
(14c-TS1)	*G* = -1083.746565 a. u. (Gas phase) *G* = -1083.802252 a. u. (In methanol)			**(14c-TS2)**	*G* = -1083.719218 a. u. (Gas phase) *G* = -1083.773376 a. u. (In methanol)		
O	3.69667600	0.69014100	-0.67321000	O	-2.98398100	-0.44627500	-1.20996300
C	2.46969800	1.19513800	-0.82113200	C	-2.82031600	0.85475800	-0.85947800
C	1.30481700	0.24320800	-0.70297100	C	-1.63353600	0.92681000	0.10131900
C	1.58813700	-0.98989400	0.11938600	C	-1.72275800	-0.03596200	1.26204500
O	2.87013600	-1.38830400	0.13742400	O	-2.31585300	-1.19584900	1.00121500
C	3.99026900	-0.51101300	0.04815100	C	-2.97668700	-1.53491900	-0.26825000
O	2.31551700	2.33703500	-1.16009200	O	-3.37378900	1.76922400	-1.37625400
O	0.73113800	-1.72409600	0.53173800	O	-1.34946300	0.31455300	2.34756600
C	4.46010700	-0.14416400	1.44150400	C	-2.21533000	-2.68400300	-0.87160500
C	5.03065800	-1.24611400	-0.77295000	C	-4.41557700	-1.79051700	0.12997400
C	-1.22685700	0.59411100	-0.14612600	C	0.90120100	0.67615900	-0.41329200
C	-1.67491200	-0.66793700	-0.60040100	C	1.22328900	-0.37567800	0.50310500
C	-3.02314900	-0.97692500	-0.55441300	C	2.53106700	-0.78232000	0.63478900
C	-3.93819000	-0.05131500	-0.04767700	C	3.54030900	-0.12219500	-0.16152000
C	-3.51448000	1.20027200	0.40598200	C	3.25261500	0.86170300	-1.03551600
C	-2.17210000	1.52498600	0.34830300	C	1.94700500	1.27255600	-1.18838600
C	0.12261100	1.02138200	-0.21704600	H	-1.52837800	2.09764100	1.03303600
H	1.10958000	-0.12333000	-1.72785500	H	-1.17286700	-2.40124600	-1.03958100
H	3.64164000	0.35413400	1.96982900	H	-2.25686300	-3.53956700	-0.19602100
H	4.74455100	-1.05781200	1.96857400	H	-2.67174800	-2.95047800	-1.82576500
H	5.32958900	0.51189400	1.36208000	H	-4.47052800	-2.22273700	1.12582700
H	5.29781300	-2.17721800	-0.27069300	H	-4.79652700	-0.78006300	0.04098700
H	4.62991100	-1.47175000	-1.76318000	H	-4.92961000	-2.41400500	-0.60222500
H	5.91934200	-0.62143900	-0.87653900	H	0.44865400	-0.85552500	1.09023500
H	-0.95785000	-1.39014500	-0.96752900	H	2.78441600	-1.58027500	1.32318400

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
H	-3.36810600	-1.94258400	-0.90627400	H	4.04584900	-1.61448700	1.32030600
H	-4.23355600	1.91225200	0.79483600	H	1.69769800	-1.89918500	2.05558700
H	-1.82176800	2.49328700	0.69264100	C	-0.38390900	0.62714300	1.16018700
H	0.32901200	2.07239200	-0.04476100	H	-0.50283700	-1.41744100	1.90649600
O	1.64671300	0.76428300	1.90997900	O	-1.35800500	3.54955900	1.47386600
H	1.08045800	0.13385300	2.37689600	H	-1.04652800	3.74902600	0.58797800
N	-5.36602400	-0.39698500	0.00430300	N	4.93230600	-0.60399100	0.04352700
O	-6.13390300	0.41496900	0.43963200	O	5.16240700	-1.48064800	0.82898600
O	-5.70604100	-1.47715800	-0.39069700	O	5.78229600	0.61334600	-0.07065900
(14a-Int)	*G* = -879.3931200 a. u. (Gas phase) *G* = -879.4303725 a. u. (In methanol)			**(14b-Int)**	*G* = -993.8458079 a. u. (Gas phase) *G* = -993.8865184 a. u. (In methanol)		
O	-2.69833100	1.11303500	0.15859700	O	-3.46209200	1.01452700	0.21995200
C	-1.44997500	1.48582700	0.43341600	C	-2.22828900	1.45364100	0.46037200
C	-0.38206100	0.43434500	0.25728000	C	-1.11024400	0.46346000	0.24451600
C	-0.71613300	-0.55875800	-0.82864100	C	-1.42203800	-0.53994200	-0.83855900
O	-2.01524600	-0.71296300	-1.05575200	O	-2.71701900	-0.76387700	-1.02811200
C	-3.01659600	-0.23764700	-0.20366200	C	-3.71675800	-0.34939000	-0.14300900
O	-1.17927700	2.58984100	0.81149000	O	-2.00712700	2.56856100	0.83866800
O	0.12270400	-1.16568000	-1.42742800	O	-0.56966900	-1.09628000	-1.46665300
C	-4.26898600	-0.16361200	-1.04225300	C	-4.99600600	-0.33919200	-0.94339500
C	-3.12209400	-1.11483500	1.03081800	C	-3.73689300	-1.23845300	1.08731300
C	2.17183700	0.49458100	0.02300000	C	1.42832000	0.66523900	-0.06513800
C	2.37325300	-0.88351700	0.29990800	C	1.71306700	-0.70136000	0.19510300
C	3.63936500	-1.41350600	0.23284100	C	3.00368000	-1.16061800	0.08636100
C	4.72257800	-0.10383100	-0.58056200	C	4.02907800	-0.26744600	-0.27598900
C	4.55959000	0.37068700	0.78909800	C	3.78344800	-0.52739000	1.09277800
C	3.29914000	-0.30569500	1.33493700	C	2.49755600	-0.42077000	1.56818600
H	-0.34433800	1.18837200	-0.17479800	H	-1.01123600	1.16938500	-0.14827900
H	-4.09596400	-1.91666800	0.46689600	H	-4.88414200	-1.81771800	0.30511000
H	-4.55337200	-1.37782600	-1.16294500	H	-5.23527500	-1.27800100	-1.35059700
H	-5.08672000	-0.45693900	0.25716500	H	-5.81753700	-0.33082000	0.03252400
H	-3.38637000	0.74196600	-2.13442500	H	-3.95357700	0.79865300	-2.26926100
H	-2.16657400	1.56036200	-1.13155600	H	-2.76637800	1.58806500	-1.20586700
H	-3.89027900	1.70051300	-0.72517100	H	-4.50472900	1.78251800	-0.89558900
H	1.53075000	-1.51678500	0.55402500	H	0.91450100	0.46930700	-1.38144800
H	3.80109500	0.42931700	-2.46718100	H	3.22865000	0.26987100	-2.20498600
H	5.71738500	-0.16687100	-1.01343600	H	4.59371100	-0.80887900	1.75480700
H	5.41299200	-0.63162400	1.40363800	H	2.28889100	-0.59320700	2.62003100
H	3.15376400	-0.49065800	2.39527100	C	0.15697500	-0.01959700	1.19371100
C	0.93063500	0.02706000	1.09214000	H	0.06919600	-0.2070810	2.27405500
H	0.90792100	-0.16947300	2.17420200	O	-0.96911500	-1.57634600	1.64658500
O	-0.39490100	1.67520000	-1.59933700	H	-0.68191200	-2.19830100	1.00001600
H	-0.12318100	-2.24100100	1.04132300	O	5.36421800	-0.76380700	-0.40218900
				C	6.18046100	-0.20615200	0.63109200
				H	7.09723700	-0.75404300	0.69618100
				H	6.39228400	0.81794000	0.40467100
				H	5.66261600	-0.26508700	1.56557800
(14c-Int)	*G* = -1083.789539 a. u. (Gas phase) *G* = -1083.845576 a. u. (In methanol)			**(15a)**	*G* = -918.5995480 a. u. (Gas phase) *G* = -918.6267384 a. u. (In methanol)		
O	-3.73723100	0.93165400	0.13743700	O	-2.80628400	-1.18477300	-0.20227400
C	-2.53737500	1.42541300	0.43650100	C	-1.59458600	-1.70550400	-0.49851100
C	-1.36631200	0.48834200	0.27040400	C	-0.42577600	-0.77187200	-0.41239200
C	-1.58103300	-0.52290400	-0.82885000	C	-0.66816400	0.73404200	-0.62915700
O	-2.85416200	-0.80475100	-1.07936400	O	-2.08906700	1.02707400	-0.35314100

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	-3.91197800	-0.44066100	-0.24082400	C	-2.86221400	0.12503000	0.38182300
O	-2.38537100	2.54738800	0.82782000	O	-1.50468300	-2.86962600	-0.79452700
O	-0.67574700	-1.03668200	-1.41794800	O	-0.28074600	1.24787900	-1.70530600
C	-5.15167800	-0.48490200	-1.10011500	C	-2.44885200	0.02227600	1.85710900
C	-3.94865700	-1.33575300	0.98473600	C	-4.30349500	0.57280100	0.24200500
C	1.17201200	0.80724500	0.08034200	C	0.77106900	1.35096100	-0.20321800
C	1.50662100	-0.54620300	0.34981300	H	0.74095100	2.43532400	-0.09529000
C	2.82057800	-0.94556300	0.30025700	C	2.1091550	-0.75170700	-0.06229500
C	3.81975400	-0.01127000	-0.00477000	C	3.01908200	-1.38932000	0.79556300
C	3.52405900	-0.27009900	1.34405100	C	4.30121000	0.98115000	-0.88153500
C	2.21417300	-0.22239600	1.75976900	C	4.70377200	0.28448900	0.25728700
H	-1.28257600	1.19718700	-0.12278100	C	3.81911900	-0.59852100	0.87718600
H	-5.02883800	-1.96645700	0.16812300	C	2.52884700	-0.77435600	0.38351300
H	-5.32852700	-1.44835200	-1.50451300	O	-0.02100600	0.46371600	1.36691700
H	-6.01701300	-0.52559000	-0.15406700	C	0.12000900	0.37217300	2.82537200
H	-4.10422000	0.68339600	-2.37394100	H	-1.46681000	1.98135100	-0.45159100
H	-3.00503200	1.53040600	-0.52290400	H	-2.45477800	2.31194800	1.01944400
H	-4.76293900	1.64423000	-1.03169600	H	-3.16243300	2.39930400	-0.60190100
H	0.72813800	0.58448900	-1.26335500	H	-4.42930700	0.69892500	1.55706700
H	3.08435200	0.49118200	-1.97946900	H	-4.54676800	-0.81949300	0.63605700
H	4.31538100	-0.51155400	2.04373100	H	-4.96825300	0.72713600	-0.14503800
H	1.96581000	-0.40147800	2.80183400	H	2.71133500	1.32237400	-2.28912700
C	-0.12294400	0.0678600	1.27693500	H	4.98885200	1.65629000	-1.38097300
H	-0.25128400	2.35305800	-0.12052000	H	5.70801300	0.41514900	0.64842800
O	-1.19736600	-1.54976800	1.67186300	H	4.14068000	-1.16655000	1.74501300
H	-0.85217200	-2.15478700	1.03770300	H	1.84132400	-1.47691600	0.84629400
N	5.21872200	-0.07810300	-0.45122500				
O	5.46053600	0.14452400	-1.60464700				
O	6.06240700	-0.35259000	0.35578300				
(15b)	*G* = -1033.048469 a. u. (Gas phase)			**(15c)**	*G* = -1123.009546 a. u. (Gas phase)		
	G = -1033.082918 a. u. (In methanol)				*G* = -1123.057317 a. u. (In methanol)		
O	3.39856300	1.46310300	-0.04220600	H	-0.37523400	1.32954600	1.09130400
C	2.14506400	1.97186700	0.07977300	H	0.66859600	1.26324100	3.12244800
C	1.03591300	1.01004400	-0.18330400	H	0.67985900	-0.54059300	2.99874600
C	1.37332200	-0.23876700	-0.91067300	H	-0.87679200	3.25973200	0.31066300
O	2.67924000	-0.60956300	-0.86087500	O	3.77677500	1.01149500	-0.14578000
C	3.55970000	0.05114200	0.04206400	C	2.62733700	1.62414700	-0.49689600
O	1.99970900	3.13454300	0.34935100	C	1.37812400	0.79222900	-0.43394500
O	0.61834900	-0.87064400	-1.60150600	C	1.50084100	-0.73465400	-0.60829200
C	3.32965700	-0.41562300	1.47244600	O	2.88054100	-1.13543700	-0.28670200
C	4.95832100	-0.24152500	-0.45522000	C	3.70305500	-0.28788100	0.46161900
C	-0.21059100	1.44088000	0.12551900	O	2.64033500	2.78249600	-0.82377900
H	-0.22468600	2.46651400	0.49608200	O	1.10057700	-1.22950500	-1.68906900
C	-1.51718800	0.80701600	0.07388600	C	3.24929800	-0.12143400	1.91855100
C	-2.63282200	1.65472900	0.10184500	C	5.10465700	-0.85738400	0.37859900
C	-3.93150200	1.16310200	0.06193300	C	0.22944200	1.47664500	-0.29729700
C	-4.12859400	-0.21990700	0.03329800	H	0.34097200	2.55813000	-0.22099000
C	-3.02363600	-1.08517300	0.05153200	C	-1.15688500	0.98372400	-0.20400200
C	-1.73830200	-0.58591500	0.06453600	C	-2.04394600	1.69092500	0.62406300
O	0.95487200	-2.33556700	0.92358500	C	-3.36536700	1.28851900	0.76775300
C	1.54196600	-3.33533700	0.10501200	C	-3.79318000	0.18091400	0.04640800
H	2.30589200	-0.20829300	1.79163900	C	-2.95671100	-0.51932400	-0.81453600
H	3.49758400	-1.49322100	1.53564600	C	-1.63198400	-0.11548900	-0.93849100
H	4.02912500	0.10248900	2.13278400	O	0.77059700	-1.29152000	0.47353800

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
H	5.13300200	-1.31965100	-0.44184700	C	0.50368800	-2.73636200	0.38522300
H	5.06091900	0.12828300	-1.47703600	H	2.30479100	0.43182900	2.00050700
H	5.68929200	0.25576500	0.18559300	H	3.16104000	-1.10558600	2.39282900
H	-2.47848600	2.72998100	0.14241300	H	3.99169700	0.45559400	2.47393600
H	-4.76699600	1.85229600	0.06630000	H	5.13153700	-1.84026200	0.85438500
H	-3.21235000	-2.15327800	0.05347500	H	5.37741900	-0.95977300	-0.67259000
H	-0.89790400	-1.26902200	0.09575400	H	5.81074400	-0.18919400	0.87588500
H	1.00623800	-2.62427600	1.84457700	H	1.68902500	2.56316400	1.16534500
H	1.04929900	-4.30628800	0.23688500	H	-4.05923400	1.81435900	1.41207600
H	1.41359600	-3.00201800	-0.92459600	H	-3.34906700	-1.35702000	-1.37880900
H	2.61603800	-3.44774600	0.30588200	H	-0.95382200	-0.62980900	-1.61357100
O	-5.34053800	-0.81695600	0.00443900	H	1.14198000	-1.05261100	1.34361300
C	-6.48346600	0.01270400	-0.02013100	H	-0.05420100	-2.98420600	1.28548100
H	-7.34153500	-0.65766100	-0.05535500	H	-0.08206700	-2.86455500	-0.51832400
H	-6.54186500	0.63409300	0.88111200	H	1.45975300	-3.25211800	0.31077100
H	-6.48577400	0.65728000	-0.90669900	N	-5.19240800	-0.25895600	0.19138800
				O	-5.91129300	0.38474800	0.93511700
(16a)	*G* = -918.6116490 a. u. (Gas phase) *G* = -918.6401859 a. u. (In methanol)			**(16b)**	*G* = -1033.060570 a. u. (Gas phase) *G* = -1033.093537 a. u. (In methanol)		
O	-2.4878550	0.12888600	-0.92568100	O	-5.54201700	-1.24261600	-0.43617600
C	-1.3153520	0.79170900	-1.02428100	O	-3.3660070	0.15566300	-0.97732200
C	-0.1645580	0.18593800	-0.28965000	C	-2.1519600	0.70371300	-1.20850700
C	-0.5245640	-0.67208100	0.87029600	C	-1.0218450	0.14592500	-0.40578100
O	-1.7181890	-1.29299100	0.78814400	C	-1.3930740	-0.48539800	0.88048500
C	-2.4968390	-1.19889700	-0.40409900	O	-2.6474640	-0.98357900	0.94966400
O	-1.2598490	1.81359200	-1.66005400	C	-3.4457700	-1.05023100	-0.23173300
O	0.13738500	-0.79826600	1.86989800	O	-2.0403080	1.59213200	-2.01181900
C	-1.9748390	-2.17584100	-1.44791500	O	-0.7056690	-0.51757900	1.87239700
C	-3.9243910	-1.46790800	0.01513900	C	-3.0104780	-2.23200900	-1.08701400
C	1.06708500	0.56334300	-0.69401900	C	-4.8778280	-1.14923400	0.24467700
H	1.03333300	1.28809500	-1.50790300	C	0.22124000	0.43017800	-0.86011200
C	2.42984500	0.19531600	-0.30366200	H	0.19326400	1.02912400	-1.77095400
C	3.45831700	0.97109200	-0.86760800	C	1.57432800	0.10549800	-0.43415000
C	4.79472600	0.70736400	-0.59012000	C	2.60833600	0.70237900	-1.17198400
C	5.12824500	-0.35915700	0.24208400	C	3.94888600	0.47289500	-0.89224700
C	4.11950200	-1.15171400	0.79183900	C	4.28253700	-0.39770100	0.14827400
C	2.78180100	-0.87957600	0.53031300	C	3.26573200	-1.01973400	0.88893300
O	-2.0510950	1.52653000	1.56982700	C	1.93820300	-0.77198700	0.60983400
H	-1.4711990	1.68764700	2.32247000	O	-2.4957530	1.89902200	1.43368400
C	-2.5918490	2.75473000	1.10394000	H	-2.4445660	1.40815800	2.26675800
H	-0.9409430	-1.94537300	-1.71972500	C	-1.3652100	2.75048700	1.36031100
H	-2.0142610	-3.19034700	-1.04559200	H	-1.9698130	-2.12126700	-1.40479400
H	-2.5957460	-2.11607000	-2.34430700	H	-3.1062410	-3.15560600	-0.51156900
H	-3.9977420	-2.46886500	0.44463600	H	-3.6438320	-2.29149800	-1.97495900
H	-4.2136410	-0.72802900	0.76384700	H	-5.0035910	-2.04575800	0.85532800
H	-4.5823840	-1.39120000	-0.85265800	H	-5.1109320	-0.26393400	0.83955300
H	3.19792300	1.79283200	-1.52940500	H	-5.5488530	-1.19417700	-0.61554500
H	5.57149200	1.32568400	-1.02790900	H	2.35246700	1.37007400	-1.99048700
H	6.16955500	-0.57593100	0.45914600	H	4.71188300	0.96273800	-1.48468800
H	4.37630800	-1.98630500	1.43614400	H	3.55538200	-1.69332000	1.68816300
H	2.01431500	-1.49165600	0.98332100	H	1.17399500	-1.24879600	1.20711200
H	-3.2034760	3.24027000	1.87270000	H	-1.4364700	2.07171500	3.58261500
H	-3.2227460	2.51070400	0.24746900	H	-1.3445270	0.34540400	3.15425400
H	-1.8067440	3.44062200	0.76715300	H	-0.4322680	1.54021400	2.20034500

