

## Effect of water content on the homogeneous catalytic process of N-vinyl pyrrolidone synthesis from acetylene

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### 1. Solvent model parameter customisation

The SMD model in Gaussian supports custom solvent parameters. In this study, the pure liquid-phase reactant 2-pyrrolidone is treated as the solvent in the calculation process. Eps and epsinf correspond to the static and dynamic dielectric constant of 2-pyrrolidone, respectively, and the value of epsinf can be approximated as the square of the refractive index ( $n_{20/D}=1.487(\text{lit.})$ ). See the Table S1. for solvent parameter settings.

**Table S1.** 2-Pyrrolidone SMD model parameterisation

2-Pyrrolidone SMD Model Custom Parameters	
eps	28.173 <sup>1</sup>
epsinf	2.211169

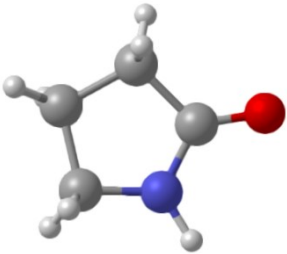
### 2. Resonance Correction Factor Setting in Shermo Programs

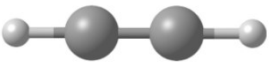
Geometry optimization and frequency calculation were performed at the B3LYP/6-311G\*\* level, and the corresponding thermodynamic correction amounts were obtained. The resonance correction factors<sup>2</sup> at this level were defined within the Shermo program as follows.

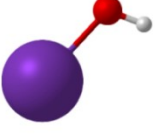
sclZPE= 0.9888 //Frequency scale factor for ZPE

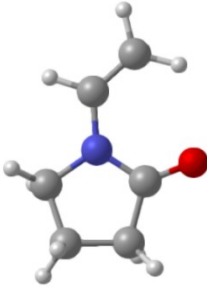
sclheat= 1.0062 //Frequency scale factor for U(T)-U(0) (the same as that for H(T)-H(0))  
 sclS= 1.0104 //Frequency scale factor for S(T)

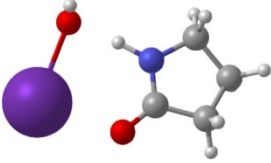
### 3. XYZ Coordinates of the Computed Structures

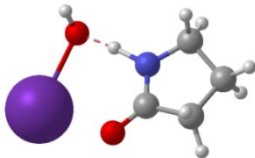
Compound	XYZ Coordinates			
2P	0 1			
	C	-1.32829400	-0.81380400	0.12416100
	C	0.89092000	-0.00211200	-0.00510500
	C	-0.00768500	1.21727700	0.14135500
	C	-1.41337600	0.69248200	-0.18826000
	H	-1.93346500	-1.42317700	-0.54914200
	H	-1.63362100	-1.03627500	1.15278500
	H	0.07235700	1.56444400	1.17800300
	H	0.33488600	2.02862900	-0.50290700
	H	-2.20441300	1.18353100	0.37969700
	H	-1.62356800	0.83425300	-1.25155400
	N	0.09581100	-1.09141200	-0.06036600
	O	2.12290100	-0.00628600	-0.04736700
	H	0.48455400	-2.02428900	-0.03829100
	E = -286.6343098 a.u.			

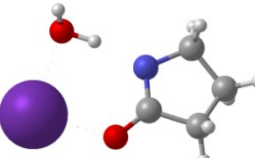
Compound	XYZ Coordinates			
C <sub>2</sub> H <sub>2</sub>	0 1			
	C	0.00000000	0.00000000	0.60034500
	C	0.00000000	0.00000000	-0.60034500
	H	0.00000000	0.00000000	1.66881200
	H	0.00000000	0.00000000	-1.66881200
E = -77.3268891 a.u.				

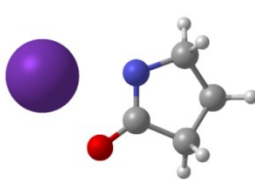
Compound	XYZ Coordinates			
KOH	0 1			
	K	0.03199300	-0.77785200	0.00000000
	O	0.03199300	1.60179800	0.00000000
	H	-0.86382000	1.96481500	0.00000000
E = -675.7955274 a.u.				

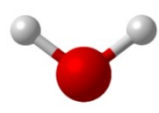
Compound	XYZ Coordinates			
NVP	0 1			
	C	-0.85301600	-1.39429800	0.13791500
	C	-0.18041500	0.87081800	0.01393900
	C	-1.69277200	0.86347100	0.13277900
	C	-2.09319000	-0.57053100	-0.23098900
	H	-0.69264700	-2.24768000	-0.52221700
	H	-0.89354800	-1.75916100	1.16963700
	H	-1.94538600	1.11115700	1.17076200
	H	-2.12974400	1.63424500	-0.50389200
	H	-2.98370600	-0.91878800	0.29325800
	H	-2.28067800	-0.64519600	-1.30522100
	N	0.25554100	-0.42935000	-0.00278900
	O	0.53836200	1.86472900	-0.03638900
	C	2.70248600	-0.13647900	-0.03571200
	C	1.58554800	-0.87038200	-0.00332000
	H	2.70880400	0.94305000	-0.06285900
	H	1.65273300	-1.95359600	0.02118600
H	3.65664700	-0.65200300	-0.03769200	
E = -364.0191048 a.u.				

