Crystal Engineering of *o*-Carboranyl Alcohols: Synthesis, Crystal Structures and Thermal Properties

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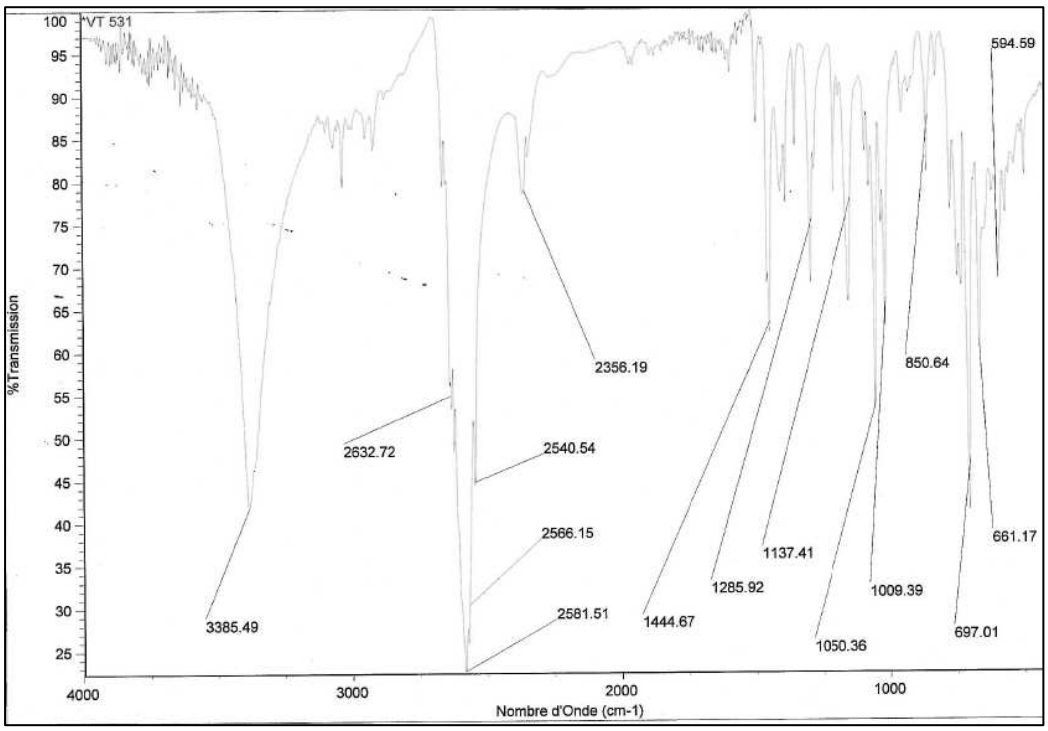
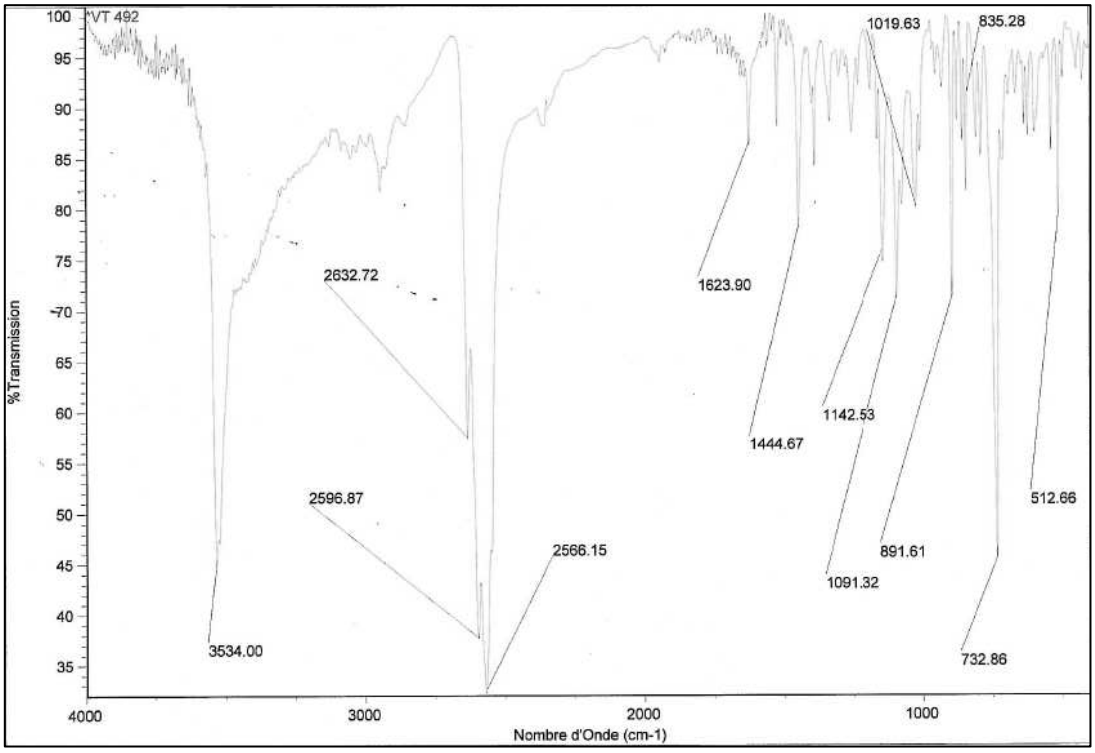
Electronic Supplementary Material for CrystEngComm

