ELECTRONIC SUPPORTING INFORMATION

Understanding Metastable Phase Transformation during Crystallization of RDX, HMX and CL-20: Experimental and DFT Studies

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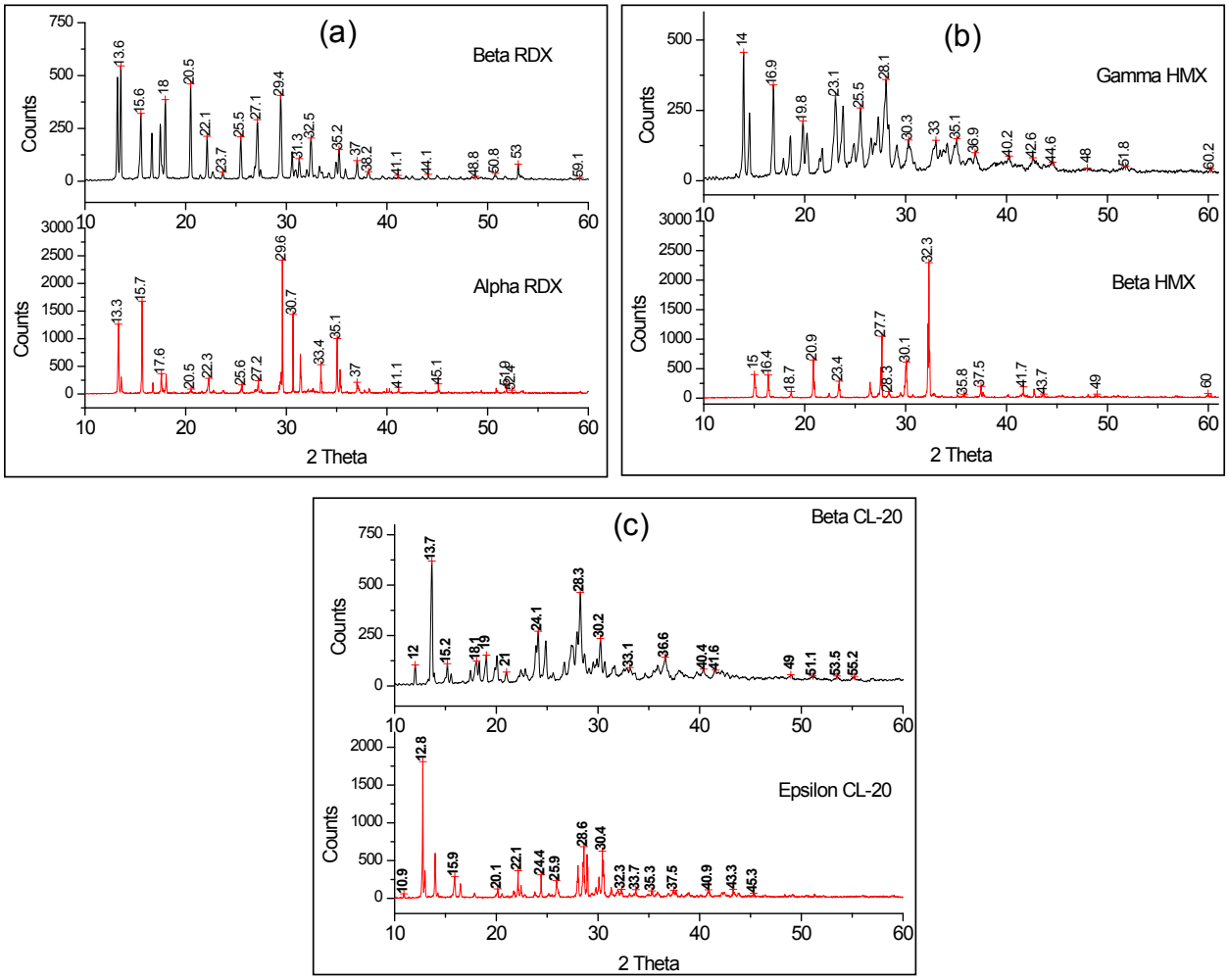


Figure S1 Powder XRD patterns of β- and α RDX (a), γ- and β HMX (b), and β- and ε CL-20 polymorphs (c).

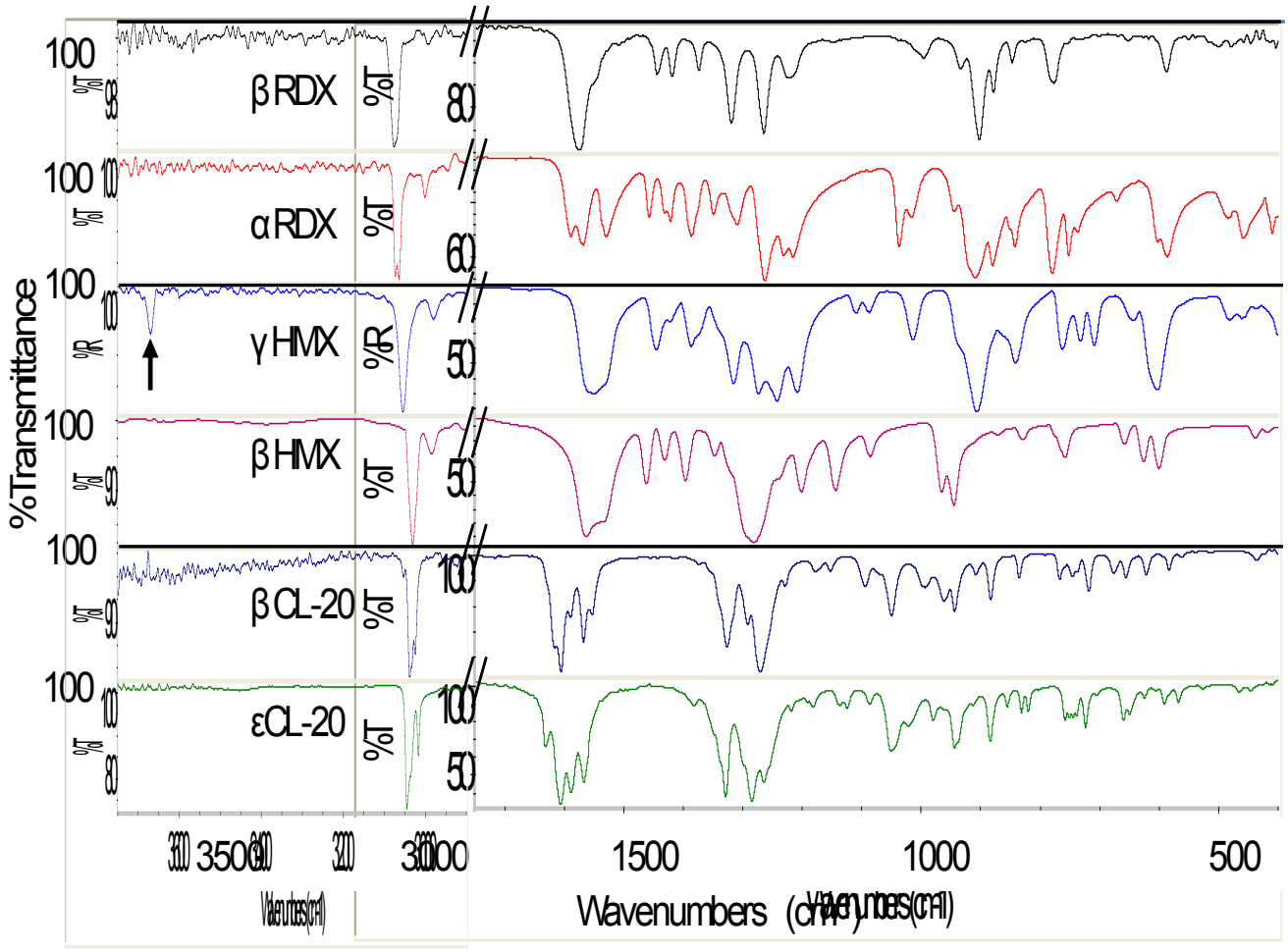


Figure S2 FTIR spectra of β- and α RDX; γ- and β HMX; and β- and ε CL-20 polymorphs. γ HMX show an absorption peak at 3670 cm^{-1}.