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
				O	5.54566400	-0.70487700	0.51197400
				C	6.60397700	0.20194500	-0.09871500
				H	7.52299500	0.24801500	-0.47226800
				H	6.57629900	-1.26195200	-0.37625100
				H	6.56864100	-0.11019200	0.99291700
(16c)	*G* = -1123.021641 a. u. (Gas phase) *G* = -1123.066911 a. u. (In methanol)			**(17a)**	*G* = -918.6749400 a. u. (Gas phase) *G* = -918.7031981 a. u. (In methanol)		
O	-3.4034050	0.01791400	-0.99758400	C	-2.89666500	0.03701200	0.33707100
C	-2.5360370	1.05565600	-0.48159800	O	-1.32461400	-2.94580100	-0.57631700
C	-1.2294300	0.40004800	0.06330600	O	-0.29188700	1.26978900	-1.67510500
C	-1.4603350	-0.73213100	0.99046300	C	-2.52415900	0.13277900	1.81240000
O	-2.6722520	-1.33495500	0.78057200	C	-4.34585300	0.39152300	0.08123900
C	-3.2048190	-1.30672500	-0.57533000	C	0.85897700	-1.27065300	-0.17266300
O	-2.4302160	2.08102500	-1.16517200	H	0.87042000	0.07417100	-2.35586200
O	-0.8053880	-1.06243600	1.94490800	C	2.18660200	0.05883300	-0.65386900
C	-2.2718760	-2.06290100	-1.51148600	C	3.17614600	0.57266900	-1.42542100
C	-4.5676120	-1.96139600	-0.47240800	C	4.46807500	-0.9393680	0.74368700
C	-0.0757810	0.92269700	-0.37951200	C	4.80123200	0.32266200	0.25649800
H	-0.2528050	1.74778600	-1.07275700	C	3.83665800	-0.40124000	1.08690300
C	1.33621800	0.55846700	-0.19815900	C	2.53951300	-0.55762400	0.61052400
C	2.22152800	1.01433300	-1.19091300	O	-0.13104600	1.38769300	0.57085200
C	3.57567300	0.72217900	-1.13919000	C	-0.26671300	2.80521300	0.53400900
C	4.04146600	-0.01999700	-0.06257100	H	-1.49720800	-0.18803300	1.99562200
C	3.20619400	-0.46920200	0.95048900	H	-2.62422500	1.16868800	2.14610600
C	1.85003000	-0.17753500	0.88168000	H	-3.20456000	-0.49978800	2.38666700
O	-3.3217100	1.36418000	0.74394900	H	-4.53658200	1.41459700	0.41212200
H	-3.5475410	0.56134900	1.26134300	H	-4.55541500	0.30963800	-0.98670900
C	-2.8420680	2.46932000	1.55327800	H	-4.99334900	-0.29559500	0.62900800
H	-1.2988290	-1.57232600	-1.58487000	H	2.91981300	2.41567300	0.93991200
H	-2.1346930	-3.08856700	-1.15997800	H	5.21346300	-1.54757400	1.24583100
H	-2.7188630	-2.07909000	-2.50795400	H	5.81012000	0.70480700	0.37728600
H	-4.4706490	-2.99608000	-0.13643300	H	4.09865600	0.80090800	2.06159600
H	-5.1891560	-1.40714500	0.23549600	H	1.80738800	-1.08836000	1.20444700
H	-5.0496470	-1.93750800	-1.45182100	H	0.06407500	1.51062100	3.15792600
H	1.83222400	1.59911400	-2.01894100	H	0.36164200	-0.25065800	3.23459900
H	4.26694400	1.05866500	-1.90170700	H	-1.30924200	3.09181900	0.36623200
H	3.62296800	-1.03270400	1.77612800	H	-0.91527700	1.01759900	-2.36802000
H	1.18826400	-0.50782800	1.67086500				
H	-3.6671460	2.78598400	2.18771200				
H	-2.5775290	3.22951100	0.82161000				
H	-1.9745700	2.15150300	2.13468200				
N	5.47860700	-0.33113700	0.01207000				
O	6.18814700	0.07534400	-0.88937300				
O	5.86506200	-0.97502100	0.96943000				
(17b	*G* = -1033.123861 a. u. (Gas phase) *G* = -1033.154788 a. u. (In methanol)			**(17c)**	*G* = -1123.08494 a. u. (Gas phase) *G* = -1123.13303 a. u. (In methanol)		
O	3.45073200	1.29287000	-0.03238500	O	3.73770300	1.11700000	-0.05980600
C	2.20650000	1.77248300	-0.26997100	C	2.55851300	1.68861100	-0.38718800
C	1.09187500	0.77642200	-0.31810700	C	1.35206300	0.79455000	-0.38883000
C	1.42836100	-0.69650900	-0.47150300	C	1.56069800	-0.71132200	-0.47022600
O	2.82727300	-0.89010200	-0.48873900	O	2.93370800	-1.02784900	-0.40045300
C	3.58966200	-0.07247000	0.37076800	C	3.73150500	-0.22512500	0.44290700
O	2.05923000	2.95709200	-0.43160500	O	2.51860000	2.86080000	-0.65312600
O	0.98367300	-1.23885400	-1.67873100	O	1.14041500	-1.24999800	-1.68808400

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	3.20507700	-0.21466900	1.83926500	C	3.26694600	-0.23045800	1.89412700
C	5.03779300	-0.43340300	0.11428200	C	5.14940800	-0.73044900	0.28421900
C	-0.1478100	1.29613800	-0.20347000	C	0.16930100	1.42397500	-0.28901200
H	-0.1435360	2.37965400	-0.08686900	H	0.24957300	2.50839600	-0.22132900
C	-1.4877400	0.71519900	-0.17131600	C	-1.2081500	0.91539800	-0.20561300
C	-2.5121470	1.54766300	0.29821000	C	-2.1381960	1.73713900	0.45030300
C	-3.8313510	1.12012500	0.39735100	C	-3.4632450	1.35259800	0.59650600
C	-4.1535820	-0.17677300	-0.00564800	C	-3.8529130	0.13931000	0.04883400
C	-3.1495980	-1.01803300	-0.50620000	C	-2.9720440	-0.68702800	-0.63689000
C	-1.8415530	-0.58488400	-0.58595900	C	-1.6465300	-0.29685000	-0.76122300
O	0.81965700	-1.38765800	0.55800400	O	0.83170100	-1.29250900	0.54468400
C	0.95991000	-2.80161000	0.49463300	C	0.82083200	-2.71630600	0.53709900
H	2.18114700	0.11652600	2.02208300	O	3.73770300	1.11700000	-0.05980600
H	3.28673700	-1.26246300	2.14030000	C	2.55851300	1.68861100	-0.38718800
H	3.88857700	0.38798600	2.44214000	C	1.35206300	0.79455000	-0.38883000
H	5.21691100	-1.46963300	0.40980300	C	1.56069800	-0.71132200	-0.47022600
H	5.25426800	-0.31739200	-0.94940200	O	2.93370800	-1.02784900	-0.40045300
H	5.69000900	0.22743100	0.68872200	C	3.73150500	-0.22512500	0.44290700
H	-2.2668580	2.56104500	0.60526200	O	2.51860000	2.86080000	-0.65312600
H	-4.5869270	1.79768400	0.77598600	O	1.14041500	-1.24999800	-1.68808400
H	-3.4337350	-2.01270200	-0.83294100	C	3.26694600	-0.23045800	1.89412700
H	-1.0905020	-1.24284500	-1.00097600	C	5.14940800	-0.73044900	0.28421900
H	0.66119700	-3.17395900	1.47488200	C	0.16930100	1.42397500	-0.28901200
H	0.31113000	-3.22502200	-0.27699200	H	0.24957300	2.50839600	-0.22132900
H	1.99765200	-3.08065200	0.29003700	C	-1.2081500	0.91539800	-0.20561300
H	1.54646300	-0.88084400	-2.38141500	C	-2.1381960	1.73713900	0.45030300
O	-5.3985370	-0.70565200	0.03628800	C	-3.4632450	1.35259800	0.59650600
C	-6.4415940	0.11156000	0.52364600	C	-3.8529130	0.13931000	0.04883400
H	-7.3462840	-0.49382700	0.47705100	C	-2.9720440	-0.68702800	-0.63689000
H	-6.2570950	0.41391000	1.56120500	C	-1.6465300	-0.29685000	-0.76122300
H	-6.5681910	-0.09740600	1.00612100	O	0.83170100	-1.29250900	0.54468400
				C	0.82083200	-2.71630600	0.53709900
(18a)	*G* = -918.6689090 a. u. (Gas phase) *G* = -918.6979001 a. u. (In methanol)			**(18b)**	*G* = -1033.117830 a. u. (Gas phase) *G* = -1033.149873 a. u. (In methanol)		
O	1.45490500	1.91889800	0.09204100	O	-2.26460300	-1.89860200	0.12179900
C	0.33118400	1.42744000	-0.47430100	C	-1.13525000	-1.45638500	-0.47619900
C	0.21397200	-0.06041200	-0.46498600	C	-0.95433200	0.02167600	-0.48254400
C	1.52968300	-0.82008200	-0.63507800	C	-2.24048900	0.84169200	-0.58735800
O	2.63638700	-0.02214900	-0.33622800	O	-3.37234400	0.09452100	-0.25761800
C	2.43775800	1.00453100	0.60832300	C	-3.18271600	-0.94372400	0.67268100
O	-0.4828410	2.19365400	-0.92281600	O	-0.37211800	-2.26558300	-0.93796700
O	1.74531100	-1.16100100	-1.97334500	O	-2.49254900	1.21898700	-1.90747400
C	2.01359300	0.49159900	1.98018200	C	-2.68537400	-0.45631400	2.02923900
C	3.73361000	1.78515300	0.65767200	C	-4.51035500	-1.66526300	0.76939200
C	-0.9199090	-0.75887900	-0.27048000	C	0.21568200	0.68404500	-0.37620900
O	1.48713800	-1.95645300	0.17422300	O	-2.11110300	1.95866800	0.24100000
C	2.67722500	-2.73927500	0.15570300	C	-3.25338600	2.80380000	0.25937200
H	0.95323500	-1.60924200	-2.29638400	H	-1.68399600	1.63883400	-2.23752200
H	1.06349300	-0.04356600	1.94325500	H	-1.71311100	0.03350300	1.95519100
H	2.77909300	-0.19021300	2.35934500	H	-3.40231900	0.25967400	2.43986300
H	1.91887100	1.33998400	2.66143800	H	-2.60430600	-1.30994300	2.70638000
H	4.53180000	1.14466900	1.03883200	H	-5.26560700	-0.99093800	1.17936200
H	3.98749700	2.12224900	-0.34846000	H	-4.81469600	-1.98707300	-0.22800200
H	3.61598100	2.65058300	1.31245600	H	-4.41020000	-2.53791400	1.41793500

Atom	*x* / Å	*y* / Å	*z* / Å
H	2.45399100	-3.63535600	0.73411600
H	2.95038600	-3.01032600	-0.86734400
H	3.50400600	-2.19337400	0.61923300
C	-2.3270090	-0.37158100	-0.07073000
C	-2.9667640	0.71704800	-0.68226700
C	-3.08266400	-1.21559800	0.76269600
C	-4.31521900	0.96307600	-0.43305200
H	-2.41007900	1.36049000	-1.34907300
C	-4.42225500	-0.95511900	1.02327200
H	-2.60315700	-2.07844500	1.21815600
C	-5.04342600	0.14046600	0.42357900
H	-4.79821800	1.80629100	-0.91640000
H	-4.98281000	-1.60993300	1.68271300
H	-6.09243800	0.34396100	0.61485600
H	-0.75750600	-1.83157700	-0.16093700

Atom	*x* / Å	*y* / Å	*z* / Å
H	-2.97393700	3.67563100	0.85140000
H	-3.52954700	3.11023800	-0.75295600
H	-4.10339700	2.29650900	0.72537500
C	1.62448700	0.29388300	-0.27150700
C	2.19795400	-0.91338700	-0.71756300
C	2.47939900	1.24742100	0.30008000
C	3.55123000	-1.14774500	-0.56340000
H	1.57481000	-1.65609600	-1.19498600
C	3.83848800	1.01778000	0.47308300
H	2.06516500	2.19601400	0.63264100
C	4.38106100	-0.19423800	0.03927000
H	4.00149100	-2.07158400	-0.91052600
H	4.45631900	1.78064100	0.93117400
H	0.08329800	1.76203500	-0.27733400
O	5.68825000	-0.52893000	0.14486200
C	6.55955800	0.40850500	0.74001800
H	6.26522000	0.62390800	1.77400700
H	7.54771300	-0.05044400	0.73222000
H	6.58708600	1.34404800	0.16883100

(18c) *G* = -1123.078909 a. u. (Gas phase)
G = -1123.124370 a. u. (In methanol)

O	-2.26238200	-1.93824800	0.19395800
C	-1.19743600	-1.40995400	-0.44227100
C	-1.16935500	0.08390700	-0.49400000
C	-2.53311900	0.76239300	-0.62875200
O	-3.57505400	-0.08402300	-0.25177900
C	-3.27356600	-1.05995300	0.71727000
O	-0.35780500	-2.14105700	-0.89768800
O	-2.82127200	1.03347400	-1.96579200
C	-2.81969500	-0.46959000	2.04709900
C	-4.51744600	-1.91121800	0.85482100
C	-0.06908900	0.84559000	-0.38373100
O	-2.51070700	1.92735600	0.13542800
C	-3.74177900	2.64147900	0.14338300
H	-2.10381500	1.59209900	-2.30192700
H	-1.90747300	0.12043700	1.94351500
H	-3.60694400	0.17939700	2.43960000
H	-2.63974600	-1.28172800	2.75525600
H	-5.33626100	-1.30314400	1.24567500
H	-4.79257100	-2.30266700	-0.12596400
H	-4.32279200	-2.74181400	1.53616900
H	-3.54049800	3.58254200	0.65504400
H	-4.08790100	2.83379700	-0.87537900
H	-4.50920300	2.08085300	0.68461600
C	1.36117200	0.51072700	-0.24939800
C	2.00653200	-0.52736700	-0.93591800
C	2.11908100	1.35346900	0.58165500
C	3.37051100	-0.73596900	-0.76845200
H	1.43875900	-1.16811500	-1.59523400
C	3.47606800	1.14598800	0.77049000
H	1.62875700	2.17605600	1.09435700
C	4.07626900	0.09697400	0.08665100
H	3.88940500	-1.52998000	-1.29103900
H	4.07096200	1.77673600	1.41909200

(19a) *G* = -1014.342830 a. u. (Gas phase)
G = -1014.376818 a. u. (In methanol)

O	-0.47186600	2.17040000	0.01805000
C	-0.42307800	1.20073000	0.80681300
C	-0.25865100	-0.17191700	0.10990900
C	1.13800700	-0.61061900	-0.10081300
O	1.72619700	0.75150800	-1.14042600
C	1.81502500	1.94670800	-0.79100200
O	-0.41367200	1.19142700	2.05074200
O	1.34593700	-1.61293100	-0.90735100
C	2.26591000	2.40808900	0.56270200
C	1.65370500	2.98581000	-1.85390400
C	-1.24020000	-0.96353900	-0.34962100
O	2.03040700	-0.48844800	0.91772300
C	1.58208000	-1.09246900	2.15160700
H	2.33935400	-1.81095900	-0.93076100
N	4.05057300	-1.76400400	-0.91566400
H	4.51083600	-2.10426900	-1.75464100
C	4.61374400	-2.39175300	0.28480200
H	1.80200500	1.85458300	1.37749200
H	3.35201300	2.25739400	0.60523200
H	2.04584500	3.46885600	0.67546800
H	2.52890000	3.64141400	-1.88088000
H	1.48253200	2.52023000	-2.82291000
H	0.78109100	3.57718900	-1.56216200
H	2.40554200	-0.95097800	2.85146600
H	0.68409300	-0.58156800	2.50599700
H	1.40877600	-2.16210400	1.99501400
H	4.09793700	-1.98492300	1.15600800
H	4.42792400	-3.46676600	0.24817700
H	5.69032000	-2.22810300	0.40408900
H	4.19249000	-0.75729000	-0.88220300
H	-0.95131300	-1.86823900	-0.88241800
C	-2.68647700	-0.73993100	-0.23383100
C	-3.53111800	-1.42953600	-1.11474500

Atom	*x* / Å	*y* / Å	*z* / Å
H	-0.26987400	1.91381100	-0.30075900
N	5.52022900	-0.12676900	0.26571100
O	6.11442400	0.62223100	1.01934500
O	6.02763300	-1.04470100	-0.35048400