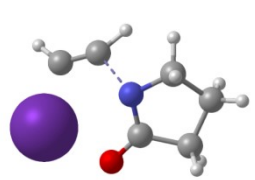
Compound	XYZ Coordinates			
2P • • • KOH	0 1			
	K	-2.68842100	-0.44877500	-0.07472100
	O	-1.67958000	1.83553300	0.01513600
	H	-1.71527800	2.16101200	0.92493800
	C	2.03198300	1.25479800	0.03766600
	C	0.72841800	-0.68444900	0.04899600
	C	2.17101500	-1.15343300	0.17859400
	C	2.98880600	0.07773500	-0.23748800
	H	2.13889300	2.06673800	-0.68523800
	H	2.18638300	1.67822000	1.03791700
	H	2.34164300	-1.43177000	1.22553900
	H	2.34951600	-2.04287800	-0.42862800
	H	3.93297100	0.17739300	0.30036600
	H	3.21455100	0.03020300	-1.30641700
	N	0.70564500	0.64537500	-0.05794800
	O	-0.27143500	-1.43430300	0.06433300
	H	-0.22140100	1.19243500	-0.04550200
E = -962.4558781 a.u.				

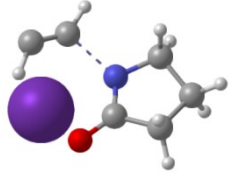
Compound	XYZ Coordinates			
2P+KOH (TS)	0 1			
	K	-2.67860000	-0.43256200	-0.08096800
	O	-1.53708300	1.83874300	0.01894100
	H	-1.61170300	2.23778500	0.89507400
	C	2.01869900	1.22589300	0.03374000
	C	0.69830600	-0.66870800	0.05760800
	C	2.13497900	-1.17329700	0.17643700
	C	2.96656800	0.04188500	-0.25115300
	H	2.13693400	2.04213800	-0.68481200
	H	2.19685200	1.64805200	1.03257800
	H	2.31439800	-1.45427500	1.22173300
	H	2.28974000	-2.06770200	-0.43121100
	H	3.91999300	0.13200100	0.27371600
	H	3.17888600	-0.01050600	-1.32326500
	N	0.67324300	0.65268900	-0.04445100
	O	-0.30730800	-1.42950900	0.07889800
	H	-0.40058200	1.29385100	-0.01677500
E = -962.4557379a.u.				

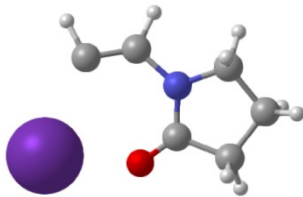
Compound	XYZ Coordinates			
2PK+H2O	0 1			
	K	-2.66204900	-0.52135900	-0.13759000
	O	-1.70826100	1.88920900	0.07910600
	H	-1.79670100	2.33709000	0.92884300
	C	2.08582000	1.22006500	-0.01858300
	C	0.72755500	-0.60621300	0.10585900
	C	2.15417200	-1.16306100	0.19842000
	C	3.00322900	0.00882400	-0.30023800
	H	2.20984500	2.01687900	-0.76033600
	H	2.31941100	1.66789600	0.95980500
	H	2.36475700	-1.41388300	1.24634000
	H	2.25966300	-2.08384100	-0.38117700
	H	3.98020100	0.09271700	0.18298700
	H	3.17238300	-0.08466900	-1.37808600
	N	0.71294300	0.70301800	-0.02791100
	O	-0.29041600	-1.37027900	0.17870500
	H	-0.75645200	1.54336800	0.03597700
E = -962.4594199 a.u.				

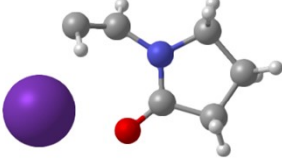
Compound	XYZ Coordinates			
2PK	0 1			
	C	-1.48301400	-1.34731800	0.12955900
	C	-0.33969600	0.61110400	0.02021400
	C	-1.81407100	1.02482700	0.11994900
	C	-2.54258200	-0.27653200	-0.22471600
	H	-1.54780900	-2.22578100	-0.52318900
	H	-1.63297100	-1.71609300	1.15700000
	H	-2.01702000	1.35860200	1.14603600
	H	-2.03797400	1.86495800	-0.54288000
	H	-3.48702400	-0.41705200	0.30790400
	H	-2.75800300	-0.31006600	-1.29796600
	N	-0.17523600	-0.69451400	0.00812900
	O	0.60190900	1.47629200	-0.01862200
	K	2.47201900	-0.29346300	-0.02236100
	E = -886.0061721 a.u.			