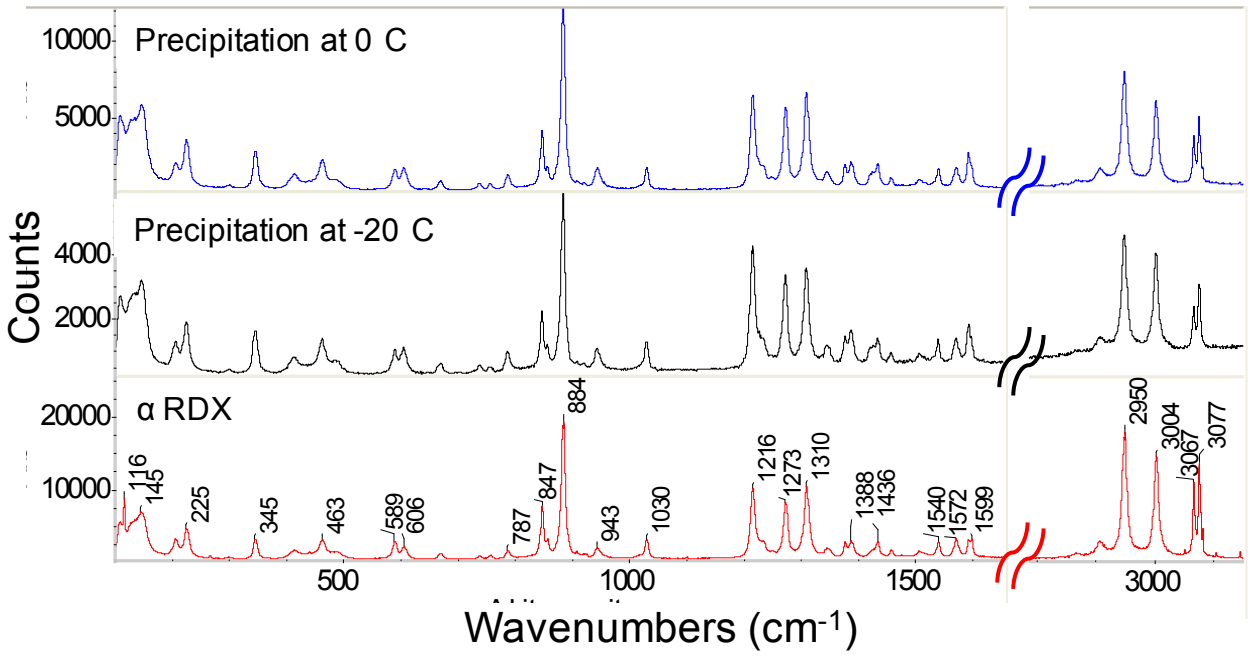


Figure S3 Raman spectra of RDX precipitated at 0 °C and -20 °C showing isolation of thermodynamic α phase

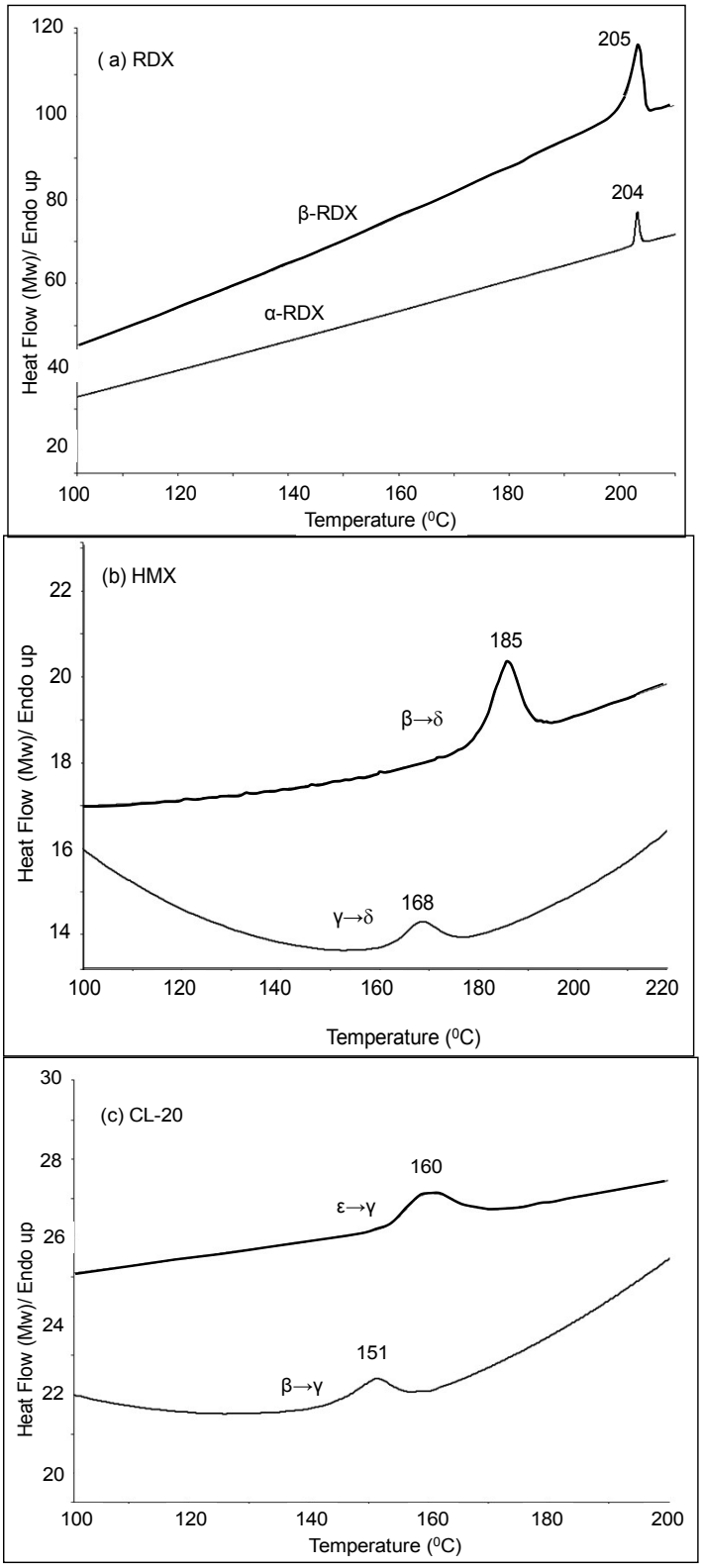


Figure S4 DSC profiles showing thermally assisted phase transformation of RDX, HMX and CL-20 polymorphs. RDX phases do not show solid-solid phase transformation, endotherm at 205 °C represents melting.

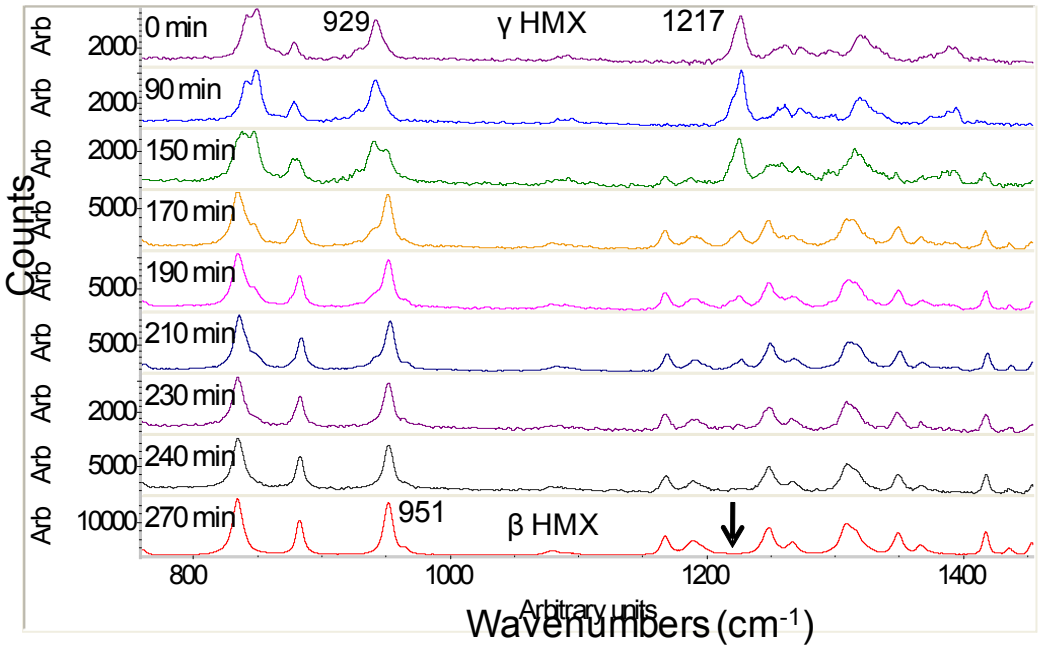


Figure S5 Raman spectral profiling of $\gamma \rightarrow \beta$ -HMX transformation in Ethylacetate/n-heptane system. The initial spectrum at 0 min matches well with that of γ phase and converts completely to β phase at 270th minute indicated by complete disappearence of Raman shift at 1217 cm^{-1}. This indicated considerably slower conversion rate in ethylacetate/ n-heptane system compared to that of acetone/ n-heptane system.