(19b)	*G* = -1128.792180 a. u. (Gas phase) *G* = -1128.833428 a. u. (In methanol)		
O	1.70529000	2.10528800	0.32881400
C	0.54390300	1.49580900	0.66938200
C	0.41400900	0.08611600	0.22953100
C	1.77467400	-0.54350900	-0.01280500
O	2.46458200	0.24649000	-0.95786000
C	2.60425700	1.62878900	-0.67768600
O	-0.2409210	2.11367800	1.34455100
O	1.67508600	-1.80619600	-0.49684100
C	4.00017300	1.91087000	-0.14766800
C	2.29123000	2.36499000	-1.97004000
C	-0.7074890	-0.62675400	0.01274000
O	2.57078900	-0.48585500	1.16068200
C	2.07491100	-1.26713000	2.23387500
H	2.61778400	-2.10473400	-0.68921400
N	4.31973300	-2.12149000	-1.00768800
H	4.66788000	-2.72347400	-1.74982200
C	5.15920100	-2.22619200	0.18998500
H	4.14944500	1.35080700	0.77670000
H	4.74000800	1.59961900	-0.89109000
H	4.11948800	2.97937600	0.04733900
H	2.97475400	2.03813300	-2.75775600
H	1.26676400	2.13641300	-2.27536500
H	2.39426800	3.44226500	-1.82251000
H	2.80323100	-1.17701200	3.04113000
H	1.10304500	-0.89672000	2.58069700
H	1.97504600	-2.31673700	1.93937300
H	4.76467800	-1.53453100	0.93681900
H	5.08838700	-3.24079400	0.58963200
H	6.21714900	-1.99608200	0.01219800
H	4.33044200	-1.16512200	-1.35980300
H	-0.4911000	-1.63647800	-0.33299300
C	-2.1453750	-0.34905400	0.06045900
C	-2.9669850	-1.29551700	-0.56835000
C	-2.7745370	0.75157300	0.67608000
C	-4.3492580	-1.16259600	-0.62426700
H	-2.5075540	-2.16094300	-1.03902400
C	-4.1487850	0.89164100	0.63358400
H	-2.1765100	1.48441100	1.19953400
C	-4.9474890	-0.05566700	-0.01909100
H	-4.9394930	-1.91778800	-1.12924800
H	-4.6401260	1.73339000	1.11007200
O	-6.2814870	0.18085700	-0.00174300
C	-7.1198570	-0.75556600	-0.64261000

Atom	*x* / Å	*y* / Å	*z* / Å
C	-3.25730400	0.11308800	0.72262000
C	-4.90784100	-1.24918100	-1.07249500
H	-3.09412500	-2.10416600	-1.84641400
C	-4.63592200	0.28468700	0.76619400
H	-2.62524600	0.61391800	1.44805000
C	-5.46399300	-0.38655700	-0.13107300
H	-5.54610700	-1.78308900	-1.76924800
H	-5.06676600	0.94497000	1.51188400
H	-6.53946000	-0.24537500	-0.09047600

(19c)	*G* = -1218.735900 a. u. (Gas phase) *G* = -1218.789775 a. u. (In methanol)		
O	1.71536900	1.99618500	0.67393100
C	0.58560000	1.26382000	0.78130200
C	0.61617300	-0.06725500	0.11136100
C	2.03265000	-0.57250200	-0.08213700
O	2.74306200	0.41705700	-0.79351700
C	2.77890500	72648300	-0.25111200
O	-0.3252460	1.68407100	1.44529900
O	2.06071600	-1.72669300	-0.78807300
C	4.06765600	1.94875900	0.52229100
C	2.61639900	2.67679400	-1.42566600
C	-0.4397640	-0.81162600	-0.24047700
O	2.69212200	-0.67973300	1.16637400
C	2.16612000	-1.68266200	2.01947900
H	3.03061600	-1.90969100	-1.01027100
N	4.69253200	-1.77957800	-1.36475800
H	5.09987200	-2.39142200	-2.06771800
C	5.50570700	-1.76965600	-0.14279400
H	4.10415000	1.26180900	1.36842700
H	4.92029400	1.76499200	-0.13785800
H	4.11213300	2.97861900	0.88468400
H	3.42641900	2.52105200	-2.14267700
H	1.66316200	2.47823100	-1.92242700
H	2.63534700	3.71108200	-1.07593000
H	2.81428600	-1.70893700	2.89602000
H	1.14365200	-1.44186900	2.33419700
H	2.17169400	-2.65778500	1.52322900
H	5.02556300	-1.10500200	0.57819800
H	5.51899700	-2.77594200	0.28277000
H	6.54106600	-1.44558900	-0.30349400
H	4.65162900	-0.84263300	-1.76200200
H	-0.1849690	-1.79292700	-0.63791600
C	-1.8859890	-0.53316600	-0.18985900
C	-2.7417800	-1.63964400	-0.08693600
C	-2.4463410	0.74663500	-0.30692700
C	-4.1204060	-1.48477600	-0.05675700
H	-2.3147920	-2.63629300	-0.02372800
C	-3.8222060	0.91841800	-0.29490100
H	-1.8059880	1.61327400	-0.40392000
C	-4.6343330	-0.20084900	-0.16200200
H	-4.7926500	-2.32862300	0.03487000
H	-4.2733610	1.89854500	-0.38599000
N	-6.0938480	-0.02041700	-0.14628700
O	-6.7824200	-1.01717800	-0.02421900

Atom	*x* / Å	*y* / Å	*z* / Å
H	-7.0334460	-1.74723800	-0.18262700
H	-8.1372350	-0.38555400	-0.51825900
H	-6.8872660	-0.83169900	-1.71151100
(20a-TS)	*G* = -1014.339900 a. u. (Gas phase)		
	G = -1014.374887 a. u. (In methanol)		
O	-2.35625400	-1.80987300	0.39362000
C	-1.08283700	-2.08582600	0.70420200
C	-0.05299600	-1.07449200	0.34327300
C	-0.65991400	0.27484700	0.00252000
O	-1.68362000	-0.95154600	0.02845800
C	-2.74496200	-0.85084600	-0.62379400
O	-0.85005000	-3.11577100	1.31151500
O	0.21984000	-0.56135900	1.13122100
C	-3.94507000	-0.10755700	-0.07151300
C	-3.05954000	-1.63531800	-1.88183300
C	1.22067700	-1.50259300	0.30193900
H	1.34361600	-2.57251100	0.47293300
C	2.48826700	-0.79985900	0.03670400
C	3.45372100	-1.47790300	-0.72367700
C	4.68868400	-0.89167700	-0.98994000
C	4.99082000	0.36414000	-0.46256500
C	4.05252000	1.02743300	0.33035900
C	2.80782200	0.45365800	0.57593700
O	-1.32374200	0.82669400	1.12230400
C	-0.47340100	1.21308000	2.19763500
H	-0.29283400	-0.78599000	2.0223500
N	-1.07902200	-1.06561100	3.32710900
H	-0.62801600	-1.79326200	3.87887000
C	-1.21877700	4.13150900	0.15830300
H	-3.68748500	0.40820800	0.85417100
H	-4.27742200	-0.81411500	0.62266500
H	-4.75861400	-0.81309200	0.11603800
H	-3.35377700	-0.94455400	-2.67626700
H	-2.17237500	-2.19064400	-2.19940800
H	-3.87908500	-2.33217400	-1.69231800
H	3.22583100	-2.46646900	-1.11445100
H	5.41835000	-1.42063400	-1.59562700
H	5.95795900	-0.65644100	0.81864700
H	4.29181100	1.99496800	0.76153200
H	2.08722100	0.97004400	1.19889500
H	-1.13109100	1.56341600	2.99433900
H	0.11295700	0.36220800	2.56437000
H	0.19732500	2.02521100	1.89947800
H	-1.73444200	3.54086500	0.91918800
H	-0.22553200	4.38826500	0.53401800
H	-1.78044600	-0.00504700	5.05710100
H	-2.00026700	-1.42434000	3.08010400
(20c-TS)	*G* = -1218.733800 a. u. (Gas phase)		
	G = -1218.786246 a. u. (In methanol)		
O	-3.23953500	-1.71765500	0.20973700

Atom	*x* / Å	*y* / Å	*z* / Å
O	-6.5221350	1.11334700	-0.25733800
(20b-TS)	*G* = -1128.792990 a. u. (Gas phase)		
	G = -1128.833689 a. u. (In methanol)		
O	-2.87120300	-1.91330400	0.27355400
C	-1.54906300	-2.19397500	0.37400700
C	-0.59940600	-1.05774600	0.16014200
C	-1.28991600	0.28248900	0.03544500
O	-2.40043000	0.12968100	-0.82437100
C	-3.38743700	-0.82897500	-0.49735700
O	-1.22001800	-3.31025800	0.68519300
O	-0.49115900	1.23630700	-0.50089300
C	-4.51345800	-0.21462200	0.31951000
C	-3.87061300	-1.39391500	-1.82422100
C	0.70308800	-1.40196500	0.13820800
H	0.83263000	-2.48127700	0.22136500
C	1.98706800	-0.70072500	0.04316300
C	3.09957400	-1.50628700	-0.23560000
C	4.38895900	-0.99406500	-0.32798100
C	4.59260600	0.36886800	-0.10892800
C	3.49989100	1.19031900	0.19770600
C	2.22272700	0.66931000	0.26968300
O	-1.83657300	0.66911500	1.28662300
C	-0.87016900	1.03534800	2.25254100
H	-1.08032100	2.02962100	-0.70738400
N	-2.38976800	3.08181400	-1.07338300
H	-2.25938000	3.87111300	-1.70112700
C	-3.10301000	3.48786400	0.14262100
H	-4.12554900	0.13626200	1.27545100
H	-4.94360200	0.62606400	-0.23333200
H	-5.29266700	-0.96125100	0.49225200
H	-4.29390000	-0.59417500	-2.43791800
H	-3.02616800	-1.83939400	-2.35572600
H	-4.63163700	-2.15711900	-1.64875300
H	2.95057400	-2.57176100	-0.39020800
H	5.21333200	-1.65881900	-0.55624500
H	3.68744300	2.24395900	0.37576900
H	1.39364300	1.32490900	0.49279400
H	-1.40461100	1.15273700	3.19625400
H	-0.10430800	0.25787500	2.36635600
H	-0.38515500	1.98089800	1.98598100
H	-3.20177900	2.61040300	0.78551100
H	-2.50428900	4.23161500	0.67426200
H	-4.09665200	3.91292500	-0.04638100
H	-2.92841600	2.37660700	-1.57316400
O	5.79880300	0.98366500	-0.16079700
C	6.92443700	0.18838700	-0.46421700
H	6.82780200	-0.27669000	-1.45244900
H	7.78048100	0.86263100	-0.46246100
H	7.07388200	-0.59334700	0.29003700
(21)	*G* = -193.014512 a. u. (Gas phase)		
	G = -193.021701 a. u. (In methanol)		
C	0.0000000	0.18648300	0.00000100

Atom	*x* / Å	*y* / Å	*z* / Å
C	-1.98919400	-2.13008300	0.51019400
C	-0.89073600	-1.12685500	0.32062500
C	-3.52109000	-0.62435100	-0.67045400
O	-1.82100600	-3.23811200	0.94732800
O	-0.44695900	1.13827200	-0.28605600
C	-4.68546100	0.13163400	-0.05238000
C	-3.85429300	-1.20603800	-2.03467300
C	0.35601700	-1.62036100	0.31206600
H	0.39232900	-2.70557900	0.41030000
C	1.68440500	-0.99758300	0.16579000
C	2.66496300	-1.75884800	-0.48887800
C	3.95717700	-1.28201200	-0.65498600
C	4.26689300	-0.03908200	-0.12221100
C	3.33578700	0.72997300	0.56321600
C	2.04320000	0.24621800	0.70270900
O	-2.07643600	0.71732900	1.29595900
C	-1.22239900	0.99268800	2.38924300
H	-0.91254900	1.98780600	-0.58465200
N	-2.00081500	3.16880700	-1.12692100
H	-1.66198900	3.93936600	-1.69769800
C	-2.83047700	3.65881400	-0.01977700
H	-4.40667900	0.48889700	0.93880000
H	-4.94267700	0.98168500	-0.69118700
H	-5.55304100	-0.52797000	0.02733000
H	-4.09855700	-0.40071000	-2.73225400
H	-2.98892000	-1.75380600	-2.41600000
H	-4.70551100	-1.88495900	-1.95257000
H	2.40259800	-2.73714500	-0.88075400
H	4.71884400	-1.85229200	-1.17180100
H	3.63310600	1.68659600	0.97442000
H	1.30444700	0.83767200	1.22517200
H	-1.86941200	1.20300600	3.24159400
H	-0.58662000	0.13007700	2.62739200
H	-0.59043900	1.86391600	2.18499400
H	-3.14923800	2.79814500	0.57234300
H	-2.22298200	4.30329400	0.62019500
H	-3.71290900	4.22326000	-0.34431400
H	-2.54952200	2.55887100	-1.73027300
N	5.63523800	0.47671000	-0.27764100
O	6.43295000	-0.21702100	-0.88121100
O	5.88479100	1.56574700	0.20601600

(21-TS) *G* = -192.9250900 a. u. (Gas phase)
G = -192.9441254 a. u. (In methanol)

C	-0.0385780	0.05179900	0.00002300
O	0.38345800	1.21434100	-0.00004100
C	1.22100600	-0.75247100	-0.00008800
C	-1.4807920	-0.32291400	0.00003900
H	1.46200500	0.45050300	-0.00051800
H	1.37789600	-1.34934900	0.90122800
H	1.37738100	-1.35128600	-0.90017800
H	-2.1184440	0.56075900	0.00032400
H	-1.6881770	-0.94160300	-0.87830100
H	-1.6881410	-0.94223300	0.87793200

Atom	*x* / Å	*y* / Å	*z* / Å
O	-0.0000000	1.39562400	0.00000000
C	-1.2875800	-0.61340900	0.00000300
C	1.28758400	-0.61340800	-0.00000300
H	-2.1415110	0.06424800	0.00016500
H	-1.3297200	-1.26273700	-0.88099000
H	-1.3295790	-1.26300900	0.88080100
H	2.14151200	0.06424900	-0.00017200
H	1.32972400	-1.26273000	0.88099400
H	1.32957600	-1.26301300	-0.88079700

(21-Enol) *G* = -192.9953020 a. u. (Gas phase)
G = -193.0120207 a. u. (In methanol)

C	1.39916500	0.24153400	0.00000900
C	-0.0842000	0.04961200	-0.00002100
C	-0.993549	1.02815200	-0.00000500
O	-0.3951570	-1.27990500	-0.00001900
H	1.65415000	1.30155700	-0.00028300
H	1.83576500	-0.23477700	0.88276200
H	1.83585500	-0.23529000	-0.88241900
H	-2.0592250	0.82018500	0.00001300
H	-0.6805100	2.06375100	0.00002200
H	-1.3532840	-1.39197100	0.00016300

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
(22a-E)	*G* = -821.4560600 a. u. (Gas phase) *G* = -821.4812002 a. u. (In methanol)			**(22b-E)**	*G* = -935.9049820 a. u. (Gas phase) *G* = -935.9404095 a. u. (In methanol)		
C	1.16636600	0.21661300	-0.06285300	C	-1.7303900	-0.47993500	-0.03095400
C	0.49909700	1.38008100	-0.06395900	C	-0.7196580	-1.36195500	-0.07283700
C	2.65099400	0.15365000	-0.02230400	C	3.15147000	-0.90493000	0.00926600
C	0.51027200	-1.13985500	-0.05686800	C	-1.5455590	1.01357900	0.01898900
O	3.27070000	-0.87588400	0.11534200	O	-4.0741010	-0.14667800	0.19160100
O	0.03240200	-1.47562800	1.12233600	O	-1.0352720	1.42622400	1.16146200
O	0.43577600	-1.82911200	-1.05747000	O	-1.8276730	1.73661000	-0.91730600
C	-0.9605900	1.56348200	-0.08264100	C	0.71413600	-1.06141200	-0.12468700
C	-1.4989180	2.69997900	0.53677300	C	1.62139900	-1.99062100	0.38829200
C	-2.8738480	2.91060100	0.56710400	C	2.99294800	-1.75260900	0.39034500
C	-3.7313290	1.99692300	-0.04431800	C	3.47956800	-0.56393300	-0.15639000
C	-3.2043120	0.87895900	-0.69057000	C	2.58658600	0.36392100	-0.70923700
C	-1.8301680	0.66178700	-0.71338400	C	1.22787000	0.11747100	-0.69382600
O	3.23835900	1.35713400	-0.13701400	O	-3.3114950	-2.23133800	-0.15823400
C	4.66550000	1.33824700	-0.07145600	C	-4.6638820	-2.67544000	-0.08638200
H	1.09500200	2.28943900	-0.02443100	H	-0.9855230	-2.41696200	-0.05837600
H	-0.8295030	3.41404500	1.00916100	H	1.24665400	-2.91887800	0.81180900
H	-3.2755600	3.78909300	1.06192000	H	3.66300300	-2.49333700	0.80981600
H	-4.8040040	2.16221500	-0.02902800	H	2.99350600	1.26479300	-1.15647900
H	-3.8663490	0.17815300	-1.18999900	H	-5.2633550	-2.19508500	-0.86260100
H	-1.4269130	-0.19095700	-1.25051300	N	-0.8578730	4.02103800	0.62435700
H	4.97787400	2.37523800	-0.17991000	C	0.29388400	4.10254000	-0.28084400
H	4.99486900	0.93197600	0.88709900	H	-0.8621880	4.79046900	1.28894900
H	5.07201100	0.72458600	-0.87781000	H	-0.9452440	2.44483500	1.10567200
N	-1.0159680	-3.82756300	0.58587700	H	-1.7184340	4.06261200	0.08092500
C	-2.2462320	-3.49475200	-0.14607500	H	1.21214400	3.93045300	0.28591200
H	-1.1758390	-4.56350000	1.26696900	H	0.37590700	5.06221700	-0.80418100
H	-0.3777390	-2.41649400	1.04422300	H	0.18703500	3.30869600	-1.02323900
H	-2.6910240	-4.35085100	-0.66431500	O	4.79108500	-0.22599300	-0.21487000
H	-2.0005300	-2.72744700	-0.88373800	C	5.72550400	-1.13979200	0.31709600
				H	6.70612600	-0.68624100	0.17563500
				H	5.55205600	-1.30856700	1.38659000
				H	5.68794500	-2.09992100	-0.21127600
(22a-z)	*G* = -821.4491640 a. u. (Gas phase) *G* = -821.4738072 a. u. (In methanol)			**(22b-z)**	*G* = -935.8980820 a. u. (Gas phase) *G* = -935.9350404 a. u. (In methanol)		
C	0.73967700	-0.61428600	-0.52753200	C	1.47208000	-0.63299200	-0.48153900
C	-0.3663110	-1.29790500	-0.19582800	C	0.34308900	-1.32121300	-0.24659000
C	0.74191000	0.87358400	-0.68298700	C	1.47216900	0.85160200	-0.65105500
C	1.99731100	-1.40428400	-0.83779100	C	2.75051000	-1.41864200	-0.68945000
O	1.38040800	1.65736500	-0.01121000	O	2.03351200	1.65507800	0.06321400
O	1.90699200	-2.50535200	-1.33125300	O	2.69892700	-2.56896600	-1.05619900
O	3.15821900	-0.83163300	-0.57917900	O	3.89618200	-0.78424200	-0.50003100
O	-0.0644880	1.25434900	-1.67497700	O	0.74524100	1.21189000	-1.71229800
C	-0.2000320	2.66660900	-1.85314200	C	0.59926800	2.61881300	-1.89843900
H	-0.8680790	2.79019100	-2.70272600	H	0.01392500	2.73560800	-2.80842200
H	-0.6317380	3.11444100	-0.95424100	H	0.07343600	3.05663800	-1.04537200
H	0.77310600	3.11922600	-2.05161900	H	1.57627100	3.09498300	-1.99978000
N	3.42867300	0.62584900	1.57919800	N	4.11586700	0.75176100	1.64178000
H	3.18948100	-0.16449800	0.20586500	H	3.89522200	-0.06186700	0.22252600
C	2.51346300	0.06475800	2.58082600	C	3.22059400	0.08929900	2.59434700
H	4.39061000	0.59318000	1.90339500	H	5.07194700	0.76540200	1.98755900
H	3.18363700	1.59019700	1.37488300	H	3.81145600	1.70708000	1.47911700