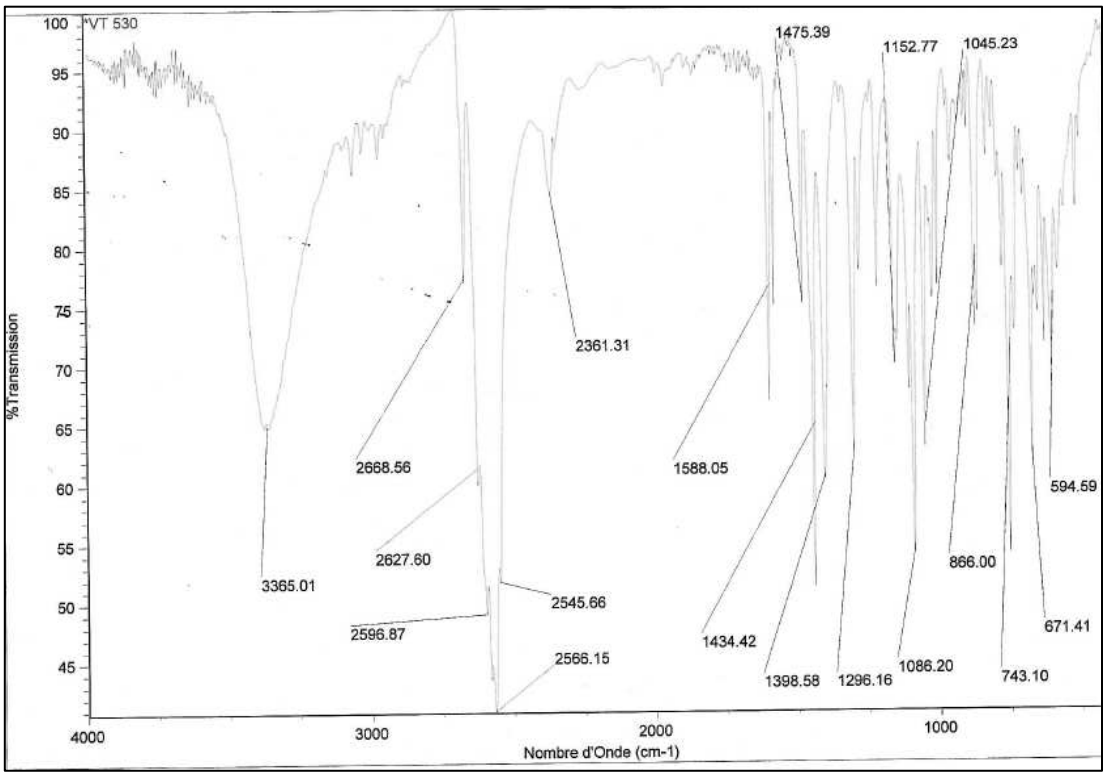
IR Spectrum (KBr) for compound (1)



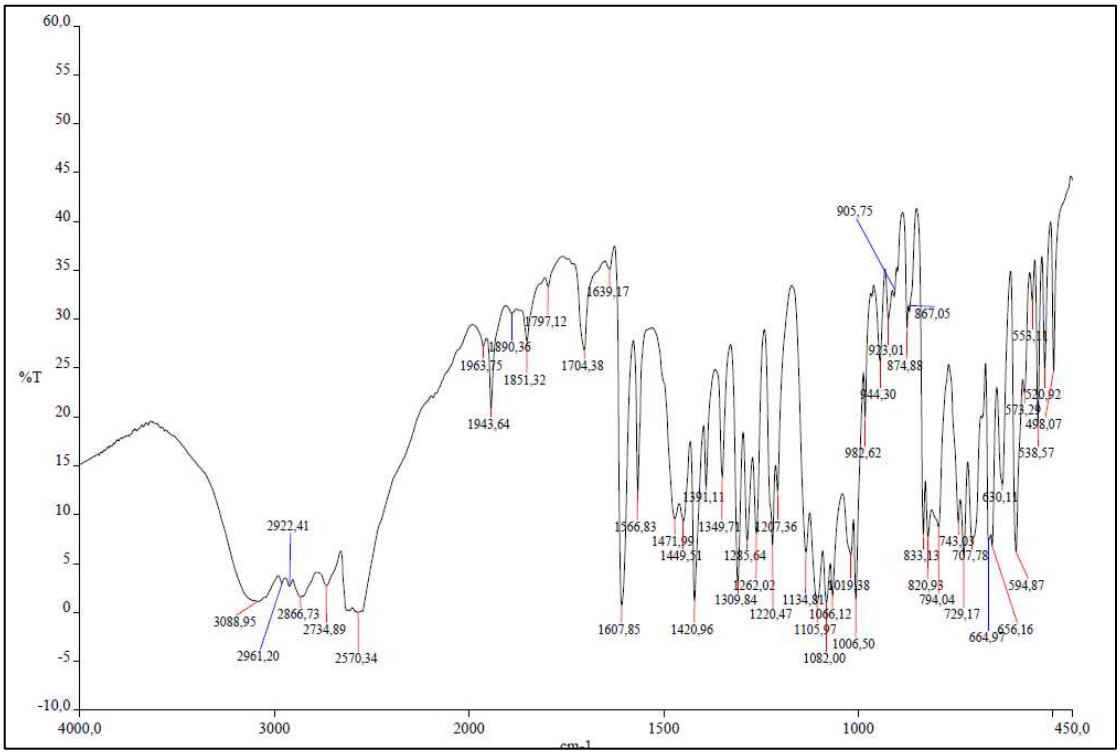
IR Spectrum (KBr) for compound (2)