In situ Raman spectral profiling of prenucleation clustering during crystallization of RDX.

Methodologies: An slightly under saturated solution of RDX in acetone (2-3ml) was taken in an Aluminium cup and placed under Raman microscope objective. Sample was focussed with 20x objective to the bottom surface of the Al cup and was then irradiated with 514nm laser source. Higher penetration of visible laser sources throgh transperant liquid media and easy escape of Raman scattered lights form bulk media facilitated to extract conformational information at various stage of saturation. Single scan data acquisitions were affeteced at every 11sec interval. Total 31 spectras were collected till acetone was completely evaporated leaving back fine crystals α RDX crystals. While under scan, acetone slowly evaporated and a saturation level is reached followed by supersaturation. At this point, RDX strarted crystallization from the solution.

Schematic Experimenatl Setup:

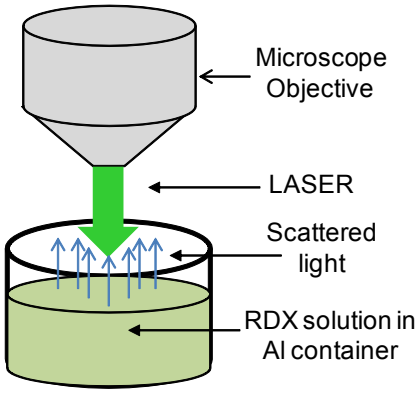
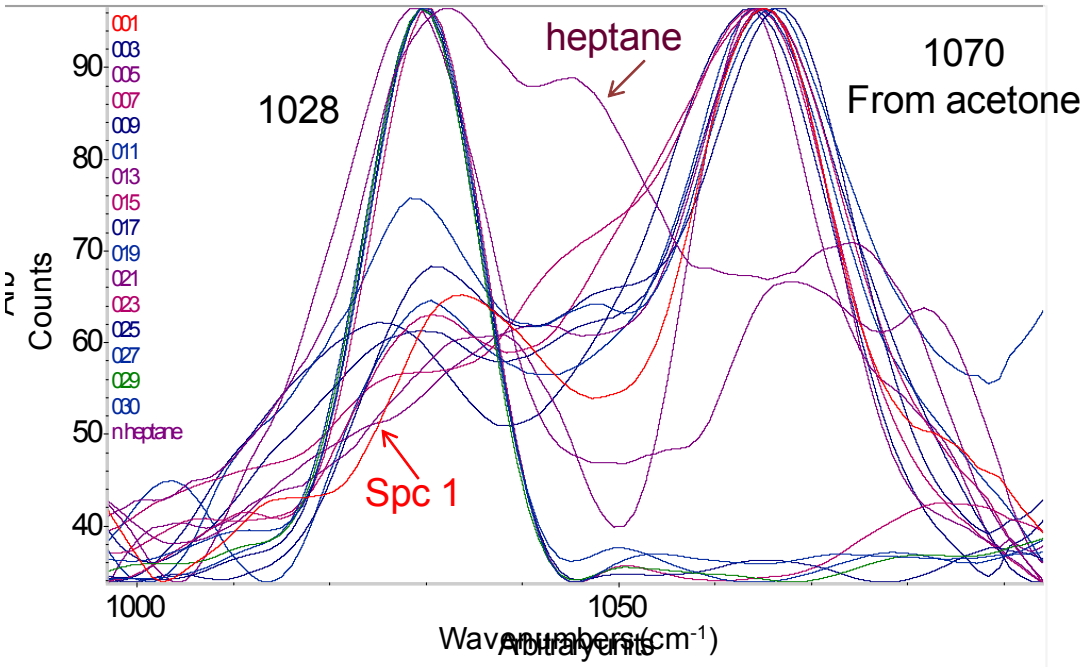
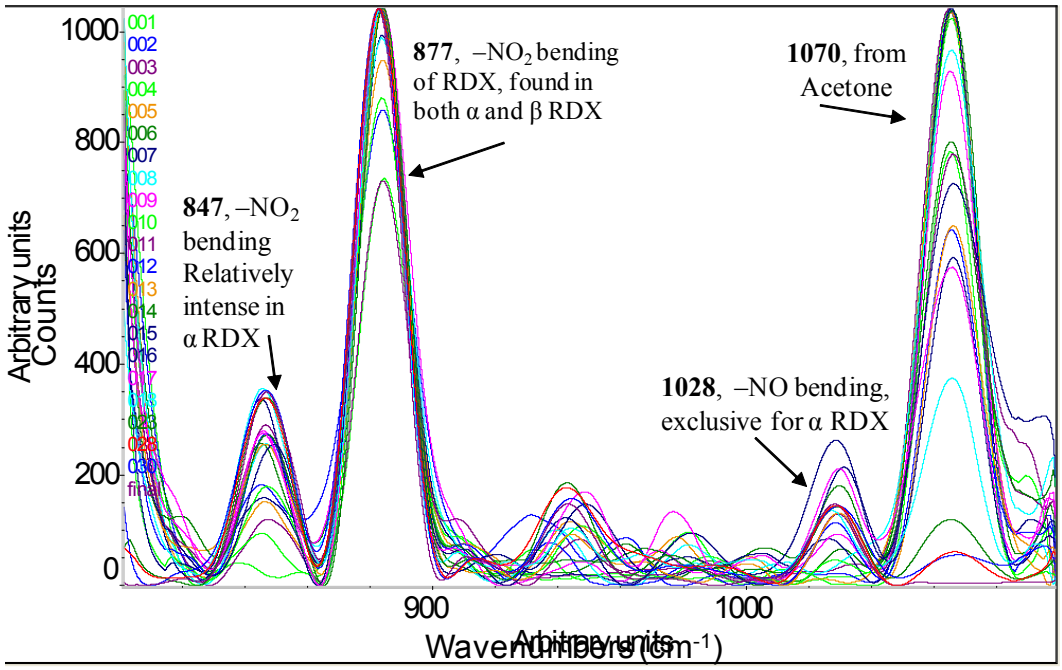
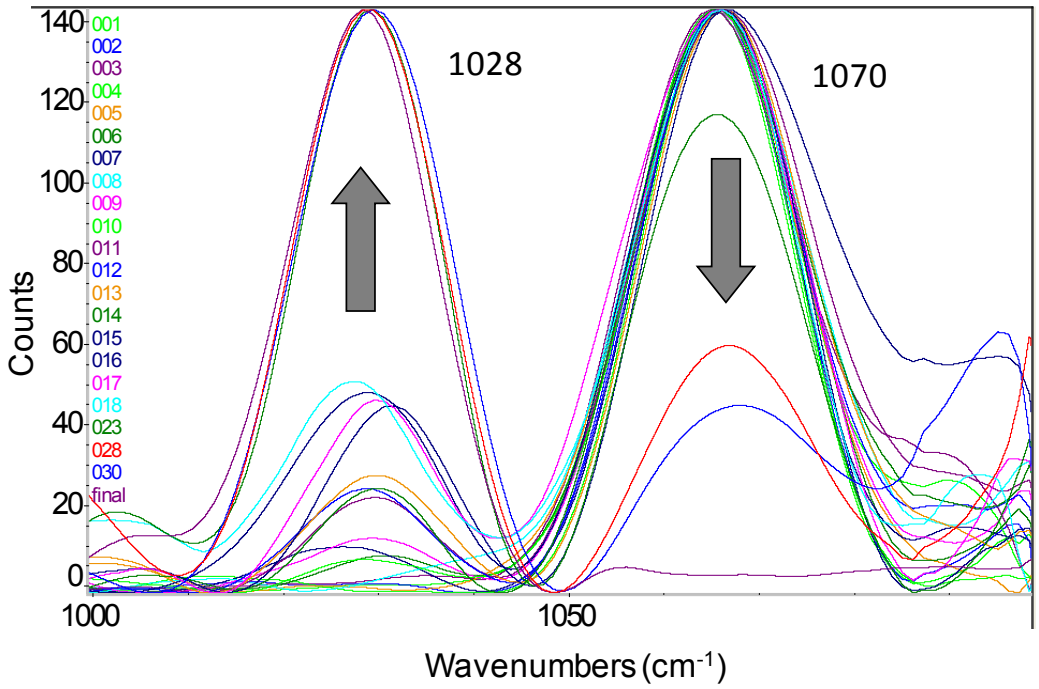


Figure below presents the results of insitu probing carried out in presence of n-heptane. A dilute solution of RDX in acetone was added with equal volume of n-heptane was probed for prenucleation clustering as solvent evaporates out and passes through saturation and super saturation stage. The results were however not conclusive as Raman shift from n-heptane severely masked the region of interest i.e. 1028 cm^{-1}, indicative of evolution of α-RDX.