Atom	*x* / Å	*y* / Å	*z* / Å
H	2.57389000	0.55978200	3.55608500
H	2.73211100	-0.99790500	2.71022300
H	1.49167500	0.15774000	2.20471500
H	-0.2684850	-2.38285300	-0.20103600
C	-1.6861600	-0.75879600	0.16533500
C	-2.8204520	-1.53573200	-0.10640900
C	-1.8557850	0.48501500	0.79163500
C	-4.0947780	-1.06440000	0.19452600
H	-2.6962020	-2.50965300	-0.57186900
C	-3.1291440	0.95078800	1.10287500
H	-0.9884270	1.07918300	1.06731400
C	-4.2526770	0.18235200	0.79764000
H	-4.9635140	-1.67304900	-0.03494000
H	-5.2449420	0.54801400	1.04184800

Atom	*x* / Å	*y* / Å	*z* / Å
H	3.23706700	0.52814900	3.59898200
H	3.49525900	-0.96618000	2.66726100
H	2.20251100	0.15088600	2.20226400
C	-2.10057700	-1.61826500	-0.28505000
C	-1.25696000	0.47744400	0.52974700
C	-3.40935900	-1.18122400	-0.10250700
H	-1.92689000	-2.61784900	-0.67446200
C	-2.54943300	0.92254700	0.72726500
H	-0.43047000	1.11703000	0.82796100
C	-3.63708500	0.10025800	0.40191900
H	-4.23192100	-1.84232400	-0.34724800
H	-2.75385400	1.90137600	1.14784400
O	-4.86286100	0.63044000	0.62786600
C	-5.98681000	-0.16916800	0.32696700
H	-6.86050500	0.43304100	0.57416700
H	-6.01349500	-0.43239000	-0.73708600
H	-5.99374300	-1.08658100	0.92739600

(22c-z) *G* = -1025.859164 a. u. (Gas phase)
G = -1025.910223 a. u. (In methanol)

C	-1.69496400	0.71925000	-0.34464000
C	-0.61662700	1.42676900	0.01820600
C	-1.59616600	-0.71026800	-0.77703300
C	-3.03071200	1.44282600	-0.41005000
O	-2.07473600	-1.65863000	-0.19372500
O	-3.04775400	2.64270200	-0.54592300
O	-4.12513500	0.70822000	-0.36446100
O	-0.88516100	-0.82396000	-1.89846400
C	-0.66022500	-2.16335900	-2.34363100
H	-0.10185200	-2.07334300	-3.27303600
H	-0.07987400	-2.71140500	-1.59666700
H	-1.61049400	-2.67450600	-2.50710100
H	-4.09230600	-0.14631200	0.20937400
C	-3.49530700	-0.69679700	2.51398400
H	-5.26131600	-1.35720600	1.67736200
H	-3.91493900	-2.10986600	1.08424100
H	-2.45800200	-0.61671900	2.17982300
H	-0.79160600	2.48021500	0.23122000
C	0.76884800	0.94612400	0.13083600
C	1.81070300	1.85108700	-0.11498700
C	1.08442800	-0.37199600	0.49500000
C	3.13722300	1.44910600	-0.04689600
H	1.57230400	2.87745900	-0.37697400
C	2.40530000	-0.78804400	0.57471600
H	0.29288000	-1.07155400	0.74704300
C	3.40770800	0.13105600	0.29361600
H	3.95489400	2.13065100	-0.24623300
H	2.67104100	-1.79869000	0.85923600
N	4.80999500	-0.30632600	0.37521400
O	5.67057800	0.52013000	0.13721200
O	5.01897100	-1.46769400	0.67382200

(23b-TS) *G* = -652.7395150 a. u. (Gas phase)
G = -652.7622322 a. u. (In methanol)

C	-1.45736700	-0.35054400	-1.25760900
C	-0.10307600	-0.65746200	-1.13027800
C	0.40927500	-1.06076000	0.10618700
C	-0.45012100	-1.16474200	1.20767000
C	-1.79960400	-0.85842000	1.07758100
C	-2.30644500	-0.44566800	-0.15747000
C	1.85552600	-1.33098800	0.27720500
O	2.63083700	-1.44255400	-0.81607600
H	2.76874100	-0.54735900	-1.21350000
C	2.63853400	0.42561400	1.23722000
C	2.23702000	1.29880800	0.14696200
O	2.77814000	1.21778100	-0.96434200
C	1.05305200	2.21099200	0.35852200
H	-1.84843100	-0.03809300	-2.22066800
H	0.55653600	-0.59267300	-1.98975500
H	-0.05088400	-1.47838000	2.16970000
H	-2.45898700	-0.94275100	1.93562600
H	2.11614600	-2.05164200	1.05093100
H	2.14654500	0.54481400	2.19878100
H	2.14654500	0.54481400	2.19878100
H	3.67877700	0.11399000	1.25229300
H	0.20712700	1.63926200	0.75784300
H	1.30677800	2.98166600	1.09400600
H	0.77337400	2.67759700	-0.58631100
O	-3.69475700	-0.13047900	-0.29217900
C	-3.91196800	1.23478300	0.07357800
H	-4.94011000	1.48663100	-0.08261700
H	-3.66409200	1.37135200	1.10547200
H	-3.29423000	1.86792600	-0.52844400

(23a-TS) *G* = -538.2956440 a. u. (Gas phase)
G = -538.3204576 a. u. (In methanol)

C	-2.10395500	0.37329300	-1.32304300
C	-0.89269800	-0.29810800	-1.15997100

(23c-TS) *G* = -742.7326040 a. u. (Gas phase)
G = -742.7693119 a. u. (In methanol)

C	-1.24401500	0.15361100	-1.15622500
C	0.08731800	-0.26012000	-1.18610700

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	-0.54147900	-0.81289900	0.09128200	C	0.61267700	-1.00304900	-0.12495100
C	-1.42022600	-0.65880800	1.17142000	C	-0.21153800	-1.33648400	0.95769800
C	-2.62697300	0.01064300	1.00571500	C	-1.53822500	-0.92291000	0.98450400
C	-2.97029200	0.53298900	-0.24404100	C	-2.05733700	-0.17158600	-0.07315400
C	0.76732200	-1.47421400	0.30012400	C	2.03997800	-1.39858300	-0.10824300
O	1.50491300	-1.81166100	-0.77268000	O	2.76461000	-1.26967500	-1.23390300
H	1.89649800	-0.99570000	-1.17168700	H	2.95442600	-0.31229700	-1.39432600
C	1.98841300	0.00564200	1.26932200	C	2.98623000	-0.00557300	1.22761400
C	1.87166500	0.94245800	0.16429300	C	2.61170100	1.14499800	0.42246900
O	2.39340900	0.69952800	-0.93258500	O	3.10457500	1.32269900	-0.69997000
C	0.98549000	2.15165900	0.34077600	C	1.50757600	2.04283500	0.92587300
H	-2.37030400	0.77041600	-2.29741000	H	0.71829700	-0.01500500	-2.03450000
H	-0.22211600	-0.43097500	-2.00297400	H	0.19782900	-1.91441500	1.78333400
H	-3.91245100	1.05570300	-0.37408300	H	-2.17048600	-1.18649200	1.82647100
H	0.79859800	-2.22919600	1.08430500	H	2.27399500	-2.31086400	0.43847000
H	1.52786900	0.26961500	2.21752000	H	2.53973200	-0.11054500	2.21274500
H	2.89943800	-0.58395700	1.31231500	H	4.00017400	-0.37489900	1.10531000
H	0.00469600	1.84407100	0.72202800	H	0.63639100	1.44095100	1.20994100
H	1.42795100	2.82995400	1.07792900	H	1.84463800	2.57769400	1.82005700
H	0.86874400	2.66589900	-0.61346600	H	1.22939600	2.75616000	0.14970700
				N	-3.46040300	0.26607700	-0.04566000
				O	-3.87733100	0.90323500	-0.97227800
				O	-4.13215300	-0.03148700	0.90229300
(24a)	*G* = -538.3707080 a. u. (Gas phase)			**(24a-TS)**	*G* = -538.3192300 a. u. (Gas phase)		
	G = -538.3947567 a. u. (In methanol)				*G* = -538.3461142 a. u. (In methanol)		
C	-2.14836500	0.10183200	-1.39051300	C	-2.23300600	-0.04497200	-1.37207300
C	-0.92796500	-0.50536300	-1.09131000	C	-1.00711600	-0.62020600	-1.03129000
C	-0.54959400	-0.70810700	0.23558200	C	-0.59238900	-0.65709600	0.29969200
C	-1.41551400	-0.30856700	1.25848800	C	-1.42838900	-0.12639400	1.28808100
C	-2.63407100	0.29662800	0.96232600	C	-2.65228300	0.44650000	0.95127400
C	-3.00147200	0.50850200	-0.36720800	C	-3.05545000	0.49369900	-0.38487600
C	0.81596700	-1.28060800	0.58945800	C	0.78288000	-1.22959700	0.65023800
O	1.40608500	-1.99788000	-0.46501700	O	1.42967500	-1.82136200	-0.37624400
H	1.90610800	-1.37920100	-1.02048900	H	2.10612500	-0.81262900	-0.87767700
C	1.88797800	0.89341400	-0.02394200	C	1.55285200	2.21728500	-0.15574800
O	2.40743200	0.58017000	-1.08136000	H	-2.54881100	-0.02493900	-2.41094700
C	1.30431800	2.26055900	0.20413400	H	-0.36025400	-1.06676500	-1.78039900
H	-2.43242700	0.25393800	-2.42721400	H	-1.12356700	-0.17176900	2.33267600
H	-0.26950100	-0.83426500	-1.88878800	H	-3.29498400	0.84964400	1.72827100
H	-1.13546400	-0.47794200	2.29673200	H	-4.00990000	0.93777900	-0.65003600
H	-3.29903300	0.59718800	1.76617100	H	0.68301100	-1.87398000	1.54039600
H	-3.95102900	0.97891300	-0.60189700	H	1.25082200	0.58404600	1.98707900
H	0.69337600	-1.98836700	1.41736400	H	2.62620800	-0.48406700	1.52404200
H	1.34102100	0.30630800	1.98881100	H	0.45378800	2.23386900	-0.10763400
H	0.22438600	2.15041600	0.36628000	H	1.92607700	2.80509600	0.68585100
H	1.72590700	2.70664900	1.11059300	H	1.88382700	2.62999200	-1.10799200
H	1.49004200	2.89945600	-0.65885600				
(24b)	*G* = -652.8196292 a. u. (Gas phase)			**(24b-TS)**	*G* = -652.7953800 a. u. (Gas phase)		
	G = -652.8375199 a. u. (In methanol)				*G* = -652.8192584 a. u. (In methanol)		
C	-1.49074900	0.00752800	-1.17434500	C	-1.55181200	-0.06451800	-1.17483000
C	-0.21548600	-0.53500000	-1.01017300	C	-0.27501200	-0.59844300	-0.98898300
C	0.27922000	-0.79534600	0.26748000	C	0.23938100	-0.76224100	0.29687900
C	-0.52518800	-0.51933800	1.37767500	C	-0.54748700	-0.40101300	1.39588200
C	-1.79825300	0.02112900	1.21625400	C	-1.82187800	0.13025900	1.21356000

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	-2.28281400	0.29146100	-0.06423700	C	-2.32569400	0.30558300	-0.07698200
C	1.70114400	-1.29713800	0.47742900	C	1.66551400	-1.28537400	0.48256800
O	2.24808700	-1.90585600	-0.66491600	O	2.26437800	-1.71442900	-0.64856800
H	2.66338300	-1.22162100	-1.21326600	H	2.84682000	-0.61506300	-1.07131800
C	2.59626000	-0.13229300	0.97025200	C	2.55916400	-0.07190300	1.09777000
C	2.58566000	0.97751300	-0.06610400	C	2.66979300	0.86908800	-0.02377100
O	3.03732100	0.76662800	-1.17858600	O	3.02962400	0.39012200	-1.13083300
C	1.93942900	2.28584500	0.29778600	C	2.18856000	2.27208300	0.04167500
H	-1.86537600	0.20543100	-2.17387800	H	-1.94497700	0.05513200	-2.18006600
H	0.39617300	-0.76862400	-1.87563100	H	0.33691600	-0.91536200	-1.82810000
H	-0.15337200	-0.73480200	2.37787300	H	-0.16348300	-0.54712200	2.40451800
H	-2.41413300	0.22569800	2.08661000	H	-2.42526800	0.40118800	2.07485700
H	1.68855200	-2.06219600	1.26222700	H	1.66687600	-2.03259300	1.29450800
H	2.23797200	0.22984200	1.93767500	H	2.13484400	0.38819700	1.99064600
H	3.61937600	-0.50606200	1.08146400	H	3.52668000	-0.53293300	1.31148200
H	0.88464900	2.09431000	0.53322200	H	1.09684300	2.21529400	0.16601600
H	2.40386500	2.70095500	1.19799900	H	2.59181100	2.78127800	0.91986500
H	2.01625200	2.98872700	-0.53136500	H	2.42502200	2.81096300	-0.87502200
O	-3.59015500	0.84511500	-0.23519000	O	-3.63488800	0.84820500	-0.2679610
C	-4.56092600	-0.20440100	-0.20326500	C	-4.60472200	-0.19763700	-0.16532200
H	-4.56789400	-0.65439600	0.76748600	H	-4.59348600	-0.59837300	0.82673900
H	-5.52894000	0.19852500	-0.41656800	H	-5.57661700	0.19483200	-0.38046700
H	-4.31232400	-0.94263500	-0.93682300	H	-4.36974300	-0.97192500	-0.86543800
(24c)	*G* = -742.7809581 a. u. (Gas phase)			**(24c-TS)**	*G* = -742.699640 a. u. (Gas phase)		
	G = -742.8153712 a. u. (In methanol)				*G* = -742.737974 a. u. (In methanol)		
C	-1.28143200	-0.14124900	-1.16903700	C	-1.33978000	-0.14163500	-1.17354600
C	0.05611300	-0.53131000	-1.08897000	C	-0.00269100	-0.53827200	-1.10495000
C	0.59955500	-0.93476600	0.13037600	C	0.55560400	-0.92439500	0.11328200
C	-0.21743300	-0.95677800	1.26520300	C	-0.24636700	-0.92533000	1.25970900
C	-1.55248800	-0.56890300	1.18751800	C	-1.58066000	-0.53175300	1.19395600
C	-2.08722100	-0.15388200	-0.03287300	C	-2.13000100	-0.13210100	-0.02611400
C	2.07784200	-1.27342700	0.26349400	C	2.03947800	-1.29172300	0.18533600
O	2.68262300	-1.60493300	-0.96083400	O	2.66272000	-1.37268900	-1.00932300
H	2.99669800	-0.78995200	-1.38332500	H	3.09437200	-0.14142700	-1.16499100
C	2.82021700	-0.10026800	0.95164500	C	2.78790800	-0.14744900	1.06856200
C	2.64920400	1.15634100	0.11647700	C	2.75627100	1.03052100	0.19281000
O	3.10796300	1.19602300	-1.01226200	O	3.14913700	0.86570400	-0.99165800
C	1.84295500	2.28880700	0.69027800	C	2.10543000	2.30943100	0.57367400
H	-1.69354000	0.17037200	-2.12383300	H	-1.76629000	0.15324100	-2.12776300
H	0.68012600	-0.53421400	-1.97684500	H	0.62580400	-0.57584600	-1.98959200
H	0.19419400	-1.28603700	2.21768300	H	0.17442700	-1.24768300	2.21111500
H	-2.17681400	-0.59576300	2.07530800	H	-2.19447700	-0.54255700	2.08973900
H	2.17705200	-2.15409000	0.90845200	H	2.15140500	-2.19794200	0.80487100
H	2.43208600	0.04440200	1.96349700	H	2.32882200	0.03980400	2.03971800
H	3.88495600	-0.34969000	1.00600600	H	3.80971000	-0.51910200	1.17858400
H	0.82588800	1.92364600	0.88239500	H	1.03223000	2.08844600	0.67336800
H	2.26247100	2.60458200	1.65084800	H	2.46083300	2.65191200	1.54809800
H	1.81488700	3.12458900	-0.00837400	H	2.25313500	3.06839200	-0.19366100
N	-3.49646900	0.25510100	-0.12037200	N	-3.53875100	0.28126000	-0.09997500
O	-4.16018500	0.23164000	0.87830200	O	-4.18803200	0.27682600	0.90840600
O	-3.92622500	0.59590300	-1.18694200	O	-3.98255700	0.60643200	-1.16567100
(24a-Int)	*G* = -538.3420010 a. u. (Gas phase)			**(24b-Int)**	*G* = -652.8139348 a. u. (Gas phase)		
	G = -538.3678514 a. u. (In methanol)				*G* = -652.8345424 a. u. (In methanol)		
C	2.20124200	-0.02412700	1.21336300	C	-1.30367400	-0.80129200	-1.23155800

Atom	*x* / Å	*y* / Å	*z* / Å
C	1.12504700	-0.86292200	0.94012200
C	0.59376800	-0.91095800	-0.35250200
C	1.13873200	-0.12223400	-1.36571600
C	2.22154900	0.71278300	-1.09423400
C	2.75012900	0.76199400	0.19534400
C	-0.5578300	-1.80563900	-0.65149700
O	-1.0428100	-2.56424600	0.15446800
H	-1.1692100	0.56479800	1.88289000
C	-2.6681650	0.62848000	-0.85341200
C	-1.8868380	1.01836900	0.15753100
O	-1.9264750	0.32763800	1.33493000
C	0.95715900	2.19402700	0.13322600
H	2.62094600	0.01532600	2.21376300
H	0.68217200	-1.49534400	1.70487400
H	0.70626500	-0.15975900	-2.36315200
H	2.64893900	1.32542300	-1.88150700
H	3.59233700	1.41264000	0.40978100
H	-0.9469700	-1.74231400	-1.68725600
H	-2.6816330	1.18925900	-1.77920300
H	-3.3146860	-0.23496400	-0.74594300
H	0.0652790	1.87783800	0.37800800
H	-0.9423450	2.66067500	-0.85269200
H	-1.2695930	2.94065000	0.87191300