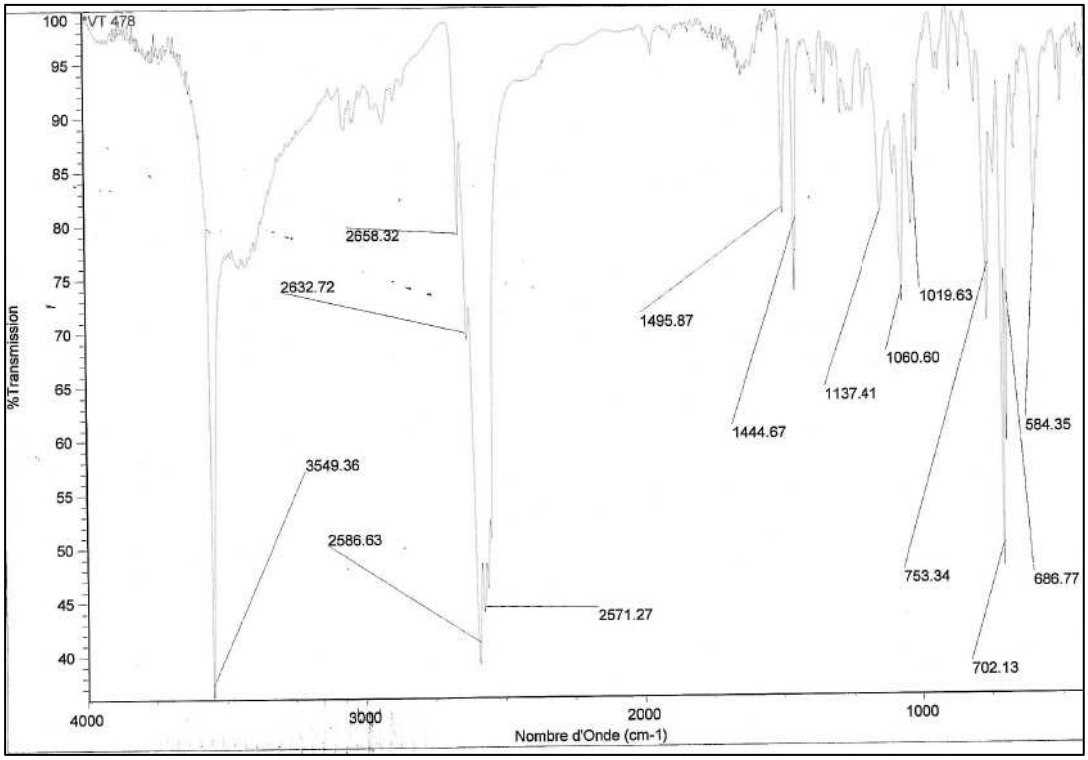
IR Spectrum (KBr) for compound (3)



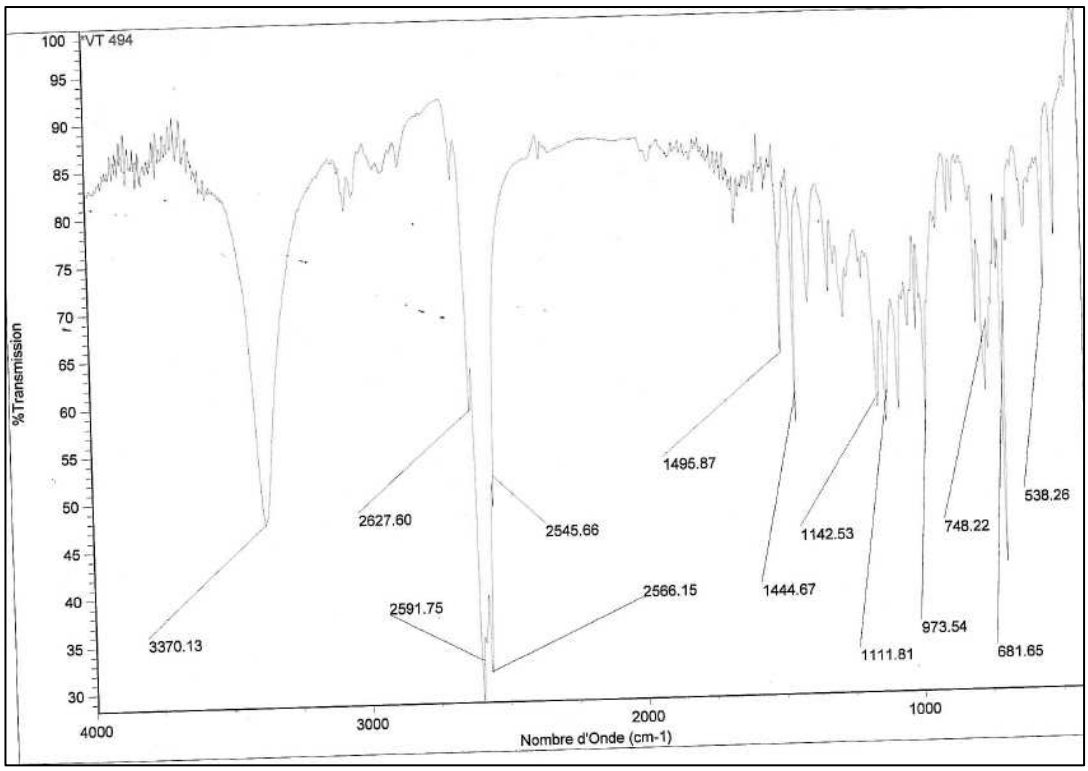
IR Spectrum (KBr) for compound (4)