The figures below show the Raman Spectral profiling of a slightly under saturated solution of RDX in Acetone. The profiling includes spectra form under saturation to saturation and super saturation levels till complete crystallization of RDX.





The very first spectrum collected at 'zero' second, showed no Raman shift at 1028 cm^{-1} indicating the conformation of RDX in solution similar to that of β-phase, previously reported as the metastable. The spectrum number 006 collected at about 55 seconds after the spectrum 001, showed slight intensity at 1028 cm^{-1}. This point is believed to be the inception of stable nucleation. The intensity further grows in subsequent spectras. Simutaneously, a decrease in intensity of 1070 cm^{-1} was recorded and which completely subsided in the final spectrum collected. This lowering in intensity, which is prominent after spectrum 018, is due to gradual evaporation of acetone and hence the final dried product donot show any intensity at 1070 cm^{-1}. The conformation in solution is same as that of metastable β phase indicating the prenuclation phase (conformation) of RDX to be exclusively the of β-form. During initial aggregation and stabilization of nucleus, the molecular conformation adopts that of thermodynamic α-phase. As the conformational energy barrier is very small (0.2 kcal/mol as aclculated by computational methods), the metstable prenuleation conformation is easily trnasformed to thermodynamically stable α-conformation. As the prenucleation phase itself is in metastable conformation, no metastable solid phase thus existed prior to formation of α phase crystals. This may be an exceptional case when compared with Ostwald's rule of stages. Even as the conformational transformation is very easy, no reversion has been encountered.

Cartesian coordinates of all the optimized stationary points at B3LYP/6-311G(d,p) in the gas phase, including corresponding charge and multiplicity were given below.

β-RDX

Charge = 0; Multiplicity = 1

C	-1.12766300	-2.31668100	1.27454400
C	-1.10261800	-2.35837900	-1.20660700
C	-3.11255000	-1.58262200	0.00193200
H	-3.59206400	-2.56344900	0.01463100
H	-3.86602300	-0.80425000	-0.01918900
H	-1.44428300	-3.39119800	-1.30913300
H	-0.46175300	-2.09647600	-2.04061300
H	-0.50313400	-2.02835100	2.11210800
H	-1.47318300	-3.34519800	1.40387100
N	-2.31478800	-1.46874800	1.22223200
N	-2.29078100	-1.51059000	-1.20505800
N	-0.34920700	-2.25883100	0.04059400
N	-2.22301600	-0.17675600	1.81872900
N	-2.19261100	-0.24273900	-1.85007200
N	0.87770000	-1.55938700	0.04144500
O	-1.29340000	0.00761300	2.57933500
O	-3.12322900	0.59813100	1.56301900
O	-1.25011600	-0.08476500	-2.60040400
O	-3.10005400	0.53780400	-1.64109500
O	1.37969200	-1.34065100	-1.04527300
O	1.35551000	-1.30045500	1.13058800
C	5.40708500	0.01897200	-0.04523200
O	6.21149400	0.66845300	-0.67342400
C	4.67105400	0.59258700	1.15216100
H	3.60645100	0.34730400	1.11768900
H	5.07145600	0.14564800	2.06922300
H	4.81664400	1.67141500	1.19212900
C	5.07686600	-1.41703600	-0.41188700
H	5.13646200	-2.06812300	0.46580400
H	4.04679300	-1.46754300	-0.77926600
H	5.75973500	-1.76595800	-1.18561200
C	-0.48706800	3.84487500	-0.08186000
O	0.01330600	4.94626000	-0.07800200
C	0.36368600	2.58463600	-0.06084900
H	0.13099600	1.98575500	0.82615100
H	0.15518100	1.96948100	-0.94241200
H	1.41854400	2.85512400	-0.04917000
C	-1.99041100	3.64468700	-0.10537500
H	-2.28616600	3.05290500	-0.97721300
H	-2.31504300	3.08341800	0.77657500
H	-2.48759000	4.61349800	-0.12957200

TS1a

Charge = 0; Multiplicity = 1

C	-0.64476300	-2.25873500	1.29897900
C	-0.52762200	-2.29969200	-1.19216600
C	-2.70949100	-2.16777600	-0.04834400
H	-2.86291700	-3.24822100	-0.03792200
H	-3.66574500	-1.66122000	-0.10141900
H	-0.54089100	-3.38911400	-1.29745100
H	0.03734000	-1.85617400	-2.00372000
H	-0.15822000	-1.78732500	2.14480700

H	-0.66909500	-3.34415200	1.43805400
N	-2.02883100	-1.81200700	1.19927600
N	-1.91408100	-1.85129400	-1.23674300
N	0.08489500	-1.93991900	0.07942900
N	-2.31923500	-0.51930300	1.73851300
N	-2.15027000	-0.57489700	-1.83969700
N	1.30352300	-1.27367600	0.12547700
O	-1.48693700	-0.03867500	2.48255200
O	-3.40357500	-0.05241400	1.45626300
O	-1.24839300	-0.11297400	-2.51047100
O	-3.25780600	-0.10455100	-1.68000000
O	1.84181800	-1.04429900	-0.94478700
O	1.73752000	-1.00180000	1.23269700
C	5.68594900	0.57876300	-0.07723900
O	6.38816200	1.31274700	-0.73443900
C	4.92594000	1.07163700	1.14074800
H	3.89042200	0.72159200	1.12826900
H	5.38940900	0.66336900	2.04601300
H	4.96344000	2.15948500	1.18287600
C	5.51381800	-0.88868200	-0.42756100
H	5.68190000	-1.52219000	0.44895100
H	4.48399000	-1.06150500	-0.75611800
H	6.20462200	-1.16028700	-1.22490600
C	-1.58203300	3.79002200	-0.05995200
O	-1.36454600	4.97977100	-0.03470000
C	-0.45356000	2.77297700	0.00342600
H	-0.56765500	2.13804500	0.88853100
H	-0.47732300	2.12256100	-0.87713300
H	0.50364900	3.29045600	0.04873500
C	-2.98960400	3.23196500	-0.15399000
H	-3.09584900	2.60738400	-1.04656700
H	-3.20499300	2.58790000	0.70443600
H	-3.70584100	4.05173800	-0.18955300

α-RDX

Charge = 0; Multiplicity = 1

C	-0.04150000	-1.89369000	1.28817800
C	0.01790800	-1.92139800	-1.19709500
C	-2.02711500	-2.58080800	0.00527700
H	-1.78154300	-3.64389200	0.02339100
H	-3.10223400	-2.45062900	-0.02167300
H	0.41362800	-2.94264100	-1.26102400
H	0.35921100	-1.34148000	-2.04496100
H	0.25995600	-1.29536600	2.13823300
H	0.34975100	-2.91335000	1.39294300
N	-1.48599800	-1.98576100	1.22790000
N	-1.42811100	-2.01326200	-1.20308900
N	0.45302800	-1.26870100	0.04958100
N	-2.21084100	-0.87567800	1.77295600
N	-2.12701300	-0.91669200	-1.80720700
N	1.77525100	-0.81337300	0.07664000
O	-1.58897100	-0.11294200	2.48482700
O	-3.39835500	-0.84207900	1.52588300
O	-1.47195400	-0.16811800	-2.50385800
O	-3.32523400	-0.88091500	-1.61916200
O	2.31605200	-0.63767000	-1.00243200
O	2.26060100	-0.60569200	1.17669800

C	6.12420000	1.12149300	-0.09221500
O	6.74091400	1.92848500	-0.74946100
C	5.41270300	1.50714800	1.19222600
H	4.39280100	1.11364100	1.20935400
H	5.93911300	1.06594200	2.04602200
H	5.40710400	2.59118900	1.29890000
C	6.01460000	-0.33454900	-0.50878400
H	6.27325300	-0.99901800	0.32148700
H	4.97800400	-0.55300700	-0.78474400
H	6.66866000	-0.52446700	-1.35896000
C	-3.17010800	3.37551800	-0.07506200
O	-3.39413000	4.56439900	-0.07232400
C	-1.75078000	2.83237900	-0.03411800
H	-1.60927900	2.21135000	0.85664200
H	-1.55946900	2.20188200	-0.90859800
H	-1.04277100	3.65987300	-0.01793300
C	-4.28480100	2.34744400	-0.11840300
H	-4.18236700	1.70836500	-1.00115700
H	-4.23138500	1.68672800	0.75263900
H	-5.24867800	2.85419100	-0.13943500