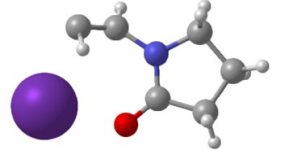
Compound	XYZ Coordinates			
H2O	0 1			
	O	0.00000000	0.00000000	0.11725200
	H	0.00000000	0.76524400	-0.46900900
	H	0.00000000	-0.76524400	-0.46900900
E = -76.4373134 a.u.				

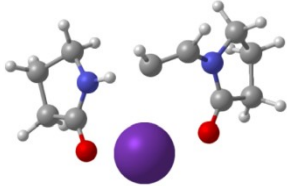
Compound	XYZ Coordinates			
2PK+C <sub>2</sub> H <sub>2</sub> (TS1)	0 1			
	C	1.62783900	0.83612100	0.99367000
	C	0.64226700	-0.70398800	-0.38788000
	C	2.14069100	-1.00579300	-0.44939000
	C	2.76834700	0.26911000	0.12123900
	H	1.63638000	1.93194100	1.03586200
	H	1.70925800	0.48355800	2.03009700
	H	2.34684200	-1.88586600	0.17232200
	H	2.44368200	-1.25210700	-1.47024300
	H	3.68731500	0.09745200	0.68638400
	H	2.99840900	0.96848900	-0.68871900
	N	0.37695600	0.34974700	0.40048800
	O	-0.22533200	-1.39275900	-0.98101800
	K	-2.19287100	-0.72442200	0.58554700
	C	-1.80532800	1.64716100	-0.88354000
	C	-0.65231400	1.84263600	-0.43498900
	H	-2.50396200	2.31054100	-1.37564700
	H	0.18158300	2.49236600	-0.22537600
	E = -963.2995319 a.u.			

Compound	XYZ Coordinates			
2PK+ C <sub>2</sub> H <sub>2</sub> (TS2)	0 1			
	C	1.68939000	1.01041000	-0.77893100
	C	0.62755200	-0.60782000	0.46338100
	C	2.11884800	-0.86592200	0.65673400
	C	2.74420300	-0.08115700	-0.50113400
	H	1.65628300	1.30395400	-1.83238700
	H	1.90329400	1.91743400	-0.19662700
	H	2.41016200	-0.46202100	1.63515900
	H	2.34424600	-1.93449900	0.66266800
	H	3.72799900	0.33561200	-0.27419800
	H	2.84809100	-0.72893300	-1.37697800
	N	0.40726500	0.42665400	-0.35426900
	O	-0.28237100	-1.28381300	1.01322300
	K	-2.15131800	-0.73410700	-0.70655500
	C	-1.67684900	1.66593400	1.21387900
	C	-0.87133000	1.78835000	0.24381100
	H	-1.82880300	0.83764100	1.89630300
	H	-0.56900800	2.50399400	-0.50175200
E = -963.3038542 a.u.				

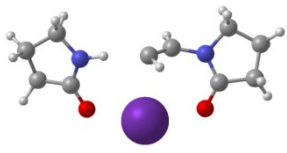
Compound	XYZ Coordinates			
NVPK1	0 1			
	C	2.27326300	0.89270300	0.28170500
	C	0.58463300	-0.67217600	-0.15759000
	C	1.84850100	-1.46494000	0.13560500
	C	2.97572200	-0.43893300	-0.01050800
	H	2.66782200	1.72422900	-0.30629400
	H	2.33886200	1.17154600	1.34023300
	H	1.77233300	-1.85226600	1.15926400
	H	1.92417300	-2.32429000	-0.53338500
	H	3.81820300	-0.61525000	0.65984600
	H	3.35383800	-0.44186900	-1.03641200
	N	0.86487200	0.64655100	-0.07588800
	O	-0.51305400	-1.19433300	-0.41578900
	K	-2.87900100	-0.50633300	0.13996300
	C	-1.33380600	1.81793700	0.06812500
	C	-0.02046800	1.78358700	-0.21125800
	H	-1.67279800	2.84762100	-0.15650400
	H	0.58183600	2.63033200	-0.56498600
E = -963.3425254 a.u.				