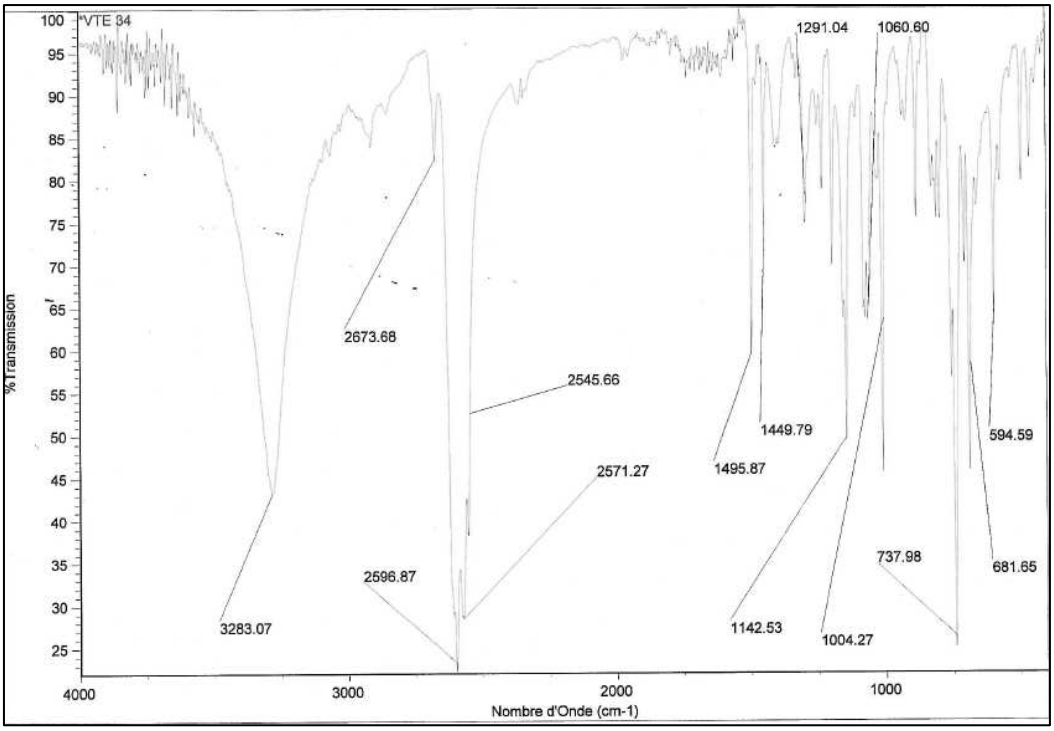
IR Spectrum (KBr) for compound (5)