γ-HMX

Charge = 0; Multiplicity = 1

C	-0.25475700	2.04349400	-1.49928300
C	-0.10046200	2.49818800	0.99131100
H	0.70117600	2.54739700	-1.67083000
H	-0.94699300	2.29184800	-2.29737500
H	0.86591900	2.99211500	0.85284200
H	-0.68935500	3.04462600	1.72111000
N	-0.84772700	2.51117600	-0.25676400
N	0.03516700	0.62058500	-1.52058300
N	-2.02275100	3.29358600	-0.32879000
N	-1.02621600	-0.25901700	-1.74802700
O	-2.40357300	3.80670200	0.70541700
O	-2.54483100	3.39709600	-1.42254400
O	-2.11822600	0.24543300	-1.94509200
O	-0.75692700	-1.44820900	-1.73099100
N	0.19731000	1.16765900	1.48957100
C	1.32917300	0.04682300	-1.21025700
C	1.45195400	0.47787200	1.28115400
N	-0.83629700	0.46407900	2.12411700
H	2.08034900	0.82578100	-1.36130300
H	1.53230500	-0.78635200	-1.87345200
N	1.41450600	-0.46338500	0.15835600
H	2.22081900	1.23262000	1.09843400
H	1.70720900	-0.09495600	2.16531900
O	-0.57320500	-0.66547400	2.49570200
O	-1.89556100	1.05271900	2.24334400
N	2.10959100	-1.66808300	0.33334800
O	2.36248500	-2.32065100	-0.66684700
O	2.40990700	-1.97832600	1.47503600
C	5.13948800	-0.22612700	-0.23957600
O	4.23978400	0.59598000	-0.22940200
C	5.67190600	-0.82299300	1.04353000
H	5.13164400	-1.75815800	1.23109000
H	6.73540100	-1.06069900	0.97854100
H	5.48143500	-0.15013800	1.87913500

C	5.73794900	-0.73013000	-1.53186500
H	6.80910400	-0.50766200	-1.56199700
H	5.63572500	-1.81845300	-1.58588600
H	5.24301200	-0.27087100	-2.38612900
C	-4.47247900	-2.84693500	0.09908300
O	-5.25071900	-3.61276000	0.62254000
C	-3.83749900	-1.70361800	0.86949700
H	-2.80079700	-1.96364400	1.11051700
H	-3.80932400	-0.78611700	0.27604600
H	-4.37666800	-1.53675500	1.80105400
C	-4.07808500	-2.98063000	-1.36007400
H	-4.52900100	-2.16122600	-1.93058500
H	-2.99697300	-2.88924300	-1.49159100
H	-4.43626700	-3.93206400	-1.75196000

TS1b

Charge = 0; Multiplicity = 1

C	0.71315500	1.51045600	-1.23604300
C	0.71785600	1.51671300	1.29076900
H	1.79772200	1.42576200	-1.32474900
H	0.30643000	2.13400300	-2.02633000
H	1.80025300	1.38848800	1.35384800
H	0.35931000	2.16876000	2.08182400
N	0.38782700	2.14443600	0.02739700
N	0.20802200	0.14336100	-1.34402400
N	-0.34734300	3.34627900	0.02525400
N	-1.16335200	-0.04374400	-1.55728300
O	-0.59409000	3.83840700	1.10956600
O	-0.62486100	3.81487000	-1.06262300
O	-1.82448200	0.96948300	-1.68641200
O	-1.56777400	-1.19473100	-1.58968500
N	0.15981700	0.17186000	1.43051000
C	1.05851700	-1.00602900	-1.28837100
C	0.97336200	-1.00607200	1.43496500
N	-1.21420800	0.04710100	1.68135300
H	2.00339600	-0.75701500	-1.76770800
H	0.58641500	-1.82007900	-1.83185400
N	1.39053000	-1.48962100	0.08542100
H	1.89063100	-0.80087000	1.98585100
H	0.42907000	-1.80090900	1.93741300
O	-1.66415600	-1.08273400	1.77767900
O	-1.83061900	1.09172200	1.77352400
N	2.46240900	-2.33091200	0.11940600
O	2.95864500	-2.66099500	-0.95758500
O	2.85601800	-2.69990200	1.22575800
C	4.81310000	0.07048000	-0.14447800
O	3.70731200	0.57934100	-0.05212800
C	5.51940800	-0.49504500	1.06514000
H	5.28106100	-1.56336500	1.12383200
H	6.60414200	-0.39847700	0.99151800
H	5.15551400	-0.01627300	1.97393500
C	5.51333300	-0.06831200	-1.47428700
H	6.47822700	0.44709000	-1.44688500
H	5.71859800	-1.12532000	-1.66958300
H	4.90144600	0.34090200	-2.27669800
C	-5.86258900	-1.32254900	-0.12630200
O	-6.65663100	-2.23025500	-0.01535000

C	-5.34045400	-0.56681900	1.08151400
H	-4.28162000	-0.79680700	1.23755300
H	-5.40806700	0.51454200	0.93088600
H	-5.90483100	-0.85862600	1.96663300
C	-5.33387500	-0.88491000	-1.47991100
H	-5.64597800	0.14438700	-1.68619400
H	-4.24049800	-0.89164900	-1.49498600
H	-5.72290200	-1.54498700	-2.25446000

IN1b

Charge = 0; Multiplicity = 1

C	-0.50628800	0.97952200	1.36712600
C	-0.44301100	0.50917000	-1.13372900
H	-1.58946100	1.11747900	1.34814100
H	-0.04471100	1.68490300	2.04884300
H	-1.52905900	0.44490100	-1.08353500
H	-0.15109700	1.08197500	-2.00794500
N	0.05133900	1.22454700	0.04094700
N	-0.27483600	-0.38611200	1.82528900
N	0.74087200	2.43988700	-0.15477000
N	1.04851600	-0.75914500	2.10236900
O	0.99662000	2.75211300	-1.30151000
O	1.02465400	3.07698300	0.84510700
O	1.85251200	0.14885600	2.18233200
O	1.27813400	-1.95140300	2.24970300
N	0.09135100	-0.83671800	-1.26883900
C	-1.27150300	-1.42422000	1.68613000
C	-0.46593500	-2.06017300	-0.64154900
N	1.32056900	-1.00995900	-1.87672500
H	-2.21251600	-1.08438300	2.10955000
H	-0.92227800	-2.30128900	2.22528100
N	-1.53090300	-1.75438100	0.27752800
H	-0.83416500	-2.73451000	-1.41133300
H	0.32662400	-2.55763500	-0.08256900
O	1.74442400	-2.16124000	-1.90761600
O	1.87085200	-0.02289100	-2.33461900
N	-2.84034400	-1.76197000	-0.18645400
O	-3.72903300	-1.66668000	0.64780800
O	-2.99468900	-1.86964200	-1.39343500
C	-4.58881600	1.32963800	-0.17314700
O	-3.37955900	1.34091700	-0.02089300
C	-5.20956000	0.84957100	-1.46420500
H	-5.31215400	-0.23892800	-1.39516200
H	-6.19906000	1.27591200	-1.63654900
H	-4.54947700	1.06703100	-2.30388000
C	-5.52776800	1.75902700	0.92772900
H	-6.08352400	2.64759600	0.61055300
H	-6.26620100	0.97408600	1.11760800
H	-4.97502900	1.98126300	1.83919600
C	5.46169500	0.25880500	-0.05298300
O	6.66712800	0.36780400	-0.01918800
C	4.55654400	1.44862100	-0.31257200
H	3.89283400	1.25111600	-1.15940800
H	3.91850000	1.63098900	0.55850000
H	5.16041100	2.33314300	-0.51092000
C	4.77513400	-1.07819300	0.16347500
H	4.05434600	-1.00979400	0.98421500