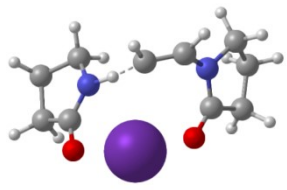
Compound	XYZ Coordinates			
NVPK2	0 1			
	C	2.18527200	1.04792700	-0.07281400
	C	0.63835900	-0.71505500	0.08255000
	C	2.01150600	-1.33663000	0.26986500
	C	2.97855700	-0.25910500	-0.23951700
	H	2.36520200	1.76563400	-0.87711500
	H	2.40127900	1.54964600	0.87768100
	H	2.14524600	-1.54273000	1.33870500
	H	2.07782500	-2.28953400	-0.25800700
	H	3.92594000	-0.23596200	0.30074900
	H	3.19807200	-0.42617000	-1.29725900
	N	0.78163800	0.61217500	-0.09064200
	O	-0.43667700	-1.34295000	0.09666700
	K	-2.83511000	-0.42343400	-0.17074100
	C	-1.31232100	1.77430000	0.63803700
	C	-0.31144500	1.56414100	-0.23249300
	H	-1.15457500	1.12161700	1.52411100
	H	-0.20951600	2.10765300	-1.17739300
E = -963.3387505 a.u.				

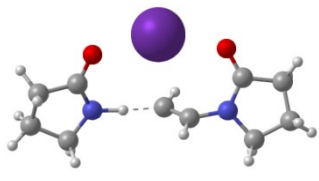
Compound	XYZ Coordinates			
NVPK2	0 1			
	C	2.18527200	1.04792700	-0.07281400
	C	0.63835900	-0.71505500	0.08255000
	C	2.01150600	-1.33663000	0.26986500
	C	2.97855700	-0.25910500	-0.23951700
	H	2.36520200	1.76563400	-0.87711500
	H	2.40127900	1.54964600	0.87768100
	H	2.14524600	-1.54273000	1.33870500
	H	2.07782500	-2.28953400	-0.25800700
	H	3.92594000	-0.23596200	0.30074900
	H	3.19807200	-0.42617000	-1.29725900
	N	0.78163800	0.61217500	-0.09064200
	O	-0.43667700	-1.34295000	0.09666700
	K	-2.83511000	-0.42343400	-0.17074100
	C	-1.31232100	1.77430000	0.63803700
	C	-0.31144500	1.56414100	-0.23249300
	H	-1.15457500	1.12161700	1.52411100
	H	-0.20951600	2.10765300	-1.17739300
E = -963.3387505 a.u.				

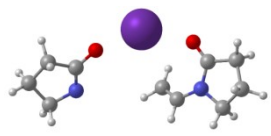
Compound	XYZ Coordinates			
NVPK1 • • • 2P 	0 1			
	C	-3.15458400	-1.58842600	0.54538500
	C	-2.31673200	0.28521500	-0.59217400
	C	-3.21210600	-0.45304000	-1.57431600
	C	-3.39273700	-1.84080800	-0.95022800
	H	-2.67304400	-2.42827200	1.04976600
	H	-4.08669600	-1.36100800	1.07745200
	H	-4.15663900	0.10021000	-1.63734300
	H	-2.76625300	-0.45852700	-2.57050800
	H	-4.37232600	-2.28044900	-1.14151300
	H	-2.63176400	-2.52503300	-1.33378800
	N	-2.26895700	-0.41145400	0.56510900
	O	-1.77077700	1.37355300	-0.83004000
	K	0.27727900	2.57313900	0.13192900
	C	-0.42105100	0.44286900	1.97167800
	C	-1.67823300	0.00123500	1.81977800
	H	-0.27304800	0.66817000	3.04411400
	H	-2.41389000	-0.14421200	2.62091800
	C	2.50102100	-1.92607500	0.61124300
	C	2.68291300	0.16966500	-0.42425300
	C	3.78240300	-0.69094300	-1.02853000
	C	3.88949300	-1.87754100	-0.05831400
	H	2.54510900	-2.23748100	1.65685500
	H	1.82113200	-2.60669600	0.08518900
	H	3.45185000	-0.99923200	-2.02730700
	H	4.70338200	-0.11781700	-1.14695600
	H	4.14324000	-2.81830400	-0.54822300
	H	4.65265700	-1.67110600	0.69654100
	N	2.02979200	-0.54527600	0.49816300
	O	2.42274100	1.34282800	-0.75461700
	H	1.16410000	-0.17672900	0.98091300
	E = -1249.9971186 a.u.			