Atom	*x* / Å	*y* / Å	*z* / Å
C	-0.02945900	-1.23927100	-0.92654600
C	0.45835200	-1.13715600	0.38389800
C	-0.35100000	-0.59441100	1.37451300
C	-1.64383200	-0.15841900	1.08791500
C	-2.12044800	-0.26272000	-0.22178300
C	1.83417800	-1.58905400	0.69716300
O	2.57018300	-2.10534400	-0.10969100
H	1.44255500	0.77837500	-1.81010000
C	3.05692500	1.32916700	0.78467000
C	2.13542400	1.46867200	-0.16868000
O	2.29484600	0.82329000	-1.36056600
C	0.90557200	2.31915600	-0.06287300
H	-1.71208200	-0.87110600	-2.23396300
H	0.62006500	-1.67217100	-1.68211100
H	0.03398100	-0.50329400	2.38758500
H	-2.25920900	0.25788300	1.87561400
H	2.15120700	-1.42556900	1.74814700
H	2.97183800	1.87811900	1.71315400
H	3.91441300	0.68683400	0.62466100
H	0.01077200	1.71365100	-0.25673400
H	0.81269600	2.75864200	0.93065700
H	0.93507300	3.12372100	-0.80532900
O	-3.35319900	0.12806500	-0.61905000
C	-4.21745000	0.67416700	0.35614200
H	0.81269600	2.75864200	0.93065700
C	-4.21745000	0.67416700	0.35614200
H	-5.14417400	0.91569300	-0.16224300
H	-4.42313000	-0.04844500	1.15401700
H	-3.79616400	1.58654400	0.79393900

(24c-Int) *G* = -742.7429060 a. u. (Gas phase)
G = -742.7801902 a. u. (In methanol)

C	-1.1941900	-0.73810400	-1.05090000
C	0.11280100	-1.17483600	-0.88412100
C	0.70421600	-1.13811800	0.38131600
C	-0.0028230	-0.65964900	1.48308800
C	-1.3144600	-0.22176900	1.33553900
C	-1.8787350	-0.27288100	0.06795500
C	2.11142200	-1.61154200	0.54092900
O	2.75237600	-2.07935100	-0.36626700
H	1.61810500	1.09600600	-1.93276700
C	3.24050000	1.24156400	0.73326800
C	2.29953600	1.47354300	-0.18362100
O	2.40583800	0.89641000	-1.41516000
C	1.08685400	2.32883600	0.02462400
H	-1.6941620	-0.75421300	-2.01138900
H	0.69979600	-1.55356600	-1.71469400
H	0.47816300	-0.62477800	2.45688300
H	-1.8987950	0.15423900	2.16577100
H	2.52714400	-1.51555400	1.56348600
H	3.18022000	1.70791700	1.70756200
H	4.09214600	0.61487500	0.49734700
H	0.17715500	1.74573000	-0.16789700
H	1.04202300	2.71094500	1.04445000
H	1.09370800	3.17863300	-0.66672000

(25b-TS) *G* = -652.7322860 a. u. (Gas phase)
G = -652.7560296 a. u. (In methanol)

C	-2.1104640	-1.20787800	0.15887800
C	-0.7515170	-1.04239700	-0.04676900
C	-0.2002170	0.25148800	-0.11411800
C	-1.0466680	1.36692300	0.02683400
C	-2.4064790	1.19658000	0.23489900
C	-2.9375310	-0.09091300	0.30102700
C	1.19518700	0.48077200	-0.34077500
O	2.44328800	0.09385900	1.91304400
H	2.79591300	0.99437400	1.96973800
C	3.62245700	0.00296900	-0.49705100
H	5.64853500	-0.56388200	-0.12853300
O	-4.3398080	-0.27058500	0.51605300
C	-5.0314190	-0.16448300	-0.73107000
H	-6.0672060	-0.38952200	-0.58477200
H	-4.9328400	0.83131100	-1.10998600
H	-4.6117100	-0.85584600	-1.43161400

Atom	*x* / Å	*y* / Å	*z* / Å
N	-3.2671050	0.19471400	-0.10175100
O	-3.8522190	0.58531200	0.89053800
O	-3.7355470	0.16194200	-1.22389100

(25a-TS) *G* = -538.2746699 a. u. (Gas phase)
G = -538.3008859 a. u. (In methanol)

C	2.93496100	1.35158300	-0.06919500
C	1.57492700	1.13169600	-0.20472400
C	1.06842800	-0.18209500	-0.20035900
C	1.96035100	-1.26160500	-0.06009900
C	3.32118200	-1.03674200	0.07763200
C	3.80764400	0.26991900	0.07322600
C	-0.32664800	-0.46774100	-0.35289500
O	-1.48353000	-0.04125600	1.94207500
H	-1.80028900	-0.95072400	2.04704000
C	-1.38121600	0.48541900	-0.60081500
C	-2.77426100	-0.08031100	-0.41159100
O	-2.98953700	-1.25009900	-0.63327400
C	-3.81455700	0.89068800	0.06885300
H	3.32307100	2.36417500	-0.07057100
H	0.89695600	1.97101500	-0.31181800
H	1.56655500	-2.27361800	-0.05568600
H	4.00316400	-1.87235300	0.18896600
H	4.87258400	0.44895600	0.18126300
H	-0.63631000	-1.50863300	-0.42800500
H	-1.22738200	1.50406300	-0.26253200
H	-1.30250200	0.67427900	-2.28333300
H	-3.53767800	1.13151100	1.09941400
H	-3.79791300	1.80798100	-0.52693200
H	-4.80058500	0.42932000	0.03158500

(25c-TS) *G* = -742.6650760 a. u. (Gas phase)
G = -742.7014658 a. u. (In methanol)

C	-1.85904200	-1.13782900	-0.17128900
C	-0.48650400	-0.98917100	-0.27352800
C	0.08800900	0.29611700	-0.24946900
C	-0.74910300	1.42038900	-0.12379200
C	-2.12275000	1.26679300	-0.01940000
C	-2.67688400	-0.01242800	-0.04298700
C	1.49938600	0.50867800	-0.36749600
O	2.57741300	0.01114900	1.95144200
H	2.93888800	0.90218800	2.06921500
C	2.50806400	-0.49747300	-0.59623100
C	3.92399200	-0.00671600	-0.37098400
O	4.20558000	1.15115300	-0.58060200
C	4.90017400	-1.03334900	0.12799000
H	-2.29962400	-2.12858000	-0.18779200
H	0.14883100	-1.86248600	-0.36964800
H	-0.30294700	2.41024900	-0.10412300
H	-2.76238500	2.13659800	0.08084300
H	1.86495400	1.53217700	-0.42913200
H	2.29297800	-1.50818900	-0.26770800
H	2.45955800	-0.67403200	-2.28122500
H	4.58662000	-1.26410400	1.15031600
H	4.84957000	-1.94568900	-0.47345600
H	5.90966600	-0.62432900	0.11663200
N	-4.13315000	-0.17938600	0.06798400
O	-4.81310000	0.80253500	0.17715800
O	-4.58315700	-1.29085800	0.04491600

(26a-TS) *G* = -538.2952901 a. u. (Gas phase)
G = -538.3226096 a. u. (In methanol)

C	-3.25334600	0.85813000	-0.14077500
C	-1.88476900	1.05089600	-0.28395600
C	-0.99997500	-0.02967800	-0.18428200
C	-1.51598800	-1.31020800	0.03468800
C	-2.88689900	-1.50193800	0.17362800
C	-3.75843200	-0.41956400	0.09143400
C	0.45150500	0.20813900	-0.36026600
O	0.73375300	2.05698500	0.58216300
H	0.68609200	1.82282400	1.51765000
C	1.44428400	-0.63235100	0.00288300
C	2.84727000	-0.28695900	-0.09413900
O	3.16788900	0.88607300	-0.30499800
C	3.89028900	-1.35783600	0.10148700
H	-3.92754700	1.70549500	-0.21208900
H	-1.48155200	2.04461500	-0.45000800
H	-0.83940200	-2.15625500	0.07130300
H	-3.27532200	-2.50192100	0.33766900
H	-4.82764000	-0.57154500	0.19904800
H	0.71813600	0.91586700	-1.14342500
H	1.23709200	-1.46979600	0.66599600
H	2.07838500	2.07097300	0.26762900

(26b-TS) *G* = -652.7496665 a. u. (Gas phase)
G = -652.7734978 a. u. (In methanol)

C	2.33778200	1.10493100	-0.01989400
C	0.96805600	1.21077200	0.18821600
C	0.14510100	0.08183700	0.09501200
C	0.72551500	-1.15881200	-0.18406200
C	2.09769900	-1.26359300	-0.38800600
C	2.90653500	-0.13319100	-0.31162900
C	-1.30848300	0.22673800	0.34081500
O	-1.74176200	2.07997000	-0.53318200
H	-1.72258300	1.87448900	-1.47639400
C	-2.26520200	-0.66203600	-0.00368600
C	-3.68034800	-0.40473300	0.16435200
O	-4.05992000	0.74067100	0.42365300
C	-4.66599100	-1.53095100	-0.01751600
H	2.96323600	1.98921900	0.04720800
H	0.51469500	2.17348000	0.40103500
H	0.09917000	-2.04286700	-0.21637000
H	2.53676800	-2.23349900	-0.59836200
H	-1.58089500	0.89564600	1.15547000
H	-2.03898100	-1.46721000	-0.69973200
H	-3.06931200	2.00423800	-0.16030300
H	-4.36118600	-2.40236700	0.56682000

Atom	*x* / Å	*y* / Å	*z* / Å
H	3.66430700	-2.22801900	-0.51934500
H	4.87443600	-0.95766200	-0.13954700
H	3.87623600	-1.69081500	1.14358900

(26c-TS)	*G* = -742.6836662 a. u. (Gas phase) *G* = -742.7191789 a. u. (In methanol)		
C	-2.05171000	1.13908300	-0.21413700
C	-0.67036700	1.24494400	-0.32066200
C	0.13910700	0.10578700	-0.23401900
C	-0.46480100	-1.14358300	-0.06566100
C	-1.84830100	-1.24813500	0.03660500
C	-2.64485500	-0.10856300	-0.03221800
C	1.60689900	0.25204400	-0.37009500
O	1.98649300	2.05024000	0.63412900
H	1.90081200	1.79288100	1.56077100
C	2.53338500	-0.66239200	-0.01045300
C	3.95791800	-0.40790800	-0.06544600
O	4.35967500	0.74693500	-0.23334600
C	4.92352600	-1.55062500	0.12092400
H	-2.66706200	2.03089100	-0.27479600
H	-0.19904300	2.21418700	-0.44737800
H	0.15386300	-2.03323500	-0.03958200
H	-2.30522800	-2.22454600	0.16145300
H	1.93829900	0.96286100	-1.12522600
H	2.25571600	-1.50306000	0.62211200
H	3.33642600	1.98431200	0.35040900
H	4.65627700	-2.38570000	-0.53095600
H	5.93733900	-1.20964700	-0.08571000
H	4.86230300	-1.91184000	1.15185800
N	-4.10654500	-0.22228400	0.07469900
O	-4.58394300	-1.31137000	0.23090700
O	-4.76331100	0.77856600	0.00145000

(27b-TS)	*G* = -652.724610 a. u. (Gas phase) *G* = -652.746241 a. u. (In methanol)		
C	-2.19966400	0.99442000	0.15793000
C	-0.88840600	1.40750600	-0.05949600
C	0.10587800	0.51634800	-0.46733200
C	-0.24477300	-0.82575600	-0.65333900
C	-1.54701300	-1.25202200	-0.44125200
C	-2.53261700	-0.34760800	-0.03786800
C	1.49667400	1.07909500	-0.70387400
O	1.88401800	1.92692400	0.37364400
H	1.50605300	1.55372100	1.18013100
C	2.59992300	0.04584500	-1.01182200
C	2.97085600	-0.83706800	0.17117100
O	2.47016700	-1.92864400	0.33553400
C	4.01719100	-0.29102300	1.11580300
H	-2.94249700	1.71776700	0.47138600
H	-0.62901000	2.45204400	0.09077400
H	0.50653200	-1.55623100	-0.93025300
H	-1.82659100	-2.29135100	-0.57333200

Atom	*x* / Å	*y* / Å	*z* / Å
H	-5.66020000	-1.19759100	0.27778100
H	-4.67929300	-1.83418100	-1.06866900
O	4.31687100	-0.24410900	-0.52032000
C	4.97968100	-0.34673300	0.74263300
H	6.02265800	-0.52592300	0.58454900
H	4.85304700	0.56565400	1.28707200
H	4.55928800	-1.15672000	1.30128400

(27a-TS)	*G* = -538.2661451 a. u. (Gas phase) *G* = -538.2944759 a. u. (In methanol)		
C	3.20128600	0.87795600	-0.32551400
C	1.96969800	1.31569000	0.12461000
C	0.95036200	0.38497900	0.44789800
C	1.22102100	-1.00047600	0.35314800
C	2.46394400	-1.42970500	-0.08485700
C	3.44444700	-0.49665500	-0.43153700
C	-0.2966870	0.90417300	0.87617300
O	-2.4108830	1.84066800	-0.88264500
H	-1.9493890	2.10798500	-1.68718000
C	-1.5568410	0.21790500	1.04534800
C	-2.0823900	-0.72592100	-0.04511600
O	-1.3429260	-1.37890700	-0.74217600
C	-3.5815770	-0.77475800	-0.13017600
H	3.97339300	1.59112800	-0.59188500
H	1.75717000	2.37774500	0.20764900
H	0.45734400	-1.71323700	0.63518900
H	2.67472200	-2.49079900	-0.15782200
H	4.41372500	-0.84266300	-0.77791600
H	-0.3345690	1.96997700	1.09426500
H	-1.2416560	-0.87957100	2.29580700
H	-2.3352500	0.85158100	1.45477000
H	-4.0118510	-0.93990100	0.86314500
H	-3.8934690	0.20595000	-0.50572900
H	-3.8792710	-1.57141600	-0.81159800

(27c-TS)	*G* = -742.6553701 a. u. (Gas phase) *G* = -742.6924335 a. u. (In methanol)		
C	2.07798700	-1.30874700	-0.11996300
C	0.73839600	-1.66683800	-0.21499000
C	-0.27065300	-0.69933900	-0.19821800
C	0.07417400	0.65207800	-0.08497700
C	1.40856800	1.02827500	0.00763200
C	2.38310800	0.03915500	-0.00909300
C	-1.71481400	-1.17055600	-0.23299800
O	-2.24816700	-1.26006500	1.08213800
H	-1.60199200	-1.70382900	1.64384500
C	-2.68103600	-0.28059800	-1.03760800
C	-3.33463500	0.81105500	-0.18507100
O	-2.81346900	1.89347000	-0.03115600
C	-4.67119700	0.47243000	0.42513500
H	2.87582900	-2.04036400	-0.13611900
H	0.47399000	-2.71655100	-0.31386000
H	-0.70349900	1.40940600	-0.08096300
H	1.70421900	2.06660800	0.09117600

Atom	*x* / Å	*y* / Å	*z* / Å
H	1.45036100	1.74291600	-1.57610700
H	2.28926100	-0.58962300	-1.84512900
H	3.48361500	0.61473300	-1.31775500
H	4.99332000	-0.33551800	0.61982300
H	3.81734400	0.76046300	1.33539600
H	4.04944900	-0.89220800	2.02408700
O	-3.77566400	-0.86469400	0.14165800
C	-4.79534300	0.01858100	0.55253900
H	-5.70086600	-0.58087700	0.63894400
H	-4.56534800	0.47075700	1.52476200
H	-4.95602100	0.81479700	-0.18416800
(28a-TS)	*G* = -538.2698250 a. u. (Gas phase) *G* = -538.2963781 a. u. (In methanol)		
C	-3.12558100	0.42929800	0.16091200
C	-1.94791500	1.04619200	-0.22992100
C	-0.79809400	0.28096200	-0.48189700
C	-0.85206200	-1.10952400	-0.32347000
C	-2.03894100	-1.72561900	0.05638500
C	-3.17514500	-0.95903700	0.29947500
C	0.40837900	0.96293200	-0.93870300
O	0.75302400	2.49590500	0.74808100
H	0.82404700	1.76234200	1.37965100
C	1.72198300	0.29056200	-1.00011100
C	2.23886200	-0.41810500	0.22362700
O	1.72941200	-0.27122900	1.31189700
C	3.42702700	-1.32796300	0.00581300
H	-4.00657300	1.02777900	0.36728300
H	-1.87013600	2.12662800	-0.29616000
H	0.02881400	-1.71525100	-0.51604300
H	-2.07524800	-2.80410100	0.16759700
H	-4.09854000	-1.44116800	0.60363900
H	0.26498200	1.79698700	-1.61605400
H	1.93294000	-0.22514300	-1.94099800
H	2.86033500	1.54248000	-1.09803600
H	3.09182400	-2.24154800	-0.49761300
H	4.17423500	-0.85299400	-0.63420600
H	3.86276400	-1.59160400	0.96845000
(28c-TS)	*G* = -742.6577320 a. u. (Gas phase) *G* = -742.6971179 a. u. (In methanol)		
C	-1.92974800	1.25969100	-0.09333300
C	-0.61431200	1.61959800	-0.33889800
C	0.35700900	0.63347500	-0.57396100
C	-0.01611700	-0.71615300	-0.54670300
C	-1.33931200	-1.07240400	-0.31264500
C	-2.29629400	-0.08742100	-0.08528300
C	1.72081800	1.05479000	-0.87702700
O	2.23775300	2.34418900	0.96260800
H	2.08708900	1.57020500	1.52854900
C	2.85409400	0.10797900	-0.90235400
C	3.08738100	-0.78560100	0.28676400