H	4.21768300	-1.36653900	-0.73376900
H	5.52107800	-1.83952500	0.38859200

TS2b

Charge = 0; Multiplicity = 1

C	-0.90231300	1.70460300	0.74814900
C	-0.40596400	0.10620800	-1.16973300
H	-1.97699100	1.61534800	0.57741400
H	-0.64290600	2.72466300	1.00841700
H	-1.47629900	-0.09614500	-1.17411300
H	-0.04820000	0.22537300	-2.18752500
N	-0.17627300	1.36545500	-0.46770800
N	-0.58822700	0.80749800	1.85763900
N	0.49958200	2.40495000	-1.14099100
N	0.72267600	0.84439000	2.36251100
O	1.00350900	2.12693300	-2.21257000
O	0.51561700	3.49467800	-0.59763800
O	1.39493800	1.79785900	2.02794300
O	1.06632300	-0.07147700	3.09786100
N	0.28511800	-1.03776000	-0.59207300
C	-1.41960600	-0.32846900	2.17988800
C	-0.18211800	-1.85070600	0.55772400
N	1.51799700	-1.41048400	-1.08867800
H	-2.44975600	-0.00339600	2.29496300
H	-1.06305900	-0.75556300	3.11400800
N	-1.40828300	-1.33880300	1.11012600
H	-0.32697100	-2.87997600	0.23772300
H	0.57233100	-1.82704900	1.34416100
O	2.05519200	-2.35577900	-0.51442400
O	1.96686200	-0.79556800	-2.03994400
N	-2.61384400	-1.83660900	0.63506600
O	-3.62680700	-1.52311000	1.24456200
O	-2.56090800	-2.55110000	-0.35440500
C	-4.72825300	0.47043800	-1.01516000
O	-3.56925100	0.79374700	-0.82090100
C	-5.07677000	-0.67528100	-1.93620300
H	-5.04642200	-1.59583700	-1.34302500
H	-6.07609300	-0.57817200	-2.36356200
H	-4.33117100	-0.76496300	-2.72614300
C	-5.87074500	1.17064100	-0.32044100
H	-6.50197600	1.67040600	-1.06253300
H	-6.50199200	0.43840900	0.19220200
H	-5.49561600	1.90415000	0.39157800
C	5.77114600	-0.26805300	-0.24257200
O	6.87049100	-0.06160000	0.22047600
C	5.53972400	-1.29534700	-1.33419700
H	4.68090700	-1.93153100	-1.10525100
H	5.30118800	-0.77959000	-2.27062100
H	6.43935800	-1.89437500	-1.47119500
C	4.54683500	0.48744400	0.24569900
H	3.91905300	0.81080300	-0.58888900
H	3.94161000	-0.18130300	0.86782700
H	4.85244600	1.34274200	0.84671600

IN2b

Charge = 0; Multiplicity = 1

C	-0.02095000	-1.62083800	-0.65250700

C	0.47461700	0.84351500	-1.05234000
H	0.95850800	-1.84711500	-1.07396200
H	-0.76487400	-2.32662400	-1.00463600
H	1.48497900	0.43883500	-1.14606900
H	0.26745500	1.50442000	-1.88611000
N	-0.42879700	-0.29004000	-1.07991900
N	0.12566300	-1.74516000	0.79762500
N	-1.69088100	-0.11146800	-1.66645300
N	-1.04553400	-1.85974500	1.56933500
O	-2.00674000	1.03825500	-1.91785700
O	-2.35434300	-1.11042000	-1.88358800
O	-2.06638700	-2.11890300	0.96237600
O	-0.93366300	-1.70327400	2.77522200
N	0.32844800	1.64470700	0.16699900
C	1.35413700	-1.41918700	1.47511300
C	0.59169300	1.06518300	1.48631900
N	0.52113200	3.03134900	0.04109200
H	2.17895700	-1.88902500	0.94521400
H	1.30437400	-1.80186500	2.49143300
N	1.62028000	0.03988200	1.47374400
H	0.87717200	1.88233000	2.14321600
H	-0.30840100	0.60238100	1.88669700
O	0.48907300	3.68201200	1.07067400
O	0.66309200	3.47228400	-1.08664100
N	2.93764500	0.43873500	1.44349000
O	3.78776100	-0.43613700	1.57949200
O	3.15116100	1.63102000	1.27619700
C	4.34178400	-1.03000500	-1.48604900
O	3.12545400	-1.10972700	-1.42884300
C	5.03762400	0.30748700	-1.56489700
H	5.24046600	0.63430200	-0.53863400
H	5.99152500	0.24817400	-2.09186600
H	4.39023900	1.04892100	-2.03283500
C	5.21416400	-2.26022400	-1.43912900
H	5.78077400	-2.34795300	-2.37174300
H	5.94508600	-2.16633700	-0.63020500
H	4.60923500	-3.15387400	-1.29350100
C	-6.02102600	0.04620300	-0.09056700
O	-7.10058400	0.54259400	0.13922600
C	-4.76331400	0.50195500	0.62940500
H	-4.20152200	-0.35303300	1.01735500
H	-4.11164000	1.02335200	-0.08024600
H	-5.03065100	1.18024400	1.43899200
C	-5.84784100	-1.06269500	-1.11138300
H	-5.00195500	-0.86283000	-1.77388500
H	-5.62214200	-2.00007000	-0.59094600
H	-6.76718500	-1.18206100	-1.68351300

TS3b

Charge = 0; Multiplicity = 1

C	-0.20422100	-0.89829200	-1.18918000
C	1.12431700	1.28381900	-1.12751600
H	0.78140000	-1.33583600	-1.35287000
H	-0.92566400	-1.31141200	-1.88590300
H	1.96252800	0.58764600	-1.19458600
H	1.25240800	2.08418400	-1.84685900
N	-0.07246800	0.53085500	-1.42677700

N	-0.65381900	-1.22455100	0.16781300
N	-1.21947500	1.25884000	-1.77981800
N	-1.91748600	-1.82229500	0.34235600
O	-1.08023400	2.45821200	-1.92559100
O	-2.24946700	0.61886000	-1.91863600
O	-2.57346600	-2.03982900	-0.65640400
O	-2.25695300	-2.05974000	1.49229200
N	1.03535500	1.90921400	0.20585000
C	0.30816500	-1.41525200	1.24992500
C	0.63536000	1.13239000	1.36950100
N	1.87847000	3.00510200	0.43126500
H	0.96918500	-2.25957300	1.05637200
H	-0.25158700	-1.59225700	2.16586200
N	1.16029800	-0.22964800	1.35581200
H	0.96720100	1.67918700	2.24879900
H	-0.44942100	1.02870900	1.39467700
O	1.86648500	3.49487500	1.54627800
O	2.52078700	3.40250300	-0.52757300
N	2.49426100	-0.41392400	1.66722500
O	2.89071800	-1.56140800	1.82942600
O	3.17422300	0.59894600	1.74236500
C	4.18533600	-1.73669400	-1.05362400
O	3.05585900	-1.37027500	-1.33227200
C	5.26882900	-0.74449700	-0.70492000
H	5.27226700	-0.62522000	0.38432700
H	6.25869900	-1.09262800	-1.00588200
H	5.05408600	0.22736700	-1.14849500
C	4.54869700	-3.20080000	-1.00518100
H	5.31067600	-3.41858500	-1.76046500
H	4.98486000	-3.44303400	-0.03150800
H	3.67001000	-3.81856300	-1.18377600
C	-6.15449200	-0.03083700	0.39541200
O	-7.19540300	0.31420300	0.90699000
C	-4.83918700	0.65706800	0.72000400
H	-4.21736500	-0.02821100	1.30704800
H	-4.28492600	0.90039700	-0.19087900
H	-5.03161300	1.55757500	1.30243000
C	-6.08787600	-1.17298000	-0.60086500
H	-5.87931300	-0.77011700	-1.59805000
H	-5.26918600	-1.85737100	-0.36400100
H	-7.04015200	-1.70173500	-0.61865500

β-HMX

Charge = 0; Multiplicity = 1

C	-0.28488900	-0.47935500	-1.08986700
C	1.23309700	1.56674400	-1.01516700
H	0.69157500	-0.90272000	-1.32218000
H	-0.98287600	-0.68890100	-1.89668600
H	1.87963200	0.90702500	-1.59236500
H	1.15291000	2.53592700	-1.50047100
N	-0.07087400	0.95751300	-0.92476500
N	-0.83070400	-1.11841600	0.10355900
N	-1.18617700	1.78493000	-0.80856700
N	-2.11297800	-1.64508100	0.03379600
O	-0.98215800	2.97540400	-0.64231100
O	-2.27273600	1.22655100	-0.85547400
O	-2.56412900	-1.90941900	-1.06689800