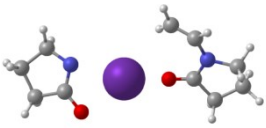


Compound	XYZ Coordinates			
NVPK2 • • • 2P	0 1			
	C	-3.55125400	-1.81077300	-0.23719700
	C	-3.09698300	0.47439300	0.08578000
	C	-4.60867200	0.32800700	0.13603200
	C	-4.86890000	-1.05474900	-0.47651300
	H	-3.28372800	-2.47871000	-1.05986600
	H	-3.57220700	-2.40586300	0.68334100
	H	-4.91724900	0.38086100	1.18705700
	H	-5.09267500	1.15330900	-0.38900100
	H	-5.72346300	-1.57053000	-0.03639800
	H	-5.05036000	-0.95822800	-1.55014400
	N	-2.55056300	-0.74181900	-0.10914800
	O	-2.47963400	1.54602100	0.21290000
	K	0.09820000	2.00919800	0.09841200
	C	-0.23937600	-0.81323900	0.84467900
	C	-1.12655800	-1.03345300	-0.13715200
	H	-0.75274900	-0.38408000	1.72971400
	H	-0.85374900	-1.48275700	-1.09773200
	C	3.68388100	-1.82460200	0.26691500
	C	3.23355200	0.42429600	-0.21028900
	C	4.69289800	0.20297100	-0.58097900
	C	5.04652600	-1.12055100	0.11340300
	H	3.60870600	-2.41107500	1.18510600
	H	3.47506500	-2.49467900	-0.57561800
	H	4.75467100	0.12910200	-1.67329700
	H	5.30593800	1.05313700	-0.27603000
H	5.76383500	-1.72626500	-0.44236600	
H	5.46964700	-0.92032300	1.10154300	
N	2.73316800	-0.71284600	0.28184500	
O	2.60800800	1.49238600	-0.36418500	
H	1.70661800	-0.81705700	0.51719900	
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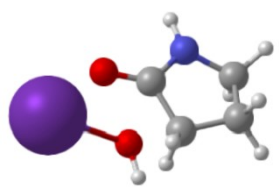
Compound	XYZ Coordinates			
NVPK1+2P (TS)  	0 1			
	C	-3.55125400	-1.81077300	-0.23719700
	C	-3.09698300	0.47439300	0.08578000
	C	-4.60867200	0.32800700	0.13603200
	C	-4.86890000	-1.05474900	-0.47651300
	H	-3.28372800	-2.47871000	-1.05986600
	H	-3.57220700	-2.40586300	0.68334100
	H	-4.91724900	0.38086100	1.18705700
	H	-5.09267500	1.15330900	-0.38900100
	H	-5.72346300	-1.57053000	-0.03639800
	H	-5.05036000	-0.95822800	-1.55014400
	N	-2.55056300	-0.74181900	-0.10914800
	O	-2.47963400	1.54602100	0.21290000
	K	0.09820000	2.00919800	0.09841200
	C	-0.23937600	-0.81323900	0.84467900
	C	-1.12655800	-1.03345300	-0.13715200
	H	-0.75274900	-0.38408000	1.72971400
	H	-0.85374900	-1.48275700	-1.09773200
	C	3.68388100	-1.82460200	0.26691500
	C	3.23355200	0.42429600	-0.21028900
	C	4.69289800	0.20297100	-0.58097900
	C	5.04652600	-1.12055100	0.11340300
	H	3.60870600	-2.41107500	1.18510600
	H	3.47506500	-2.49467900	-0.57561800
	H	4.75467100	0.12910200	-1.67329700
	H	5.30593800	1.05313700	-0.27603000
	H	5.76383500	-1.72626500	-0.44236600
	H	5.46964700	-0.92032300	1.10154300
	N	2.73316800	-0.71284600	0.28184500
	O	2.60800800	1.49238600	-0.36418500
	H	1.70661800	-0.81705700	0.51719900
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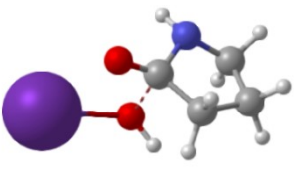
Compound	XYZ Coordinates			
	0 1			
	C	-3.55125400	-1.81077300	-0.23719700
	C	-3.09698300	0.47439300	0.08578000
	C	-4.60867200	0.32800700	0.13603200
	C	-4.86890000	-1.05474900	-0.47651300
	H	-3.28372800	-2.47871000	-1.05986600
	H	-3.57220700	-2.40586300	0.68334100
	H	-4.91724900	0.38086100	1.18705700
	H	-5.09267500	1.15330900	-0.38900100
	H	-5.72346300	-1.57053000	-0.03639800
	H	-5.05036000	-0.95822800	-1.55014400
	N	-2.55056300	-0.74181900	-0.10914800
	O	-2.47963400	1.54602100	0.21290000
	K	0.09820000	2.00919800	0.09841200
	C	-0.23937600	-0.81323900	0.84467900
	C	-1.12655800	-1.03345300	-0.13715200
	H	-0.75274900	-0.38408000	1.72971400
	H	-0.85374900	-1.48275700	-1.09773200
	C	3.68388100	-1.82460200	0.26691500
	C	3.23355200	0.42429600	-0.21028900
	C	4.69289800	0.20297100	-0.58097900
	C	5.04652600	-1.12055100	0.11340300
	H	3.60870600	-2.41107500	1.18510600
	H	3.47506500	-2.49467900	-0.57561800
	H	4.75467100	0.12910200	-1.67329700
	H	5.30593800	1.05313700	-0.27603000
	H	5.76383500	-1.72626500	-0.44236600
	H	5.46964700	-0.92032300	1.10154300
	N	2.73316800	-0.71284600	0.28184500
	O	2.60800800	1.49238600	-0.36418500
	H	1.70661800	-0.81705700	0.51719900
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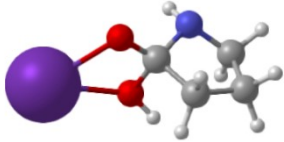
Compound	XYZ Coordinates			
NVP • • • 2PK(1)	0 1			
	C	3.87042500	1.73797700	-0.42090900
	C	3.14174500	-0.45429500	0.08630800
	C	4.52055300	-0.58486400	-0.52584400
	C	4.75740800	0.76638900	-1.21208600
	H	3.42010300	2.51503700	-1.04097900
	H	4.41120000	2.22327500	0.39757300
	H	5.23061900	-0.76395800	0.29037500
	H	4.56159600	-1.44740000	-1.19246500
	H	5.80281700	1.07552700	-1.20771300
	H	4.42124700	0.72071400	-2.25085900
	N	2.81649600	0.86903400	0.13823500
	O	2.42717400	-1.38369600	0.47126300
	K	-0.10369200	-2.00376300	0.27787800
	C	0.88093500	0.92462500	1.64084900
	C	1.63167900	1.42165300	0.65542400
	H	1.15541000	0.04171900	2.20531700
	H	1.35137200	2.34742700	0.16074900
	C	-4.57631000	1.65106000	0.11315400
	C	-3.27668200	-0.17396000	-0.18691400
	C	-4.56096700	-0.47244000	-0.97890300
	C	-5.53778400	0.56214100	-0.41762600
	H	-4.97558300	2.15834200	0.99932800
	H	-4.42660900	2.43694600	-0.64457600
H	-4.36233200	-0.32114900	-2.04860600	
H	-4.87523200	-1.51284200	-0.85543100	
H	-6.26026700	0.94334400	-1.14515100	
H	-6.10324200	0.12896200	0.41475700	
N	-3.30404800	0.98689700	0.41654500	
O	-2.30721400	-1.01279300	-0.18163200	
H	-0.03379000	1.43624300	1.91677300	
E = -1250.0346495 a.u.				