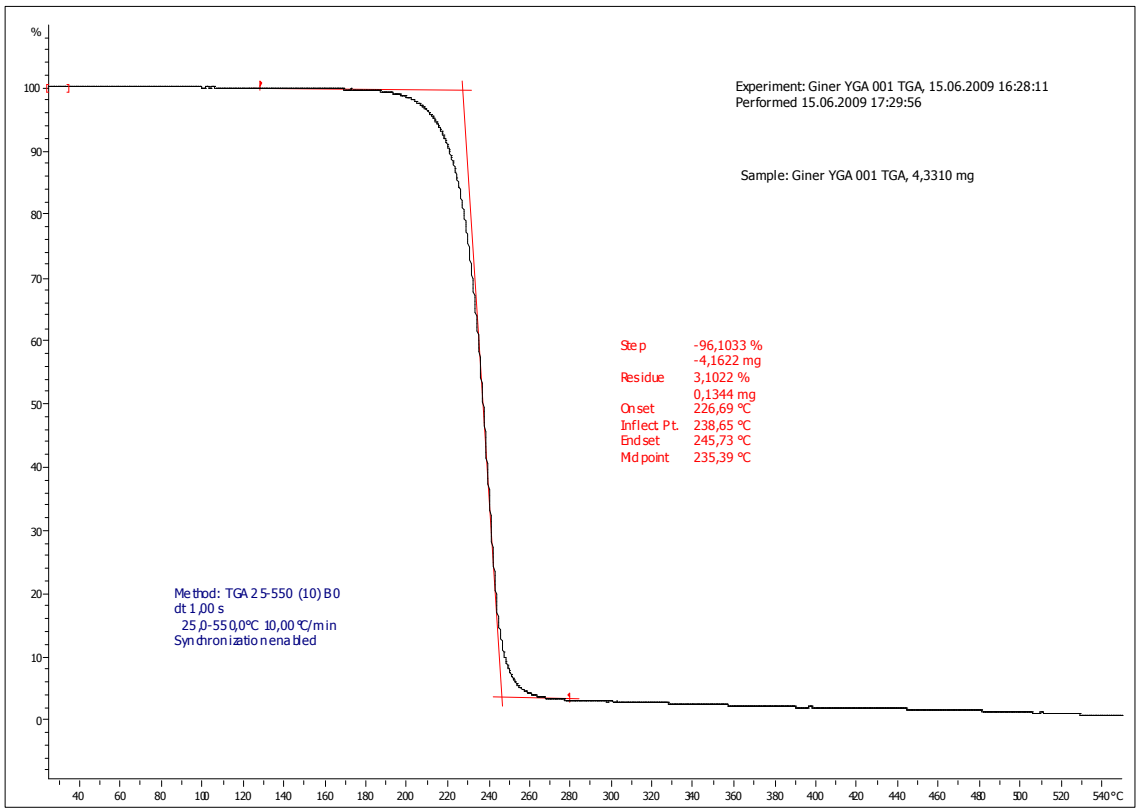
IR Spectrum (KBr) for compound (6)



IR Spectrum (KBr) for compound (7)

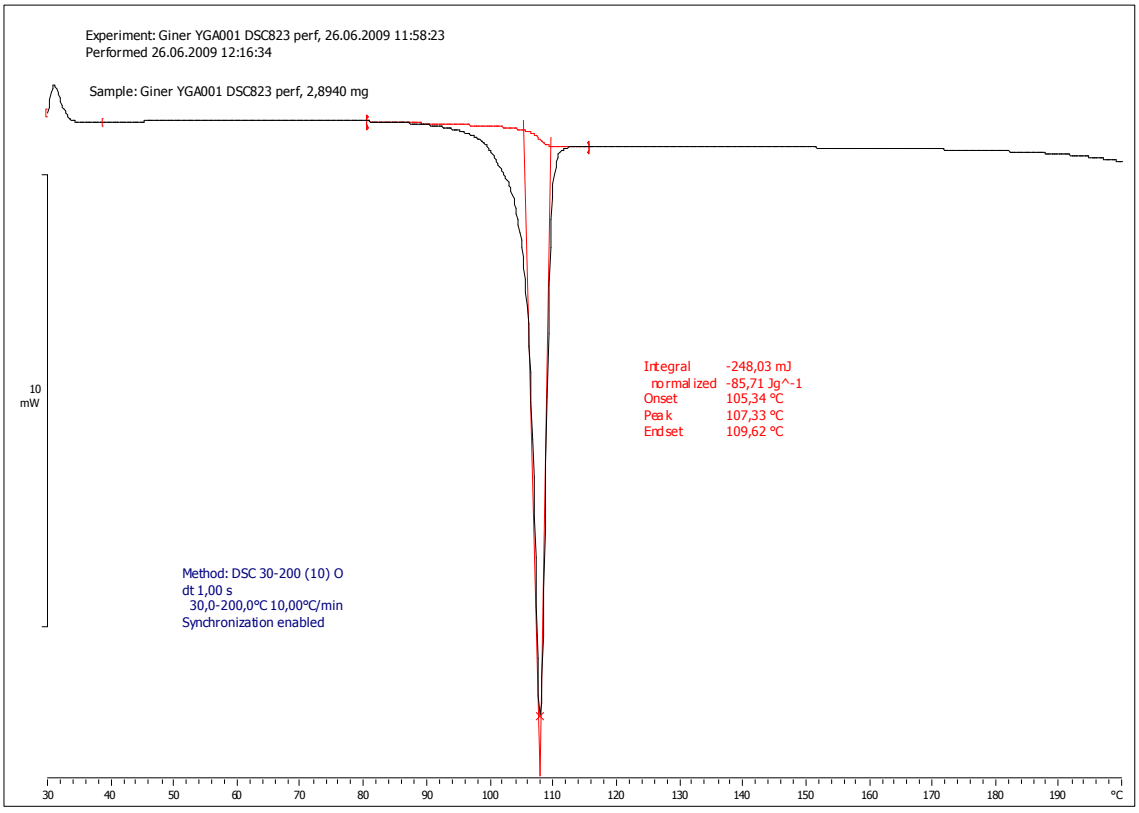


TGA and DSC for compound (1)