O	-2.66607700	-1.84115800	1.11052300
N	1.81910100	1.75469900	0.33522900
C	-0.39738700	-0.75000600	1.46727700
C	1.25788400	1.19752400	1.54705100
N	3.11426500	2.24365000	0.35737200
H	-0.45817000	-1.63569800	2.09269300
H	-1.05561300	0.01709600	1.88114800
N	0.94823800	-0.23125700	1.46935300
H	1.98001500	1.39280700	2.33594700
H	0.31730400	1.69505200	1.78506200
O	3.65281000	2.41015900	1.43744700
O	3.59380100	2.50385500	-0.74125500
N	2.00048300	-1.14073200	1.56657900
O	1.71216900	-2.32509100	1.54375900
O	3.12048300	-0.66236300	1.64742700
C	3.94989400	-1.57683400	-1.30917500
O	2.86306900	-1.09741500	-1.58813200
C	5.20232300	-0.73650600	-1.28168000
H	5.76666300	-0.92626300	-0.36454800
H	5.84628500	-1.02773700	-2.11904800
H	4.96124600	0.32242300	-1.36043700
C	4.08581900	-3.03738700	-0.95012100
H	5.05034600	-3.44831000	-1.25476600
H	4.01579000	-3.11687600	0.14041700
H	3.26785200	-3.61130500	-1.38452000
C	-6.43747000	0.10041500	-0.00614400
O	-7.62265600	0.16324300	0.23202300
C	-5.39679600	0.60372000	0.97863200
H	-4.81490500	-0.24336400	1.35698400
H	-4.69055800	1.27985400	0.48758100
H	-5.89181700	1.10816100	1.80783700
C	-5.90897800	-0.48637500	-1.30164600
H	-5.43011300	0.30217500	-1.89216100
H	-5.14126800	-1.24083300	-1.10881200
H	-6.73135100	-0.91742300	-1.87140200

ε-CL20

Charge = 0; Multiplicity = 1

C	1.26224200	-0.14120600	1.51384900
H	2.07646100	-0.20426100	2.22541100
N	1.33306200	1.07330300	0.70498600
N	2.57058000	1.78545200	0.66241600
O	2.68344300	2.59166700	-0.23143000
O	3.35241800	1.56095300	1.56484200
C	0.65237900	0.80537600	-0.57344300
H	1.19579500	1.26214300	-1.39258300
N	-0.71758500	1.26273100	-0.55991800
N	-1.08508700	2.42986100	-1.28127600
O	-2.23784700	2.78925200	-1.16783300
O	-0.22550600	2.91606800	-1.98449300
C	-1.57012200	0.76284100	0.49807400
H	-2.56747900	1.17734100	0.40026900
N	-1.01036800	0.95852400	1.84755700
N	-0.69724800	2.22775100	2.32029200
O	-1.23105200	3.15928100	1.75053300
O	0.05533900	2.26966500	3.27886800
C	-0.17494700	-0.17230500	2.22843300

H	-0.06972500	-0.25214400	3.30415500
N	-1.05006700	-1.20563400	1.69605300
N	-0.84574300	-2.54178100	2.02047000
O	-1.49032100	-3.35130100	1.38495200
O	-0.06593300	-2.75409500	2.93400500
C	-1.59651100	-0.81770200	0.39835000
H	-2.60299800	-1.18701400	0.24377700
N	-0.73145800	-1.27836600	-0.67813900
N	-1.30874600	-1.67465400	-1.89618100
O	-0.55169400	-1.81565900	-2.83714400
O	-2.51185900	-1.86270300	-1.89260000
C	0.63316500	-0.78055600	-0.67716100
H	1.15481100	-1.13112700	-1.55977100
N	1.30135500	-1.22892300	0.54210800
N	2.49045000	-1.99886600	0.41169200
O	2.57409300	-2.67448200	-0.59054900
O	3.26639700	-1.95430100	1.34402800
C	-5.35885300	-0.01996400	-0.84772800
O	-4.55318000	0.04629800	0.06182400
C	-5.10125300	0.63938500	-2.18434100
H	-6.02122900	1.00633600	-2.64450000
H	-4.38075700	1.44966900	-2.07564500
H	-4.67629600	-0.11685700	-2.85454600
C	-6.64972400	-0.79261900	-0.69672100
H	-7.49644800	-0.09871200	-0.72916800
H	-6.77873800	-1.49060000	-1.52930800
H	-6.65734800	-1.33092600	0.24973600
C	4.52068500	-0.04439700	-1.86464800
O	3.34947800	0.02535400	-1.53606300
C	4.92882500	-0.08623000	-3.31673100
H	5.46317600	0.83676600	-3.56682900
H	5.62247100	-0.91291700	-3.49662000
H	4.05294800	-0.18294600	-3.95630200
C	5.61789000	-0.11541700	-0.82696600
H	5.75455000	-1.16807300	-0.55380300
H	6.57056000	0.26023000	-1.20394800
H	5.32337700	0.42608300	0.07195400

TS1c

Charge = 0; Multiplicity = 1

C	-1.27356600	0.81217100	1.27122300
H	-2.06986000	1.19624100	1.89735400
N	-1.37283200	-0.63208300	1.08477100
N	-2.62164300	-1.26196600	1.38095200
O	-2.76938500	-2.37465800	0.93316200
O	-3.37542500	-0.64569800	2.10783000
C	-0.72475800	-0.96659000	-0.19660500
H	-1.29208700	-1.72933300	-0.71759800
N	0.64158300	-1.39302600	-0.00896800
N	0.97874000	-2.76995400	-0.13136100
O	2.13043300	-3.06189800	0.10944300
O	0.09599000	-3.50268300	-0.52220700
C	1.52200200	-0.49261800	0.70326500
H	2.51581100	-0.92138800	0.77285400
N	1.00415000	-0.06329600	2.01813300
N	0.67840400	-0.99270400	3.00115600
O	1.18336600	-2.09270800	2.89160400

O	-0.05318200	-0.59088600	3.89041900
C	0.18394400	1.13799000	1.86868600
H	0.11207100	1.70639400	2.78872600
N	0.99754100	1.80980000	0.88462300
N	1.37439800	3.13976300	0.97434100
O	2.15790800	3.53032100	0.13062300
O	0.87093100	3.77995300	1.88100400
C	1.55155000	0.88626600	-0.07937300
H	2.55924700	1.15059800	-0.37945900
N	0.67338700	0.83938600	-1.24845900
N	1.24231700	0.50683500	-2.49137600
O	0.47459100	0.16748100	-3.37138300
O	2.45121500	0.62537700	-2.58360200
C	-0.69795400	0.41056900	-0.99224700
H	-1.24200500	0.34246800	-1.92648100
N	-1.33377500	1.35409100	-0.08165300
N	-2.48672800	2.04591200	-0.51301300
O	-2.59266700	2.21085200	-1.70991700
O	-3.22364600	2.46401900	0.35963700
C	5.29021600	-0.45501200	-0.85533200
O	4.50240400	-0.09032700	-0.00245000
C	5.03124000	-1.68052300	-1.70269000
H	5.95264800	-2.22044300	-1.93203700
H	4.31584000	-2.33901800	-1.21113800
H	4.60039400	-1.34644800	-2.65358100
C	6.55987000	0.31823300	-1.13115200
H	7.42577900	-0.28792600	-0.84419100
H	6.65779700	0.52645100	-2.20067400
H	6.56426700	1.24835400	-0.56505800
C	-4.64655600	-0.59222100	-1.62673600
O	-3.46413000	-0.59484200	-1.33264200
C	-5.12762300	-1.11214300	-2.95847000
H	-5.75523300	-1.99543800	-2.79850000
H	-5.75493300	-0.36385900	-3.45268100
H	-4.28301700	-1.37345700	-3.59394300
C	-5.68079900	-0.03959600	-0.67121500
H	-5.66289400	1.05299800	-0.75206200
H	-6.69040600	-0.38378000	-0.89906200
H	-5.41483900	-0.29527600	0.35519600

IN1c

Charge = 0; Multiplicity = 1

C	-1.27170800	1.50945200	-0.07568900
H	-2.04273600	2.27048100	-0.08603300
N	-1.39871100	0.61815900	1.07349200
N	-2.65305500	0.59049500	1.76007800
O	-2.83354500	-0.35706300	2.48762600
O	-3.37624400	1.55330700	1.59786900
C	-0.79570700	-0.67682900	0.70267700
H	-1.38922200	-1.49438700	1.09532800
N	0.56870500	-0.77526200	1.15989200
N	0.88184400	-1.59145900	2.28299700
O	2.03464500	-1.56810200	2.65647400
O	-0.02190600	-2.27456000	2.71461000
C	1.47830100	0.27357100	0.74991500
H	2.47055700	0.07740300	1.14210000
N	1.01270500	1.63609400	1.05763200