Atom	*x* / Å	*y* / Å	*z* / Å
H	-1.71290600	-2.16703000	-0.69908600
H	-2.14941600	0.19132000	-1.86730000
H	-3.47050900	-0.91587100	-1.44912100
H	-5.40632000	0.30310700	-0.36873300
H	-4.57581900	-0.45401300	0.99723300
H	-5.00196200	1.28937200	1.06527100
N	3.79829000	0.43494700	0.08752800
O	4.63195900	-0.45200500	0.06927900
O	4.04479800	1.62256600	0.18047200
(28b-TS)	*G* = -652.7251860 a. u. (Gas phase) *G* = -652.7482817 a. u. (In methanol)		
C	2.20312700	1.08206000	-0.16946100
C	0.93526100	1.48452200	0.21879900
C	-0.06025700	0.53028500	0.4824920
C	0.23925600	-0.83022200	0.33835700
C	1.51606200	-1.23014600	-0.03896400
C	2.49795100	-0.27689700	-0.29374100
C	-1.36792400	0.99239400	0.93613900
O	-1.98133400	2.42161400	-0.76535500
H	-1.92200000	1.68029600	-1.38902600
C	-2.54136200	0.09843300	1.00884700
C	-2.92605000	-0.70385800	-0.20575200
O	-2.45223600	-0.48074500	-1.29715700
C	-3.93370000	-1.80759100	0.02541100
H	2.96371600	1.82502000	-0.38493500
H	0.66717800	2.53469200	0.27405400
H	-0.51995300	-1.58044200	0.54010900
H	1.74292200	-2.28623400	-0.13907300
H	-1.37379200	1.84593600	1.60430600
H	-2.65620300	-0.43630100	1.95573300
H	-3.88357200	1.12962100	1.09748400
H	-3.44107800	-2.64175200	0.53720700
H	-4.75241500	-1.46576400	0.66290500
H	-4.31710200	-2.15472200	-0.93299700
O	3.80758900	-0.69066700	-0.69191600
C	4.71623000	-0.51318400	0.39793400
H	5.63912400	-1.00749400	0.17697300
H	4.89723500	0.53109800	0.54494600
H	4.29222200	-0.93035300	1.28736400
(29a-z)	*G* = -461.9555980 a. u. (Gas phase) *G* = -461.9714807 a. u. (In methanol)		
C	-2.11707700	-1.48598200	-0.00006600
C	-0.86856400	-0.87423500	-0.00022800
C	-0.77017800	0.52666600	-0.00013500
C	-1.95941300	1.27750200	0.00011600
C	-3.20345400	0.66272800	0.00028600
C	-3.28504200	-0.72747100	0.00019100
C	0.47415400	1.30632000	-0.00030600
C	1.79600100	1.03178600	-0.00031300
C	2.54759300	-0.24706200	-0.00002100
O	2.04949600	-1.35696100	-0.00021400
C	4.05585100	-0.08545300	0.00051300

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
O	2.52481700	-0.60552700	1.34342700	H	-2.17610300	-2.56964100	-0.00014100
C	4.06095200	-1.92335200	0.07533300	H	0.03405200	-1.46865600	-0.00042800
H	-2.67252000	2.02611400	0.10109100	H	-1.89933300	2.36269000	0.00018700
H	-0.29481100	2.65606300	-0.30096900	H	-4.10572800	1.26538500	0.00048400
H	0.72367800	-1.49057900	-0.72808900	H	-4.25403900	-1.21654000	0.00030600
H	-1.62224900	-2.11961800	-0.30268100	H	0.26517300	2.37667100	-0.00044200
H	1.82753800	1.94609500	-1.48464600	H	2.44547500	1.90467000	-0.00041900
H	3.03202000	-0.37315100	-1.86805500	H	4.37524300	0.48014000	-0.88042800
H	4.24420000	1.07251600	-0.80231300	H	4.37461100	0.48006400	0.88173300
H	3.58063200	-2.69838100	-0.53217000	H	4.52546600	-1.06789000	0.00064200
H	4.95005400	-1.58566000	-0.46225500				
H	4.33745200	-2.34751900	1.03952900				
N	-3.69271000	-0.46740400	0.17266100				
O	-3.97590100	-1.63283200	0.17291700				
O	-4.49303700	0.40318700	0.37255100				
(29b-z)	*G* = -576.4117420 a. u. (Gas phase) *G* = -576.4240607 a. u. (In methanol)			**(29c-z)**	*G* = -666.3984870 a. u. (Gas phase) *G* = -666.4241604 a. u. (In methanol)		
C	1.39953700	-1.09852300	-0.29034500	C	-1.19166300	-0.95682500	-0.00021800
C	0.09107200	-0.64283300	-0.17507400	C	0.13951600	-0.55559800	-0.00032100
C	-0.16983200	0.73364300	-0.07789000	C	0.46373300	0.81081600	-0.00018700
C	0.92094800	1.62117100	-0.10082800	C	-0.58803100	1.74453200	0.00004400
C	2.22533400	1.16194300	-0.21603500	C	-1.91528800	1.33959300	0.00015400
C	2.46834600	-0.20595300	-0.31150700	C	-2.22119400	-0.01898400	0.00001900
C	-1.49373900	1.35623700	0.04808800	C	1.81800900	1.37840600	-0.00029400
C	-2.77149600	0.92476100	0.10983000	C	3.07785500	0.89318800	-0.00026300
C	-3.36707400	-0.43323600	0.07143000	C	3.61215900	-0.49059700	0.00002000
O	-2.74404500	-1.47312400	-0.03076100	O	2.94070000	-1.50505300	-0.00022000
C	-4.88045300	-0.45493000	0.17230500	C	5.12666300	-0.57566600	0.00061000
H	1.58443400	-2.16534900	-0.36449000	H	-1.42560500	-2.01657600	-0.00032400
H	-0.73395400	-1.34078300	-0.15925600	H	0.93381300	-1.28849900	-0.00050500
H	0.73482800	2.68938500	-0.02651600	H	-0.35280100	2.80562100	0.00014900
H	3.04906100	1.86801300	-0.23129400	H	-2.70791200	2.08056500	0.00033800
H	-1.41150900	2.44218200	0.10542800	H	1.78533300	2.46847800	-0.00040900
H	-3.51685400	1.71148800	0.20598400	H	3.86026000	1.64922200	-0.00032300
H	-5.20337800	0.01634500	1.10589100	H	5.53356400	-0.06932200	-0.88030500
H	-5.32181300	0.11782000	-0.64935500	H	5.53286100	-0.06933100	0.88185600
H	-5.23119200	-1.48517900	0.13640700	H	5.43077800	-1.62124400	0.00072900
O	3.80845500	-0.69054400	-0.43058600	N	-3.62354300	-0.45979900	0.00011200
C	4.49813200	-0.49598300	0.80690800	O	-3.85122300	-1.63733100	-0.00000900
H	5.40967000	-1.05628500	0.79913300	O	-4.48398400	0.37569400	0.00030500
H	4.71938600	0.54335000	0.93234300				
H	3.88139200	-0.82943300	1.61520400				
(29a-E)	*G* = -461.9762840 a. u. (Gas phase) *G* = -461.9902225 a. u. (In methanol)			**(29b-E)**	*G* = -576.419620 a. u. (Gas phase) *G* = -576.445673 a. u. (In methanol)		
C	-3.12546100	1.09443200	0.00018200	C	2.16129400	1.21602400	-0.25405500
C	-1.74466200	1.27340900	0.00013400	C	0.77897300	1.35561400	-0.16272500
C	-0.87402700	0.17528900	0.00000400	C	-0.05974000	0.23337800	-0.13079000
C	-1.42454700	-1.11572800	-0.00007500	C	0.52450600	-1.04121200	-0.19304000
C	-2.80208000	-1.29584700	-0.00002800	C	1.90360000	-1.18203600	-0.28418600
C	-3.65818900	-0.19232600	0.00010100	C	2.72767500	-0.05481500	-0.31508500
C	0.57424300	0.42770300	-0.00005300	C	-1.51136200	0.44444100	-0.03361500
C	1.54787500	-0.49638000	-0.00019800	C	-2.45754700	-0.50679200	0.00856100
C	3.00407800	-0.21847300	-0.00013100	C	-3.91778300	-0.27047300	0.10665700
O	3.78267900	-1.15603000	0.00009400	O	-4.66906500	-1.22961700	0.13582100

Atom	*x* / Å	*y* / Å	*z* / Å
C	3.54547800	1.19814300	-0.00009800
H	-3.78280800	1.95797300	0.00028200
H	-1.33050200	2.27847300	0.00019700
H	-0.77464800	-1.98472800	-0.00017100
H	-3.21233600	-2.30067100	-0.00008900
H	-4.73368400	-0.33787200	0.00013900
H	0.84463700	1.48164000	0.00007100
H	1.32409500	-1.56011600	-0.00026700
H	2.78602600	1.97846100	-0.00251800
H	4.17871500	1.31765300	0.88234300
H	4.18282700	1.31609700	-0.87976000

(29c-E) *G* = -666.405564 a. u. (Gas phase)
G = -66.4307275 a. u. (In methanol)

C	-1.85622200	1.26879800	0.01200600
C	-0.46932200	1.39186900	0.01301500
C	0.35626100	0.25954000	0.00235000
C	-0.24594000	-1.00814000	-0.00943500
C	-1.62962300	-1.13248400	-0.01045600
C	-2.44047400	0.00465500	0.00025200
C	1.81354200	0.45326100	0.00400100
C	2.74906700	-0.50934000	-0.00511400
C	4.21530400	-0.29046900	-0.00310700
O	4.95541200	-1.25866100	-0.01189100
C	4.81346400	1.10307100	0.00979600
H	-2.47816400	2.15813800	0.02038000
H	-0.01491700	2.37934800	0.02219700
H	0.36834000	-1.90263400	-0.01785100
H	-2.08011800	-2.11988000	-0.01963800
H	2.12627300	1.49537400	0.01375700
H	2.48251600	-1.56312600	-0.01492500
H	4.08614000	1.91340600	0.01492300
H	5.45106200	1.18873800	0.89303000
H	5.45500400	1.20333500	-0.86901300
N	-3.90396800	-0.13349500	-0.00089100
O	-4.57077000	0.86219500	-0.04981500
O	-4.37272900	-1.23638400	0.04714600

(30a-TS1) G = -538.2876030 a. u. (Gas phase)
G = -538.3162953 a. u. (In methanol)

C	2.92492000	1.34301600	0.02504900
C	1.56970700	1.15290500	-0.18192400
C	1.04148000	-0.15240300	-0.26878000
C	1.91528600	-1.25301200	-0.14101200
C	3.26964700	-1.05657300	0.06787500
C	3.77492200	0.24162500	0.15111400
C	-0.33970000	-0.40447200	-0.50823700
C	-1.38177100	0.61006800	-0.78114400
C	-2.75796700	0.00674700	-0.44598500
O	-3.02457800	-1.10353100	-0.84228600
C	-3.69212300	0.86256800	0.35818600

Atom	*x* / Å	*y* / Å	*z* / Å
C	-4.49633700	1.12989900	0.17104600
H	2.79360400	2.09775300	-0.27743600
H	0.33852300	2.34830000	-0.11517800
H	-0.10022600	-1.92818500	-0.17025100
H	2.34014900	-2.17459300	-0.33148300
H	-1.80972400	1.49006200	0.00580300
H	-2.20542400	-1.56353000	-0.02816700
H	-3.75974900	1.93131000	0.14194100
H	-5.18769500	1.24852600	-0.66676400
H	-5.07912300	1.21250500	1.09162700
O	4.14653900	-0.20616100	-0.40898800
C	4.72216500	-0.13072600	0.89786500
H	5.77117900	-0.33285600	0.83775200
H	4.57024400	0.84975500	1.29846000
H	4.25578700	-0.85263100	1.53523600

(30a-TS2) *G* = -538.2819840 a. u. (Gas phase)
G = -538.3119145 a. u. (In methanol)

C	3.03137000	-1.37297100	-0.11985700
C	1.66068400	-1.36597200	0.07634900
C	0.98504200	-0.14035500	0.23786500
C	1.69667300	1.07676100	0.16219000
C	3.06643700	1.05387200	-0.05315400
C	3.73273200	-0.16501600	-0.18627200
C	-0.42541800	-0.05397700	0.47786300
C	-1.39606300	-1.01519900	0.09749800
C	-2.85243000	-0.62545100	-0.09815100
O	-3.52280800	-1.35762700	-0.78955200
C	-3.33416500	0.65197500	0.52057600
H	3.56087000	-2.31447500	-0.22118300
H	1.11494500	-2.30222800	0.15333200
H	1.11169100	1.99831800	0.18914100
H	3.61742700	1.98532600	-0.13034800
H	4.80589800	-0.17811100	-0.35073800
H	-0.78414900	0.88530000	0.89879200
H	-1.10479700	-1.92046300	-0.43006200
H	-1.51091000	-1.68092900	1.95868400
H	-3.17511500	0.63282100	1.60461800
H	-2.74623500	1.50019200	0.11836300
H	-4.39631300	0.76668300	0.30516400
O	-1.04284500	2.60004800	-0.39077500
H	-0.95726500	2.42619200	-1.34259000

(30b-TS2) *G* = -652.754632 a. u. (Gas phase)
G = -652.776669 a. u. (In methanol)

C	2.18481000	-1.31870400	-0.24582800
C	0.82106500	-1.33089700	-0.00629300
C	0.13396900	-0.11491100	0.17808200
C	0.82591700	1.11202900	0.08143100
C	2.18835400	1.10833700	-0.17722300
C	2.86691500	-0.10107400	-0.33291000
C	-1.26923800	-0.04832100	0.46274600
C	-2.23804200	-1.02261700	0.11211300
C	-3.70513700	-0.65296800	-0.03681600
O	-4.38688300	-1.39381700	-0.70755300
C	-4.18467000	0.61714100	0.59846300

Atom	*x* / Å	*y* / Å	*z* / Å
H	3.32673700	2.34790000	0.09390700
H	0.91003300	2.00858800	-0.27240800
H	1.50678500	-2.25724400	-0.20127400
H	3.93427600	-1.90734600	0.16908100
H	4.83610800	0.39733100	0.31662600
H	-0.65415600	-1.43513400	-0.66086500
H	-1.20330700	1.53278200	-0.22782600
H	-1.39155800	0.84225800	-1.85959700
H	-3.26734000	0.85001500	1.36864000
H	-3.71212700	1.89053400	-0.01475700
H	-4.69206200	0.42958000	0.34873600
O	-1.44502000	-0.34074300	2.00669000
H	-1.78302300	-1.24789100	1.97364300

(30b-TS1) *G* = -652.7705461 a. u. (Gas phase)
G = -652.7911382 a. u. (In methanol)

C	-2.09729300	-1.20853700	0.19077200
C	-0.74456000	-1.06990600	-0.06705900
C	-0.17729100	0.21399800	-0.20915900
C	-1.00973400	1.34648300	-0.08379100
C	-2.36175700	1.20155400	0.17610500
C	-2.90599300	-0.07611800	0.31361500
C	1.20228100	0.41275700	-0.50209800
C	2.20059200	-0.64341200	-0.78060100
C	3.60652800	-0.07768200	-0.50942600
O	3.89540700	1.01162200	-0.94625600
C	4.53947300	-0.94187900	0.28715700
H	-2.52910300	-2.19705100	0.30199400
H	-0.11671600	-1.94946500	-0.15502400
H	-0.57097200	2.33435900	-0.18663200
H	-2.99434000	2.07667100	0.27509000
H	1.54477400	1.42764700	-0.69481200
H	2.01131800	-1.54395300	-0.19527100
H	2.16549300	-0.90552200	-1.85164500
H	4.15051900	-0.88712000	1.31054900
H	4.51297700	-1.97985300	-0.05651500
H	5.55209900	-0.54319300	0.23161800
O	2.39122400	0.38143500	1.97501300
H	2.75733800	1.27544100	1.90452600
O	-4.30187100	-0.22803800	0.58443600
C	-5.03616700	-0.15821200	-0.64064900
H	-6.06847100	-0.36537000	-0.45003500
H	-4.94036900	0.82215000	-1.05851600
H	-4.64909900	-0.87916900	-1.33006900

(30c-TS1) *G* = -742.65137601 a. u. (Gas phase)
G = -742.69025191 a. u. (In methanol)

C	-1.85003100	-1.14859100	-0.18024300
C	-0.48011300	-1.01685600	-0.32705100
C	0.11181700	0.26367000	-0.34342600
C	-0.71389400	1.39988600	-0.20772800
C	-2.08333600	1.26172400	-0.05921700

Atom	*x* / Å	*y* / Å	*z* / Å
H	2.72382300	-2.25268300	-0.36505700
H	0.29106100	-2.27470300	0.08676300
H	0.22937400	2.02535300	0.12805500
H	2.72366500	2.04741400	-0.27066300
H	-1.62742600	0.88554100	0.89600600
H	-1.95113000	-1.92331900	-0.42554500
H	-2.28461600	-1.69139500	1.97516600
H	-3.99109600	0.59931300	1.67689800
H	-3.62158800	1.47376700	0.17889300
H	-5.25459800	0.71726600	0.41694800
O	-1.95058700	2.59758300	-0.38256600
H	-1.89281300	2.42570800	-1.33683200
O	4.27283800	-0.09851800	-0.59420100
C	4.98816700	-0.04473200	0.64285700
H	6.03906400	-0.10225800	0.44997200
H	4.76715400	0.87502300	1.14296200
H	4.69352600	-0.86671400	1.26126700

(30c-TS2) *G* = -742.7359950 a. u. (Gas phase)
G = -742.7759255 a. u. (In methanol)

C	1.93350900	-1.29783600	0.06725100
C	0.55580500	-1.31628900	0.20478900
C	-0.14963400	-0.10301300	0.32740500
C	0.54098300	1.12724000	0.27225600
C	1.91889100	1.12964900	0.11568800
C	2.61364800	-0.07687500	0.02099000
C	-1.57047200	-0.04256600	0.50635400
C	-2.50524400	-1.02538400	0.09277500
C	-3.95915300	-0.66570700	-0.16793200
O	-4.58510000	-1.41590600	-0.88131400
C	-4.49145400	0.60650100	0.41931000
H	2.48491400	-2.22948900	-0.00376700
H	0.02542600	-2.26248200	0.26603600
H	-0.06227700	2.03732000	0.26676700
H	2.45461600	2.07114200	0.05449300
H	-1.96492400	0.89253800	0.90397200
H	-2.17427700	-1.92858100	-0.41452500
H	-2.68674100	-1.67966000	1.95271600
H	-4.37858000	0.59836800	1.50926600
H	-3.90332200	1.46313100	0.03565200
H	-5.54543000	0.69878500	0.15789500
O	-2.20123600	2.59244200	-0.40932600
H	-2.07168400	2.41336700	-1.35518500
N	4.07484500	-0.06773000	-0.13939000
O	4.63696200	0.99074100	-0.18502100
O	4.64651000	-1.11910800	-0.21820300