Lab: IQAC STARe SW 9.20

^exo



Lab: IQAC STARe SW 9.20

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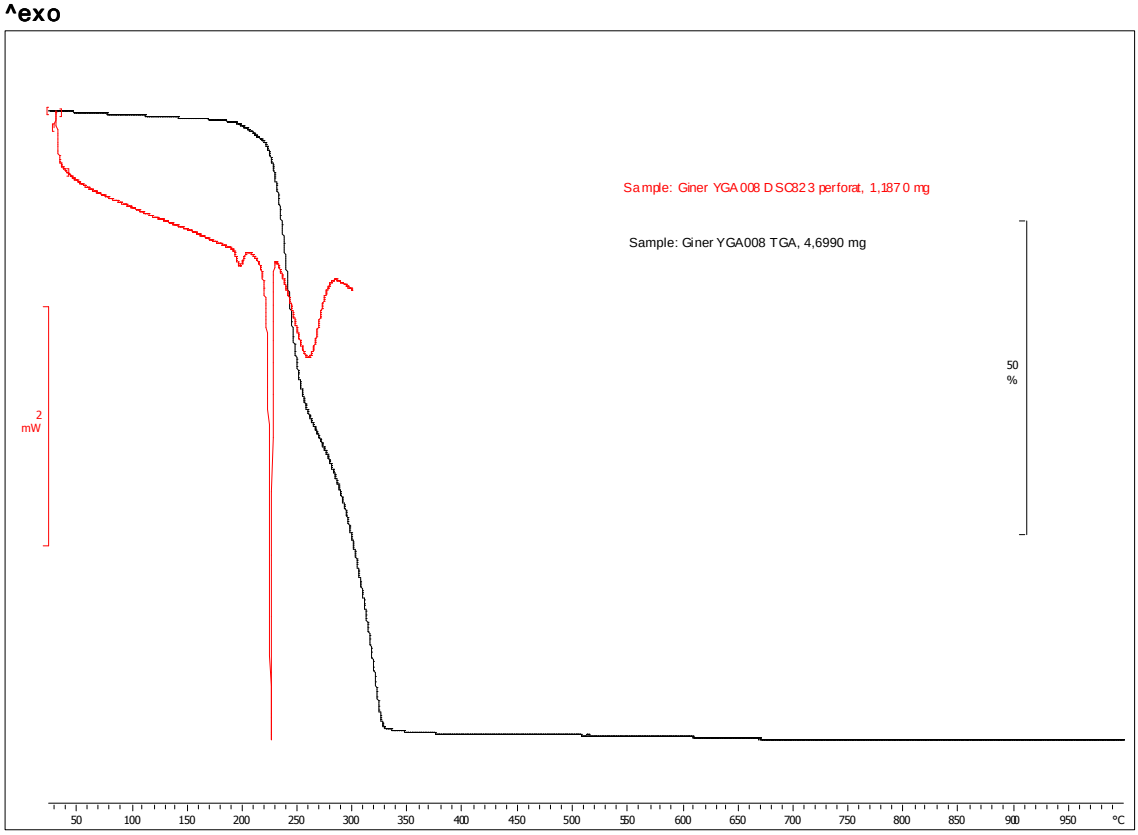