N	0.72135300	2.02372400	2.36313000
O	1.21961000	1.35734900	3.24870600
O	0.02120100	3.01574600	2.47843800
C	0.19944200	2.14833100	-0.04630000
H	0.15411000	3.23044300	-0.04316300
N	0.96837000	1.65084500	-1.17324700
N	1.84977600	2.55859900	-1.83135700
O	2.73954500	2.05667100	-2.48298700
O	1.57984200	3.73762400	-1.72691100
C	1.49084900	0.32405000	-0.83438700
H	2.49407600	0.18481500	-1.22147200
N	0.59534700	-0.68001900	-1.39383800
N	1.14496700	-1.92850500	-1.74006500
O	0.36232400	-2.84788900	-1.88501200
O	2.35191800	-1.96567200	-1.90159600
C	-0.77449300	-0.65850700	-0.88820100
H	-1.33720300	-1.48312400	-1.30811700
N	-1.37642300	0.61880200	-1.22132000
N	-2.48470900	0.67293400	-2.07785300
O	-2.62457100	-0.26715300	-2.83360100
O	-3.16467200	1.68152200	-2.01880300
C	5.20374400	-1.12896800	-0.08355900
O	4.43682900	-0.19759800	0.07436900
C	4.91677200	-2.49824100	0.49128600
H	5.82999100	-3.01622600	0.79217900
H	4.22755700	-2.42089000	1.33175900
H	4.44069500	-3.09699100	-0.29382300
C	6.47178100	-0.97050100	-0.89156700
H	7.34024100	-1.07693800	-0.23279100
H	6.54660900	-1.75917200	-1.64617700
H	6.49389800	0.00871000	-1.36719800
C	-4.74959000	-1.55259400	-0.40113500
O	-3.56504400	-1.33976800	-0.21172300
C	-5.26738600	-2.94729900	-0.65475900
H	-5.89696000	-3.25738800	0.18623300
H	-5.89957500	-2.96442500	-1.54755300
H	-4.43987200	-3.64616000	-0.76584100
C	-5.75268100	-0.42161100	-0.41669600
H	-5.81200300	-0.03887600	-1.44212600
H	-6.75158100	-0.75028200	-0.12461900
H	-5.41517400	0.39170400	0.22533100

TS2c

Charge = 0; Multiplicity = 1

C	-1.28552000	0.44736800	1.41953300
H	-2.03686800	0.64819200	2.17369500
N	-1.33028200	-0.93467800	0.95066300
N	-2.55025500	-1.65557500	1.17301800
O	-2.68442700	-2.66710200	0.52308500
O	-3.28796000	-1.22221000	2.03272500
C	-0.79525500	-0.95386100	-0.43243300
H	-1.36463300	-1.64750200	-1.03979900
N	0.60248600	-1.30214200	-0.44661600
N	1.01159800	-2.58878100	-0.89279200
O	2.19901600	-2.82410200	-0.82827900
O	0.14042000	-3.29836800	-1.34849000
C	1.49282000	-0.49830200	0.36331900

H	2.51207700	-0.84818900	0.25002400
N	1.09794500	-0.39158300	1.77617900
N	0.94876400	-1.52450600	2.57104800
O	1.51449100	-2.53051100	2.18935700
O	0.29082600	-1.37817600	3.58739900
C	0.19415400	0.74517600	1.95889500
H	0.17808600	1.08452100	2.98726400
N	0.82700300	1.71902300	1.08391800
N	1.69257200	2.68404300	1.69842200
O	2.50588700	3.20535900	0.96910500
O	1.47537400	2.92883100	2.86632000
C	1.35299500	1.01120600	-0.09312500
H	2.31312100	1.41276100	-0.40014700
N	0.39191500	1.13686800	-1.17738900
N	0.87941100	1.15821200	-2.49689300
O	0.07367600	0.93247500	-3.37906800
O	2.05707000	1.43590700	-2.63703900
C	-0.92608600	0.54836000	-0.93799900
H	-1.53864400	0.63199700	-1.82662600
N	-1.53753700	1.18456600	0.19803400
N	-2.35382900	2.29053200	0.11129100
O	-2.51279000	2.75798400	-1.00218100
O	-2.82887800	2.69198400	1.16127000
C	-4.89949100	-0.30590600	-1.38658600
O	-3.69670300	-0.30396400	-1.19474000
C	-5.55497500	0.75081800	-2.24665000
H	-5.76212600	0.32155600	-3.23358500
H	-6.51297000	1.06917300	-1.82831700
H	-4.88905100	1.60462700	-2.36489800
C	-5.79287900	-1.36046700	-0.77646200
H	-6.38946600	-0.90134000	0.01952900
H	-6.49703300	-1.75182500	-1.51611500
H	-5.19644300	-2.16704300	-0.35345300
C	5.27864500	-0.30743300	-0.99846300
O	4.43299900	0.10088500	-0.22451900
C	4.91961900	-0.74058400	-2.40397000
H	5.76229800	-0.65779500	-3.09275800
H	4.61905100	-1.79407100	-2.36653400
H	4.07277600	-0.15981500	-2.76992400
C	6.72709500	-0.42739500	-0.58384300
H	7.10736900	-1.42845800	-0.80918700
H	7.33169900	0.27903700	-1.16264500
H	6.83347400	-0.21349200	0.47843800

β-CL-20

Charge = 0; Multiplicity = 1

C	1.05891200	0.37864500	1.65559200
H	1.61425300	0.53018400	2.57254500
N	1.54175300	1.23937600	0.58810200
N	2.88005300	1.73817100	0.71823100
O	3.37164600	2.18161700	-0.29611400
O	3.36088300	1.72987500	1.83124600
C	1.20463200	0.59598500	-0.70634100
H	2.00977200	0.74499300	-1.41609900
N	-0.02624500	1.12914600	-1.22126700
N	-0.03705200	1.90917700	-2.40041100
O	-1.11548700	2.33192600	-2.75546800

O	1.03234900	2.04435500	-2.96083800
C	-1.20597200	1.01011900	-0.39663100
H	-2.06843200	1.39593900	-0.92870800
N	-1.05244900	1.62609400	0.93088900
N	-0.71571800	2.97170900	1.05778800
O	-0.96256300	3.68213500	0.10325100
O	-0.23910500	3.30184700	2.13110800
C	-0.50161200	0.65018500	1.87551300
H	-0.70619400	0.92981900	2.90127000
N	-1.24872000	-0.53570000	1.48538400
N	-2.43722700	-0.81318400	2.24850100
O	-3.25848700	-1.51967200	1.70709500
O	-2.46899200	-0.37155600	3.37669800
C	-1.40625500	-0.50759700	0.00998100
H	-2.39303100	-0.85362400	-0.28110000
N	-0.38121600	-1.29219600	-0.62133600
N	-0.69937000	-2.50867500	-1.26334600
O	0.22363600	-3.10487900	-1.77494400
O	-1.87488800	-2.81845400	-1.27624000
C	0.99398400	-0.93539000	-0.35678400
H	1.66439800	-1.57312600	-0.91977700
N	1.32649500	-0.93638200	1.07344300
N	1.16489200	-2.07998700	1.84494700
O	1.12096800	-3.13641000	1.24359300
O	1.11687600	-1.90693300	3.05180300
C	5.06831200	-1.06081100	-1.18726700
O	3.87415300	-0.88962800	-1.02872400
C	5.60579500	-2.33675700	-1.79697200
H	5.98436200	-2.12137900	-2.80222800
H	6.44772000	-2.72461700	-1.21706300
H	4.81763500	-3.08515200	-1.86486400
C	6.08033100	-0.01283700	-0.78198600
H	6.61815900	-0.36361500	0.10593200
H	6.82722200	0.13437900	-1.56700900
H	5.58451100	0.92837700	-0.55099200
C	-5.25807000	-0.24592400	-1.28272900
O	-4.15093300	0.20999500	-1.06665000
C	-5.52554000	-1.73309500	-1.22270000
H	-5.90464600	-1.97215900	-0.22253900
H	-6.28700600	-2.03878800	-1.94363700
H	-4.60388500	-2.29265000	-1.37797600
C	-6.42789700	0.65595600	-1.60432600
H	-6.71964900	0.50913100	-2.64988600
H	-7.29717500	0.39622700	-0.99311500
H	-6.15457200	1.69858600	-1.44986100