(31a-TS2) *G* = -538.2862110 a. u. (Gas phase)
G = -538.3158315 a. u. (In methanol)

C	2.13306800	-1.32358600	-0.73985300
C	0.89475000	-0.78181500	-0.39252300
C	0.82397000	0.43886200	0.32951500
C	2.02217600	1.15037000	0.60238900
C	3.25403600	0.65556900	0.18221400

Atom	*x* / Å	*y* / Å	*z* / Å
C	-2.65187900	-0.01268300	-0.04529100
C	1.51187600	0.45717200	-0.51929600
C	2.51545400	-0.59600200	-0.79010100
C	3.90368400	-0.07250700	-0.37898600
O	4.23791800	1.03723100	-0.72194900
C	4.76328100	-1.00112900	0.42756300
H	-2.30098100	-2.13470300	-0.16545900
H	0.14184800	-1.89959200	-0.42447700
H	-0.25665400	2.38471200	-0.21369400
H	-2.71090800	2.13941000	0.04853500
H	1.88024000	1.47628100	-0.62013200
H	2.27161800	-1.52848100	-0.27976900
H	2.55810800	-0.78909500	-1.87544200
H	4.29889200	-1.00473300	1.42051100
H	4.75019000	-2.01464400	0.01669100
H	5.78197800	-0.61694900	0.47347200
O	2.51000800	0.24881800	2.03236400
H	2.89123000	1.13915900	2.04712900
N	-4.10551300	-0.16182800	0.11472600
O	-4.77138700	0.82916100	0.22862100
O	-4.56755200	-1.26854500	0.12499100

(31a-TS1) *G* = -538.291147 a. u. (Gas phase)
G = -538.320535 a. u. (In methanol)

C	-2.03907500	-1.65391200	0.17160000
C	-0.83533500	-1.15603000	-0.30613100
C	-0.70049400	0.22233300	-0.56284300
C	-1.77823100	1.09002400	-0.29705500
C	-2.96864200	0.58531200	0.19639700
C	-3.10260500	-0.78682400	0.42228100
C	0.50939000	0.77367200	-1.10008600
C	1.80445600	0.05132500	-1.14119300
C	2.21145600	-0.72491200	0.12777000
O	2.68124400	-1.83304300	0.00246500
C	2.02568400	-0.04467700	1.45600300
H	-2.14936800	-2.71728600	0.35357100
H	-0.00882900	-1.83276500	-0.50414200
H	-1.61307000	2.15660700	-0.41347600
H	-3.79140300	1.25553800	0.41982200
H	-4.03813800	-1.18081800	0.80630300
H	0.41520000	1.68003500	-1.68843800
H	1.78901000	-0.67699500	-1.96487900
H	2.60103100	0.76999000	-1.35923100
H	2.00881500	1.04707200	1.36590900
H	1.03440400	-0.32376200	1.83430000
H	2.77380800	-0.42304500	2.15328100
O	0.90672600	2.69741400	0.63843800
H	1.51515600	3.19259600	0.06930000

(31b-TS1) *G* = -652.7731890 a. u. (Gas phase)
G = -652.7942097 a. u. (In methanol)

C	-1.50255700	-1.22165100	0.05763100

(31b-TS2) *G* = -652.7569190 a. u. (Gas phase)
G = -652.7781957 a. u. (In methanol)

C	-1.52353000	-1.06677700	0.30651300
C	-0.20629800	-0.63586000	0.14282100
C	0.06763700	0.60944500	-0.48214200
C	-1.01532900	1.45368400	-0.84386800
C	-2.33064300	1.06470900	-0.60407300
C	-2.58215500	-0.27849200	-0.13873200
C	1.49562200	1.05911700	-0.75854000
C	2.55122900	0.03544000	-1.24716500
C	2.78635300	-0.98890000	-0.16433400
O	1.95807900	-1.86209300	0.02953100
C	4.05633200	-0.90041400	0.63634600
H	-1.72093400	-2.01749300	0.79205100
H	0.61857100	-1.25332700	0.48347800
H	0.81440000	2.41082900	-1.32195400
H	-3.11770900	1.81148900	-0.56503000
H	1.80333800	1.67357100	-1.47231000
H	1.95523900	-0.79523500	-2.86050800
H	3.38870100	0.51389700	-1.42071300
H	4.90466000	-1.00194400	-0.05264500
H	4.13797300	0.08277000	1.11077700
H	4.08623200	-1.69074500	1.38595700
O	2.48053900	2.24142200	1.65220500
H	3.43007700	2.04225000	1.64570400
O	-3.91707800	-0.79101800	-0.12463000
C	-4.67472000	-0.12167700	0.88673600
H	-4.95674700	0.84944800	0.53705400
H	-5.55371700	-0.69000900	1.10868900
H	-4.08060400	-0.02363400	1.77122100

(31b-TS1) *G* = -652.7731890 a. u. (Gas phase)
G = -652.7942097 a. u. (In methanol)

C	-1.33594000	-0.86099600	0.41484800

Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
C	-0.22120200	-0.91908600	-0.38019000	C	-0.00042500	-0.51791900	0.19971200
C	0.14612000	0.42353700	-0.59560800	C	0.33445300	0.74768500	-0.35029300
C	-0.77989200	1.45138600	-0.32900700	C	-0.69759600	1.69523400	-0.58143000
C	-2.04963800	1.13950300	0.12462200	C	-2.02352800	1.38790300	-0.28765200
C	-2.41427200	-0.19639300	0.30942300	C	-2.35296900	0.03549000	0.09502200
C	1.44389800	0.77920100	-1.09129000	C	1.77520100	1.10979200	-0.68326100
C	2.60241400	-0.14675600	-1.12465700	C	2.71706500	0.05083100	-1.30973600
C	2.84275500	-1.00974400	0.13071100	C	2.93251800	-1.06788200	-0.32022000
O	3.12603200	-2.17714400	-0.01519600	O	2.05051400	-1.88935900	-0.13765000
C	2.73782800	-0.33994600	1.47302000	C	4.24938600	-1.13545600	0.40300600
H	-1.79170100	-2.25603100	0.20762000	H	-1.57944300	-1.82872400	0.84238200
H	0.48692900	-1.71862400	-0.57914200	H	0.79141600	-1.21919800	0.44244100
H	-0.43780800	2.47826800	-0.41222100	H	-0.44965100	2.66852300	-1.00130800
H	-2.75580600	1.93139700	0.34887200	H	-2.74576000	2.18593800	-0.14552100
H	1.51595100	1.70238400	-1.65614900	H	2.08889100	1.75241300	-1.36907900
H	2.48802700	-0.84260100	-1.96837600	H	1.96583700	-0.60755300	-2.93770700
H	3.51214000	0.43481900	-1.30554600	H	3.57828500	0.47758400	-1.50099500
H	2.90392700	0.74131000	1.41291400	H	5.04611700	-1.24680900	-0.34364900
H	1.70465600	-0.45967900	1.82209400	H	4.43534700	-0.20019000	0.94068300
H	3.39494800	-0.85365600	2.17540600	H	4.25990200	-1.98078200	1.09057400
O	2.10879800	2.56843800	0.70806100	O	2.98698700	2.02797200	1.73915800
H	2.80513300	2.96925800	0.16605400	H	3.91593500	1.75986600	1.65847300
O	-3.72835600	-0.51577400	0.77426700	N	-3.75937800	-0.38749700	0.15823000
C	-4.66757200	-0.33618800	-0.28899400	O	-4.00120400	-1.51744600	0.47940500
H	-5.60802100	-0.76361900	-0.01014200	O	-4.60882400	0.41424800	-0.11389900
H	-4.79363700	0.70890300	-0.48080700				
H	-4.30382700	-0.81947300	-1.17161800				
(31c-TS1)	*G* = -742.656059 a. u. (Gas phase)			**(32b-Int)**	*G* = -652.8139270 a. u. (Gas phase)		
	G = -742.695454 a. u. (In methanol)				*G* = -652.8403562 a. u. (In methanol)		
C	-1.32639300	-1.08961200	-0.30077200	C	-1.97741900	-1.22546400	0.04307800
C	0.00507300	-0.82618600	-0.58871100	C	-0.64232800	-1.05920100	-0.24356400
C	0.44768700	0.50672200	-0.69556900	C	-0.09031300	0.25823200	-0.31513800
C	-0.45819600	1.56248700	-0.47244200	C	-0.93752000	1.38754100	-0.08503900
C	-1.78016400	1.28848000	-0.16809200	C	-2.27377400	1.20690800	0.20429800
C	-2.21662600	-0.03639300	-0.09102600	C	-2.78660000	-0.09577700	0.26710800
C	1.80370500	0.82510500	-1.03655400	C	1.24438700	0.50527500	-0.61064200
C	2.92038800	-0.15073800	-0.99888600	C	2.31753200	-0.45767900	-0.86379000
C	2.99242300	-1.08222100	0.22814700	C	3.67276200	0.07201100	-0.28623600
O	3.24128800	-2.25325900	0.05181900	O	3.84257000	1.25799400	-0.19047100
C	2.77515500	-0.47243000	1.58549100	C	4.68037400	-0.97882500	0.07337400
H	-1.67183200	-2.11546800	-0.23494500	H	-2.40974300	-2.21839400	0.09780100
H	0.69674100	-1.64727400	-0.75515100	H	-0.01291400	-1.92500400	-0.42089500
H	-0.06744900	2.57526400	-0.46689800	H	-0.51206200	2.38538300	-0.14115500
H	-2.47284200	2.10065600	0.02328300	H	-2.92182400	2.05712700	0.38081300
H	1.97228600	1.76962100	-1.54251300	H	1.56786000	1.54741100	-0.65221500
H	2.86648300	-0.79994000	-1.88476400	H	2.09822500	-1.48386600	-0.56359400
H	3.86713600	0.39611100	-1.05524000	H	2.49411000	-0.46131300	-1.95533300
H	2.99084400	0.60163700	1.59876700	H	4.31591300	-1.55852300	0.92825000
H	1.70708600	-0.56068800	1.82016800	H	4.81709800	-1.67517300	-0.76070000
H	3.33352700	-1.04852300	2.32399300	H	5.62648800	-0.50322500	0.32829800
O	2.34947100	2.49476900	0.91164600	O	1.50199700	-0.14157300	1.90074600
H	3.11455900	2.88816300	0.46533700	H	1.36655400	0.78353400	2.01561600
N	-3.62238300	-0.32419400	0.22821900	O	-4.17188800	-0.28581700	0.56670900
O	-3.97051300	-1.47033500	0.28809300	C	-4.94194900	-0.15231300	-0.63082300

Atom	*x* / Å	*y* / Å	*z* / Å
O	-4.36501800	0.59863800	0.41605800

Atom	*x* / Å	*y* / Å	*z* / Å
H	-5.96508400	-0.38851100	-0.42514200
H	-4.87315100	0.85367300	-0.98881600
H	-4.56381000	-0.82220600	-1.37456600

(32a-Int) *G* = -538.341999 a. u. (Gas phase)
G = -538.373973 a. u. (In methanol)

C	-2.77360200	-1.36859300	-0.10328400
C	-1.43673600	-1.14767400	-0.34047500
C	-0.93323800	0.19056400	-0.37334400
C	-1.83033700	1.28338900	-0.15657000
C	-3.16790900	1.04802600	0.08306300
C	-3.63253000	-0.27386300	0.10876300
C	0.40046100	0.49232200	-0.61822000
C	1.51764800	-0.42542000	-0.84766800
C	2.83096600	0.14558000	-0.21525700
O	2.95200600	1.33543100	-0.09623300
C	3.86493100	-0.87222000	0.16402600
H	-3.16936400	-0.07830400	-2.3778290
H	-0.76901300	-1.98624800	-0.50829500
H	-1.44157100	2.29729700	-0.18311100
H	-3.85362100	1.87034100	0.24918500
H	-4.68583900	-0.46132700	0.29718600
H	0.68518600	1.54641900	-0.63315500
H	1.32742600	-1.46379200	-0.57041100
H	1.73176700	-0.40498000	-1.93228500
H	3.49359000	-1.47879300	0.99701400
H	4.05679600	-1.54952600	-0.67485300
H	4.78286100	-0.36550100	0.45890400
O	0.59581300	-0.18439700	1.89091000
H	0.42129900	0.73300900	2.01450100

(34a-TS) *G* = -862.788880 a. u. (Gas phase)
G = -62.8236322 a. u. (In methanol)

C	-5.03696800	-0.61053300	-0.55732900
C	-3.77429900	-1.19342100	-0.48185900
C	-2.65037700	-0.43777200	-0.12413800
C	-2.82002800	0.93164400	0.13058500
C	-4.08092800	1.51442700	0.05591600
C	-5.19562800	0.74661400	-0.28449200
C	-1.32961000	-1.09360700	-0.04818500
C	-0.27911700	-0.62778200	0.63638700
C	1.09814100	-1.28379700	0.82786200
O	1.49008300	-1.16189200	2.09975800
C	1.03870000	-2.76464800	0.37300000
N	2.09053600	-0.55594200	0.08388000
H	2.64986200	-0.27817800	0.91714100
C	3.03550100	-1.26343000	-0.84427000
C	3.87978200	-0.12554700	-1.39122400
C	2.83508400	0.95912100	-1.68512500
C	1.71260600	0.71815400	-0.64414300
H	-3.65452500	-2.25346300	-0.69174800
H	-1.95678300	1.54700100	0.37004900
H	-4.19308500	2.57586200	0.25498300
H	-1.25119900	-2.03911600	-0.58384500
H	-0.38532100	0.27810700	1.23418100
H	1.98618800	-3.25325500	0.61041600
H	0.79343400	-2.92572300	-0.68461300
H	0.26974200	-3.23609200	0.98502800
H	3.58528100	-2.01427000	-0.27862300
H	2.44583700	-1.74806400	-1.62645300
H	4.44694600	-0.41808400	-2.27668600
H	4.58601300	0.21516200	-0.62722300
H	3.24665600	1.96797800	-1.61594700
H	2.42014100	0.83407500	-2.68785700
H	0.73750700	0.57469700	-1.10563400
H	2.56831300	2.64261900	1.77246200
H	-6.17750400	1.20547300	-0.34431900

(32c-Int) *G* = -742.7429120 a. u. (Gas phase)
G = -742.7852963 a. u. (In methanol)

C	-1.73684200	-1.14672300	-0.28148600
C	-0.38098100	-0.99892800	-0.46057300
C	0.19834600	0.30862700	-0.44834300
C	-0.64366100	1.44738600	-0.24760300
C	-2.00114400	1.28517300	-0.06637200
C	-2.54047000	-0.00817300	-0.08389800
C	1.55593900	0.53742400	-0.63373600
C	2.62792200	-0.43896300	-0.83503800
C	3.94425800	0.04553500	-0.13983300
O	4.12741000	1.22441100	0.00600600
C	4.90247300	-1.03584100	0.26179600
H	-2.18976000	-2.13190400	-0.29116300
H	0.24458000	-1.87154100	-0.61691900

(34c-TS) *G* = -1067.241665 a. u. (Gas phase)
G = -1067.285873 a. u. (In methanol)

C	-4.27813500	-1.17576200	-0.61389100
C	-2.96054600	-1.52744800	-0.35522800
C	-2.08774500	-0.64620200	0.29799700
C	-2.56492600	0.61851800	0.67632500
C	-3.87664800	0.98790800	0.42550600
C	-4.71200100	0.07996500	-0.21504100
C	-0.70597900	-1.07745900	0.55429700
C	0.17531000	-0.46428500	1.35305700
C	1.56389800	-0.94078700	1.59551900
O	2.25065800	-0.36094600	2.41648300
C	2.06848600	-2.15562200	0.84942800
N	2.59033900	0.67972400	-0.43726900
H	2.48711700	0.75588000	-1.44987200

Atom	*x* / Å	*y* / Å	*z* / Å
H	-0.19739400	2.43765600	-0.23968000
H	-2.64550000	2.14261400	0.08725200
H	1.90021500	1.57358400	-0.61765800
H	2.36799400	-1.46909400	-0.58495900
H	2.88737500	-0.41323100	-1.90959900
H	4.46339500	-1.63357900	1.06778200
H	5.09012400	-1.70932800	-0.58110100
H	5.83466600	-0.58738500	0.60270300
O	1.60911300	-0.18998600	1.86824100
H	1.48183400	0.73378400	2.00170200
N	-3.98715500	-0.18388600	0.10878700
O	-4.43382400	-1.29680900	0.09123200
O	-4.66300900	0.79270000	0.27585100

(34b-TS) *G* = -977.2255453 a. u. (Gas phase)
G = -977.2550138 a. u. (In methanol)

C	4.40064700	1.40591300	-0.72823200
C	3.09648600	1.59270600	-0.30811500
C	2.39584700	0.58953700	0.38088200
C	3.06401800	0.63378600	-0.61278600
C	4.37465900	-0.81873500	0.22026000
C	5.05066200	0.19512500	-0.46633800
C	1.01503800	0.84291600	0.80042400
C	0.19167500	-0.00643700	1.43179100
C	-1.20400000	0.31299800	1.81022400
O	-1.90723500	-0.55780500	2.29524500
C	-1.72331000	1.71942600	1.59853500
N	-2.42430800	-0.37166600	-0.75198200
H	-2.44204800	-0.12296300	-1.73744200
C	-2.05705500	-1.80186300	-0.61749000
C	-3.29754300	-2.52716300	-0.05614700
C	-4.45651400	-1.59876300	-0.42615600
C	-3.78652100	-0.22765200	-0.22138600
C	-4.54454600	0.90275800	-0.86922100
O	-5.26701900	1.67929000	-0.29989900
O	-4.36049700	0.93839800	-2.21040600
H	4.94398300	2.17870100	-1.26113700
H	2.60010500	2.53716900	-0.51626100
H	2.55706500	-1.41100100	1.16710700
H	4.85741200	-1.76421600	0.43668200
H	0.64013800	1.83545500	0.55207100