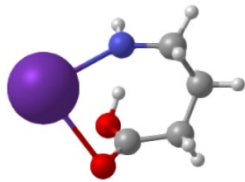
Compound	XYZ Coordinates			
NVP • • • 2PK(2)	0 1			
	C	-3.55125400	-1.81077300	-0.23719700
	C	-3.09698300	0.47439300	0.08578000
	C	-4.60867200	0.32800700	0.13603200
	C	-4.86890000	-1.05474900	-0.47651300
	H	-3.28372800	-2.47871000	-1.05986600
	H	-3.57220700	-2.40586300	0.68334100
	H	-4.91724900	0.38086100	1.18705700
	H	-5.09267500	1.15330900	-0.38900100
	H	-5.72346300	-1.57053000	-0.03639800
	H	-5.05036000	-0.95822800	-1.55014400
	N	-2.55056300	-0.74181900	-0.10914800
	O	-2.47963400	1.54602100	0.21290000
	K	0.09820000	2.00919800	0.09841200
	C	-0.23937600	-0.81323900	0.84467900
	C	-1.12655800	-1.03345300	-0.13715200
	H	-0.75274900	-0.38408000	1.72971400
	H	-0.85374900	-1.48275700	-1.09773200
	C	3.68388100	-1.82460200	0.26691500
	C	3.23355200	0.42429600	-0.21028900
	C	4.69289800	0.20297100	-0.58097900
	C	5.04652600	-1.12055100	0.11340300
	H	3.60870600	-2.41107500	1.18510600
	H	3.47506500	-2.49467900	-0.57561800
	H	4.75467100	0.12910200	-1.67329700
H	5.30593800	1.05313700	-0.27603000	
H	5.76383500	-1.72626500	-0.44236600	
H	5.46964700	-0.92032300	1.10154300	
N	2.73316800	-0.71284600	0.28184500	
O	2.60800800	1.49238600	-0.36418500	
H	1.70661800	-0.81705700	0.51719900	
E = -1250.0410943 a.u.				