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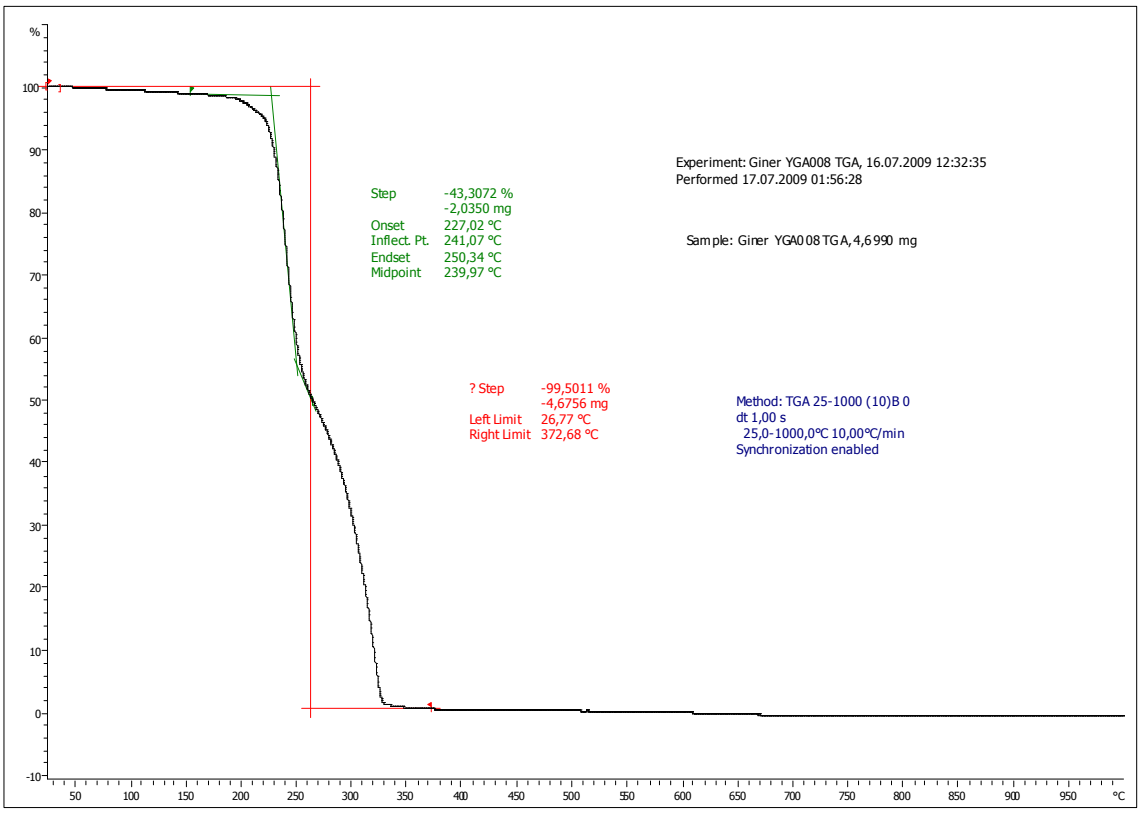
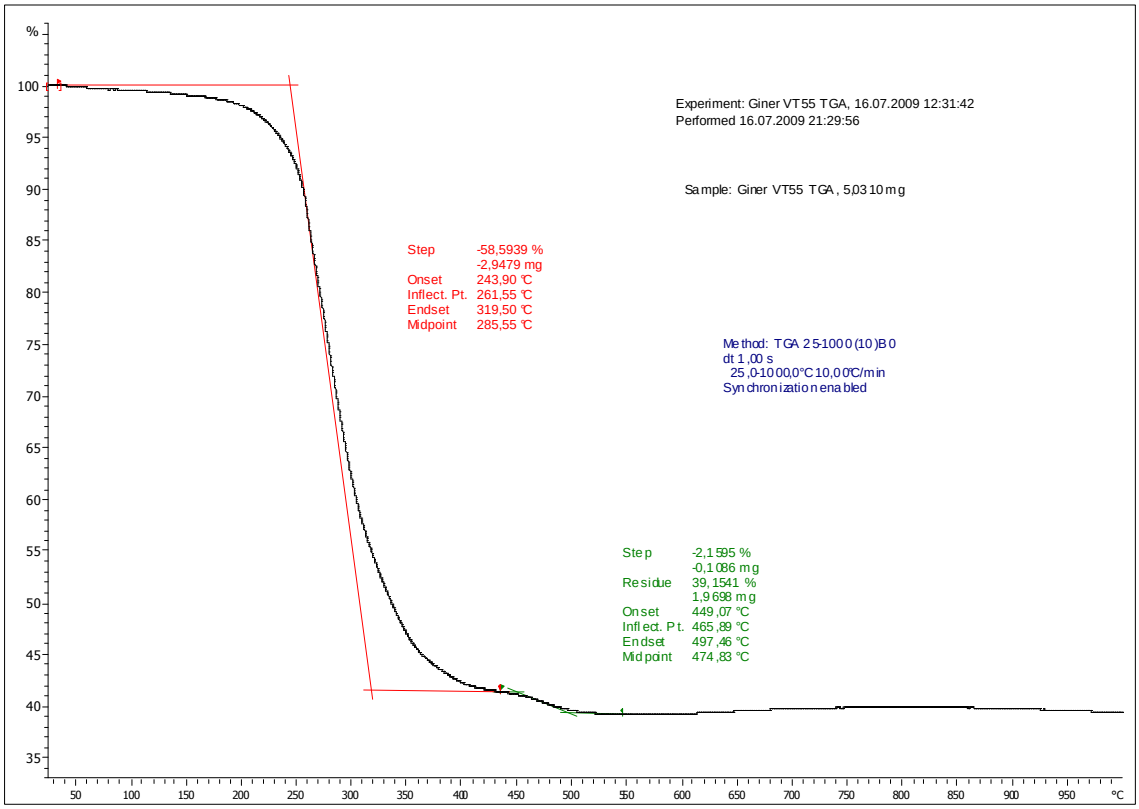