Atom	*x* / Å	*y* / Å	*z* / Å
C	2.40161100	2.00181400	0.17172800
C	3.71320000	2.79559000	-0.05352900
C	4.77040300	1.70879800	-0.36432700
C	3.99436400	0.38254800	-0.14787600
C	4.52926000	-0.74770800	-0.98957000
O	5.26401700	-1.62235400	-0.60988700
O	4.11426900	-0.65642400	-2.27382100
H	-4.96532500	-1.84745800	-1.11331000
H	-2.59910900	-2.50561800	-0.65887500
H	-1.89957600	1.32612600	1.15934600
H	-4.26163800	1.95991200	0.70820100
H	-0.40571800	-1.99024800	0.04197900
H	-0.08060500	0.43078700	1.91554400
H	3.12879500	-2.29228400	1.06811300
H	1.92886000	-2.02356500	-0.22717700
H	1.52047100	-3.05073500	1.16410100
H	1.51649900	2.48732700	-0.24651000
H	2.23453700	1.84460000	1.24333500
H	3.97931200	3.38474300	0.82726300
H	3.61520200	3.48816500	-0.89370100
H	5.10063100	1.77554700	-1.40586000
H	5.65426200	1.76992800	0.27381800
H	4.06731800	0.07182000	0.89980900
H	4.52372100	-1.39953900	-2.75046100
N	-6.10362000	0.46793600	-0.48698000
O	-6.81323400	-0.34417400	-1.05132700
O	-6.45759700	1.57662100	-0.13049400

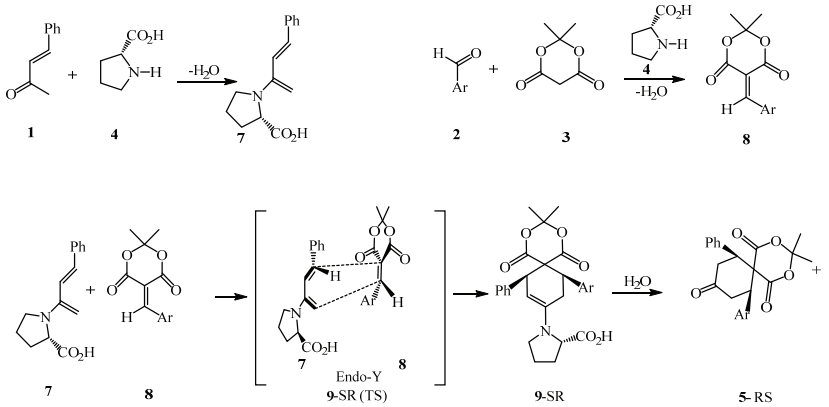
(36b-TS) *G* = -977.2232340 a. u. (Gas phase)
G = -977.2542333 a. u. (In methanol)

C	4.27058100	-1.10280400	0.85450500
C	2.88208700	-1.14174700	0.76463800
C	2.17449700	-0.11296400	0.12900200
C	2.89064400	0.97268500	-0.39804100
C	4.27641500	1.01276300	-0.30592600
C	4.97167300	-0.02584300	0.31657600
C	0.71128400	-0.20104800	0.04803300
C	-0.07758600	0.52986300	-0.75627900
C	-1.52515200	0.36094900	-0.85203200
O	-2.12684700	2.64202500	-0.59431400
C	-2.14537100	0.58719400	-2.15355100
N	-2.24931000	0.03525700	0.21365500
C	-1.86247300	0.49536000	1.57696800
C	-3.16714100	1.05492800	2.13292200
C	-4.21684100	0.11598100	1.54431700
C	-3.72366600	-0.03288800	0.09864800
C	-4.23302400	-1.32452800	-0.52652800
O	-5.35692200	-1.42679100	-0.93556500
O	-3.38294600	-2.36757700	-0.53901800
H	4.80361300	-1.91101300	1.34511300
H	2.33601600	-1.98313700	1.18380700
H	2.35995900	1.79843900	-0.86215700
H	4.81778800	1.86103400	-0.71253600
H	0.25325300	-0.95430500	0.68931500
H	0.32862700	1.24238700	-1.46695500

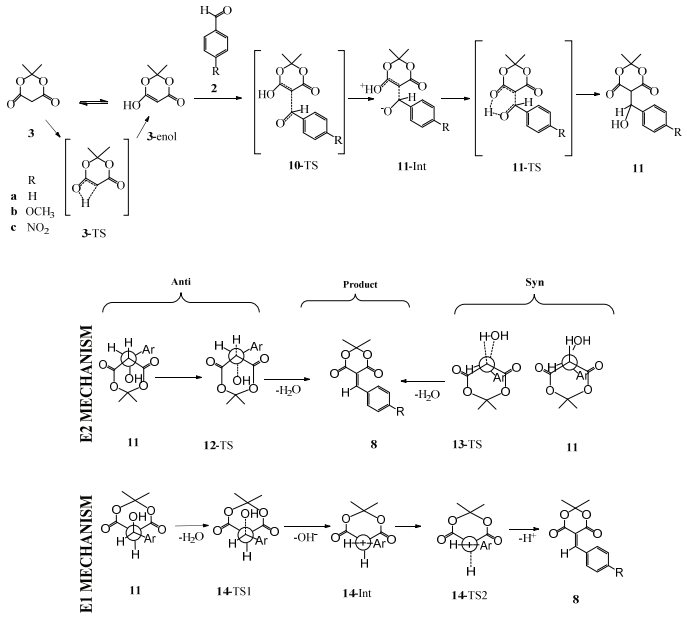
Atom	*x* / Å	*y* / Å	*z* / Å	Atom	*x* / Å	*y* / Å	*z* / Å
H	0.49643400	-1.01575800	1.69848900	H	-1.99768600	3.58406000	-0.44333700
H	-2.73186300	1.79288500	2.00751300	H	-3.06514300	0.04422600	-2.36027400
H	-1.75095600	1.93358500	0.52597100	H	-2.35981100	1.71550900	-1.90266600
H	-1.07835600	2.45659400	2.08659700	H	-1.43722000	0.50414100	-2.97554500
H	-1.76472000	-2.20258700	-1.59382800	H	-1.49171300	-0.34716700	2.17068800
H	-1.20392400	-1.91056800	0.05817200	H	-1.09307600	1.26013500	1.46435500
H	-3.21730300	-2.59181500	1.03311700	H	-3.29776800	2.06278400	1.72742800
H	-3.41176600	-3.53781700	-0.45594400	H	-3.17239800	1.08136100	3.22462500
H	-4.73582700	-1.71639900	-1.48021200	H	-4.20833300	-0.85518100	2.05497200
H	-5.34539800	-1.73670900	0.19405900	H	-5.23411100	0.50794900	1.56499300
H	-3.74412600	-0.01168400	0.85029200	H	-4.06680900	0.81934700	-0.49558000
H	-4.90199700	1.67566600	-2.54182700	H	-2.51703000	-2.08720800	-0.20694600
O	6.32627700	0.09909700	-0.91338000	O	6.39780100	0.02170300	0.41037500
C	7.01872600	-1.10570800	-0.66603000	C	6.97252400	-0.68281100	-0.69337100
H	8.01055000	-0.97801700	-1.09868100	H	8.03913900	-0.61320900	-0.64450100
H	7.11176000	-1.29736400	0.40952900	H	6.67990900	-1.71116800	-0.65143500
				H	6.62856100	-0.25120900	-1.61005500
(36a-TS)	*G* = -862.7869580 a. u. (Gas phase)			**(36c-TS)**	*G* = -1067.239282 a. u. (Gas phase)		
	G = -862.8228895 a. u. (In methanol)				*G* = -1067.283682 a. u. (In methanol)		
C	5.01272400	-1.44161200	0.48955600	C	4.00851700	-1.33981800	0.31116300
C	3.62191400	-1.41591800	0.43960400	C	2.61705400	-1.34121700	0.27461300
C	2.94068600	-0.28078400	-0.01921100	C	1.90677500	-0.18564600	-0.07648800
C	3.68670200	0.84237600	-0.40811600	C	2.62428100	0.98404500	-0.37023000
C	5.07489900	0.81758000	-0.35569100	C	4.01313600	0.98606000	-0.33111600
C	5.74305800	-0.32491700	0.08912200	C	4.71037300	-0.17590100	0.00548800
C	1.47346100	-0.30220800	-0.06499900	C	0.43998700	-0.23605900	-0.11246300
C	0.69434300	0.56571200	-0.73069700	C	-0.36436300	0.66948600	-0.69252700
C	-0.76096900	0.46591500	-0.80318100	C	-1.81779600	0.54365500	-0.76212800
O	-1.26131900	2.70657000	-0.20245000	O	-2.36093200	2.71058100	0.03862000
C	-1.40553100	0.90031400	-2.03835200	C	-2.48377600	1.07085400	-1.94886500
N	-1.46949900	0.01681400	0.22757700	N	-2.50621000	-0.01066700	0.23033400
C	-1.02818000	0.26080400	1.62959900	C	-2.05656100	0.11836100	1.64494600
C	-2.29358400	0.78205900	2.30146500	C	-3.32636300	0.54949600	2.37026300
C	-3.39619900	-0.02275400	1.61848300	C	-4.41783300	-0.21649500	1.62736400
C	-2.94793400	0.02042800	0.15133000	C	-3.98505100	-0.03370700	0.16632600
C	-3.52632400	-1.14780700	-0.63563500	C	-4.54554800	-1.14058000	-0.71645300
O	-4.66389200	-1.14843800	-1.01885200	O	-5.68654200	-1.13302200	-1.08927000
O	-2.72049100	-2.20879100	-0.82454600	O	-3.71867900	-2.16225200	-1.00492400
H	5.52484100	-2.33126500	0.84208200	H	4.54333900	-2.24535600	0.57946800
H	3.05296600	-2.28825400	0.75131200	H	2.07034200	-2.25030900	0.51228900
H	3.17835000	1.74547000	-0.73200000	H	2.09321100	1.90052200	-0.60884500
H	5.63976900	1.69508200	-0.65384000	H	4.55579200	1.89900700	-0.55479700
H	6.82750300	-0.33944700	0.13000400	H	-0.00820100	-1.11159800	0.35763300
H	1.00194100	-1.12269100	0.47621100	H	0.02847800	1.52197700	-1.23722500
H	1.11059800	1.35784100	-1.34472000	H	-2.20621300	3.59091500	0.39636400
H	-1.08958000	3.61154900	0.07759400	H	-3.42214300	0.60064900	-2.23505300
H	-2.35199700	0.42717000	-2.29106900	H	-2.66448500	2.11331400	-1.43637700
H	-1.56668000	1.98776000	-1.62180100	H	-1.81035400	1.17147400	-2.79764600
H	-0.72336100	0.91065800	-2.88604800	H	-1.68051900	-0.84249300	2.01260200
H	-0.67682700	-0.67167400	2.08441200	H	-1.27631000	0.87970500	1.67810500
H	-0.23122400	1.00490700	1.60300500	H	-3.45164900	1.62509800	2.21327500
H	-2.39331800	1.84200200	2.04880800	H	-3.28818200	0.32362600	3.43800300
H	-2.26890300	0.65087400	3.38531200	H	-4.40964400	-1.27924700	1.90028800
H	-3.41415000	-1.05708000	1.98433100	H	-5.42506100	0.17168600	1.78134900

Atom	*x* / Å	*y* / Å	*z* / Å
H	-4.39558500	0.39939800	1.72765600
H	-3.27131700	-0.30348100	0.96156000
H	-1.83530500	-2.01141500	-0.48369700

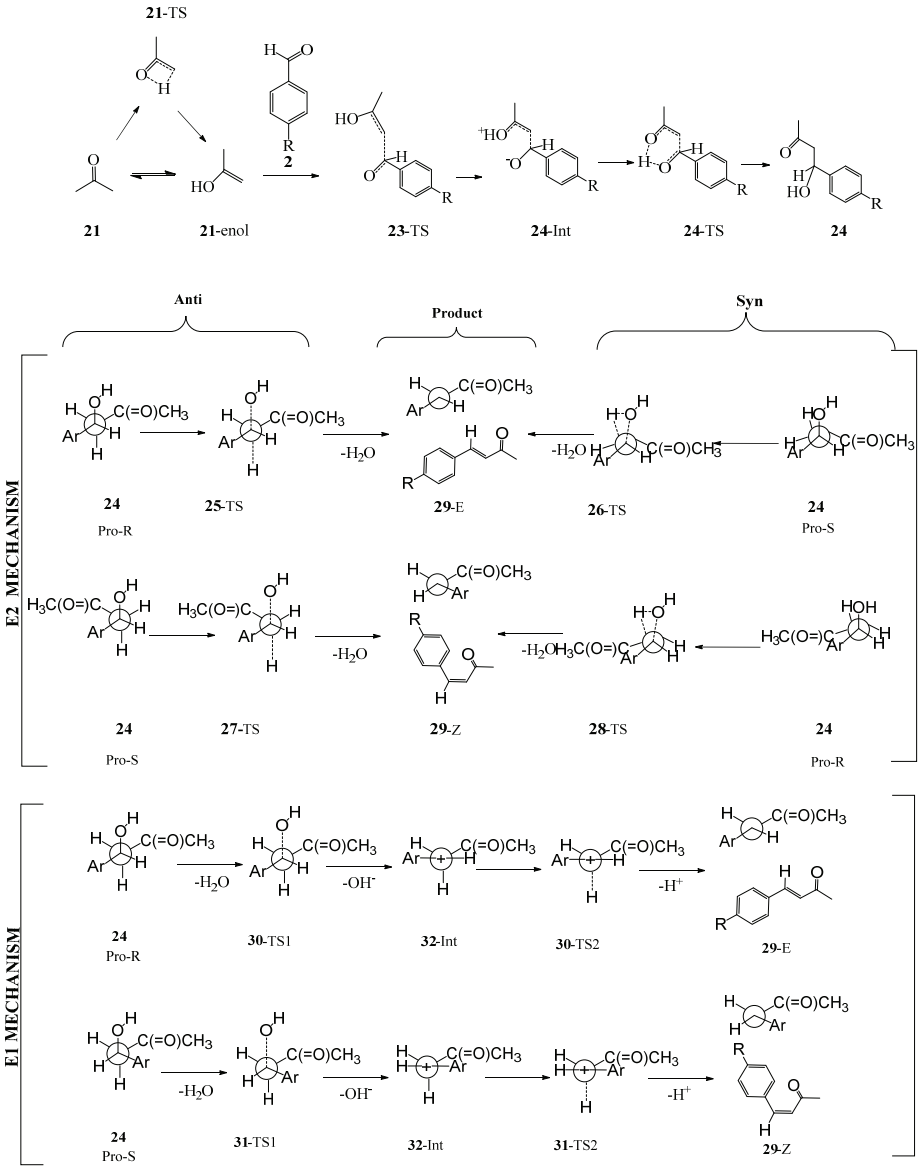
Atom	*x* / Å	*y* / Å	*z* / Å
H	-4.33331900	0.93639600	-0.20078200
H	-2.83469900	-1.97583800	-0.65489800
N	6.17975100	-0.16723100	0.04735700
O	6.74971700	0.87001600	-0.14674500
O	6.74991500	-1.19775400	0.27394900



Scheme S-1. Mechanism of multicomponent domino Knoevenagel/Diels–Alder reaction.



Scheme S-2. Mechanism of knoevenagel reaction to produce dienophile **8**.



Scheme S-3. Mechanism of aldol reaction to produce compound **22**.

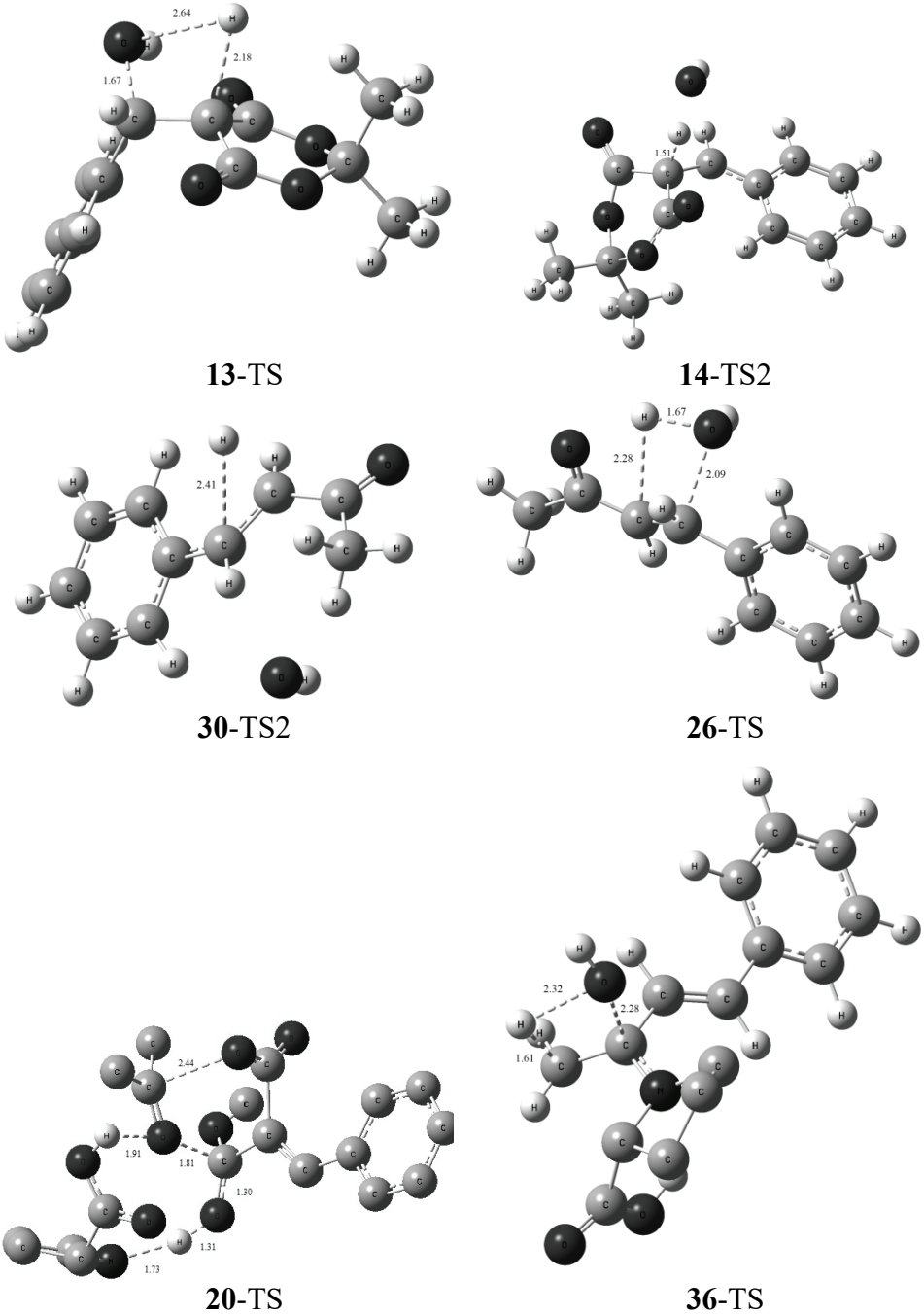


Fig. S-1. Optimized structures of selected transition states involved in Knoevenagel step of reaction (Bond lengths in Å).