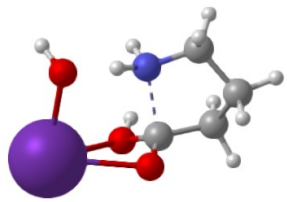
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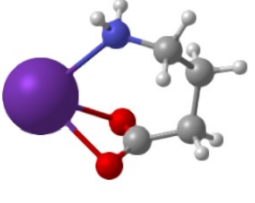
Compound	XYZ Coordinates			
2P • • • KOH	0 1			
	C	-2.22264000	0.64361500	-0.78211300
	C	-0.59303900	-0.87618500	-0.04549900
	C	-1.26968800	-0.33541200	1.20208800
	C	-2.56436800	0.30394200	0.67800700
	H	-1.74156100	1.62413600	-0.86275500
	H	-3.08296500	0.61179600	-1.45150800
	H	-1.41079500	-1.12005700	1.94725900
	H	-0.59124000	0.41508400	1.62085100
	H	-3.38215400	-0.42114500	0.70690100
	H	-2.87116900	1.18527600	1.24239300
	N	-1.25276200	-0.40303700	-1.11762200
	O	0.41149500	-1.60315400	-0.07937200
	K	2.58545500	-0.11346800	0.01749800
	O	1.15781000	1.92829800	-0.02878200
	H	-0.85171700	-0.48938800	-2.04261500
	H	0.92126400	2.15453000	0.88069000
	E = -962.4469941 a.u.			

Compound	XYZ Coordinates			
2P+KOH (ts1)	0 1			
	C	-2.30680500	-0.91549400	-0.00678500
	C	-0.31713300	0.22739400	0.47587300
	C	-1.19836400	1.25631100	-0.25443000
	C	-2.51708200	0.51271400	-0.56412000
	H	-2.01193000	-1.60662600	-0.80558200
	H	-3.20653700	-1.31465300	0.46804000
	H	-1.36085600	2.09259700	0.43310600
	H	-0.69467700	1.65521200	-1.13514900
	H	-3.35914000	0.99566100	-0.06267200
	H	-2.74965500	0.48685600	-1.63090500
	N	-1.23360000	-0.73989500	0.97377500
	O	0.68883500	0.55968100	1.18098300
	K	2.72763400	-0.05183100	-0.15965800
	O	0.44051100	-0.64219900	-0.98427600
	H	-0.77205900	-1.59867100	1.25303100
	H	-0.03345700	-0.37173300	-1.77969000
	E = -962.426424 a.u.			

Compound	XYZ Coordinates			
intermediate	0 1			
	C	-2.39717800	-0.80426700	-0.25466700
	C	-0.26791300	0.01877300	0.37365500
	C	-1.14853300	1.27106900	0.09206400
	C	-2.54056000	0.73401500	-0.31357000
	H	-2.18939100	-1.21238400	-1.25596800
	H	-3.30578300	-1.29338200	0.10718000
	H	-1.19790000	1.84903300	1.01816400
	H	-0.68823400	1.90732500	-0.66742100
	H	-3.30454900	1.06973000	0.39223400
	H	-2.85539300	1.06365900	-1.30682200
	N	-1.28311300	-1.00482600	0.67785200
	O	0.71420300	0.11329500	1.23631000
	K	2.78350000	0.02559200	-0.17043100
	O	0.39047600	-0.36914000	-0.99108700
	H	-0.86648200	-1.92684000	0.58280300
	H	-0.20931700	-0.18039400	-1.72362000
E = -962.4328818 a.u.				

Compound	XYZ Coordinates			
ts2	0 1			
	C	-1.44123700	1.56132900	-0.33924800
	C	-0.22070500	-1.21923500	0.02393100
	C	-1.63598800	-0.97297400	-0.43745300
	C	-2.30202000	0.33030800	0.02481900
	H	-2.03373900	2.46216600	-0.08584800
	H	-1.35708300	1.57538800	-1.44038100
	H	-1.62182500	-1.02753800	-1.52903000
	H	-2.21252100	-1.83761900	-0.08226800
	H	-3.29904600	0.38268800	-0.43463200
	H	-2.46063700	0.30942800	1.11123400
	N	-0.11285800	1.53483200	0.25120900
	O	0.63752900	-1.71275100	-0.68947500
	K	2.22245500	0.50226200	-0.15774500
	O	0.06811800	-1.05001900	1.35134700
	H	-0.20875200	1.91767700	1.19870700
	H	-0.28850400	-0.16340100	1.57364000
E = -962.3929261 a.u.				

Compound	XYZ Coordinates			
ts2 H <sub>2</sub> O	0 1			
	C	-1.95006500	1.43258300	0.10009600
	C	-0.57169400	-0.86360700	0.00234500
	C	-2.09288900	-1.01582100	0.02062500
	C	-2.64199700	0.25447100	-0.62691100
	H	-2.56557600	1.77479600	0.93473600
	H	-1.79369900	2.28072900	-0.56934600
	H	-2.35769900	-1.91857100	-0.53586900
	H	-2.45938100	-1.11862300	1.04749000
	H	-2.37868000	0.25620400	-1.68810800
	H	-3.72885800	0.32549300	-0.55161100
	N	-0.65576900	0.93729500	0.61287400
	O	0.04203300	-0.87830000	-1.09348200
	K	2.47095800	-0.39344100	-0.18846300
	O	0.13709400	-1.49052700	1.04776600
	H	-0.63354800	0.94526500	1.62849400
	H	-0.38812700	-1.49373200	1.85962000
	O	1.73300500	2.01998100	-0.06405200
	H	1.96675000	2.37302200	0.80348000
H	0.22381600	1.43473100	0.26300700	
E = -1038.8699275 a.u.				

Compound	XYZ Coordinates				
potassium 4-aminobutyrate	0 1				
	C	-1.68527400	1.33721700	-0.37044200	
	C	-0.05113400	-1.30677600	-0.06088800	
	C	-1.57696300	-1.25269700	-0.10990200	
	C	-2.13376400	0.08953600	0.40198600	
	H	-2.45920300	2.11014400	-0.26671400	
	H	-1.61185000	1.10940000	-1.43885000	
	H	-1.91375800	-1.42476600	-1.13613600	
	H	-1.97897300	-2.05785500	0.51468000	
	H	-3.22691000	0.03828500	0.35764800	
	H	-1.87772100	0.21024900	1.46134600	
	N	-0.36632300	1.85242700	0.07276200	
	O	0.58413800	-1.26759600	-1.15523600	
	K	2.12088100	0.50780100	0.04468400	
	O	0.49680500	-1.31551600	1.08052000	
	H	-0.16910300	2.69992200	-0.45646600	
	H	-0.45969700	2.16062300	1.03935100	
	E = -962.475935 a.u.				



#### 4. Calculated solubility data

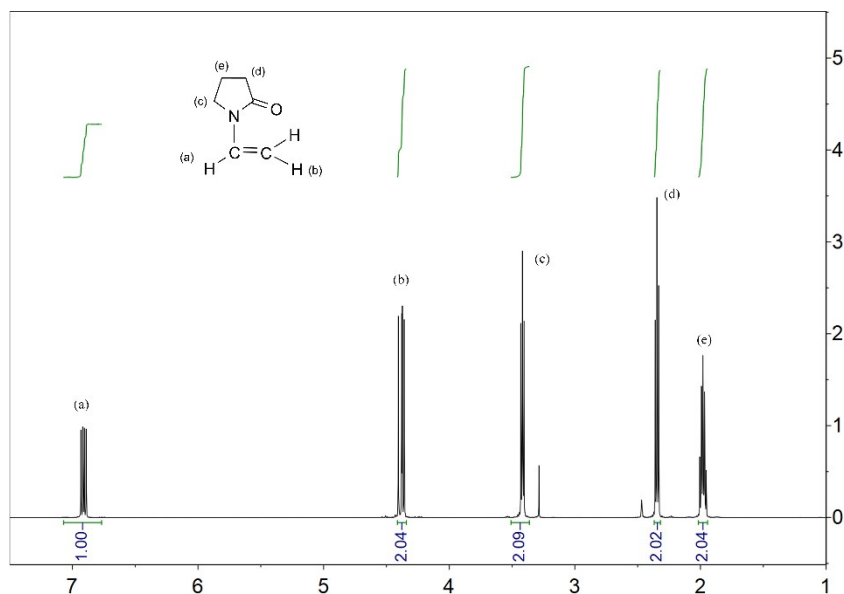
The solubilities of acetylene in 2-pyrrolidone, DMSO and NMP were obtained by COSMO-RS<sup>3</sup> calculations as shown in Table S2. The results show that the solubility of acetylene in DMSO and NMP is almost twice as much as in 2- pyrrolidone under the same conditions.

**Table S2.** Predicted acetylene solubility (P=0.1MPa)

T/K	Solvent	Acetylene solubility (mole fraction)
303.15	2- pyrrolidone	0.051
	DMSO	0.095
	NMP	0.105
423.15	2- pyrrolidone	0.006
	DMSO	0.008
	NMP	0.008

#### 5. <sup>1</sup>H NMR spectrum for product NVP

The purified product NVP is analyzed by <sup>1</sup>H NMR as shown in Fig. S1. There are four different methylene groups and one monohydrogen group in the compound, which is consistent with the structure of NVP. Also, there are few spurious peaks in the figure, which can prove the high purity of the product.



**Fig. S1** <sup>1</sup>H NMR spectrum for product NVP

## Reference

1. J. George and N. V. Sastry, *Journal of Chemical & Engineering Data*, 2004, **49**, 235-242.
2. D. O. Kashinski, G. M. Chase, R. G. Nelson, O. E. Di Nallo, A. N. Scales, D. L. VanderLey and E. F. Byrd, *J Phys Chem A*, 2017, **121**, 2265-2273.
3. A. Klamt, *J Phys Chem-Us*, 1995, **99**, 2224-2235.
4. C. Legault, CYLview20, Université de Sherbrooke, 2020.