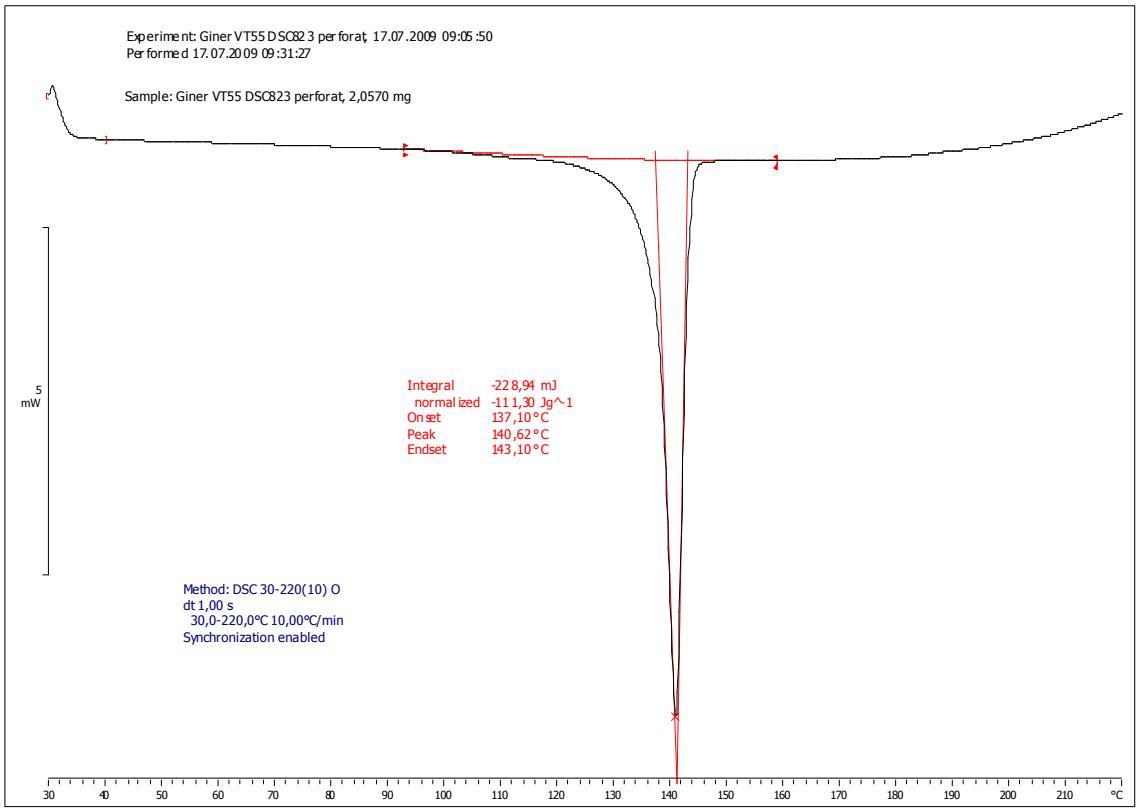
Lab: IQAC STARe SW 9.20

TGA and DSC for compound (3)



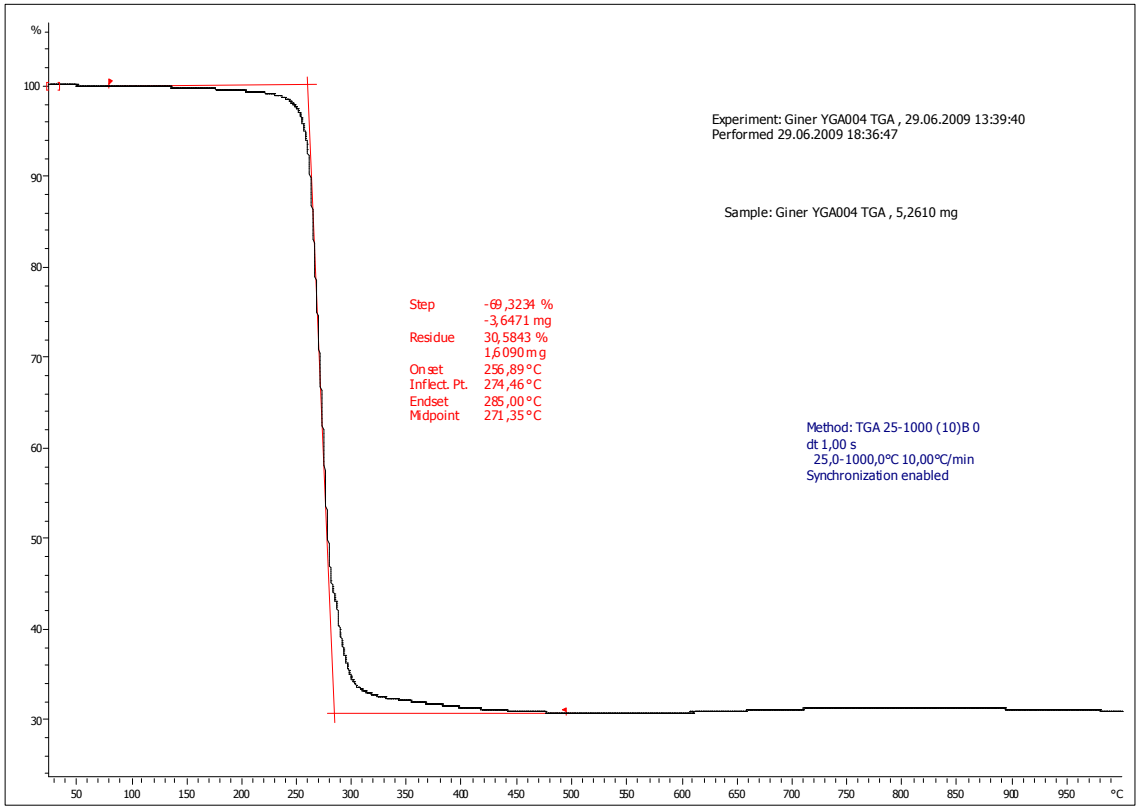
Lab: IQAC STARe SW 9.20

^exo

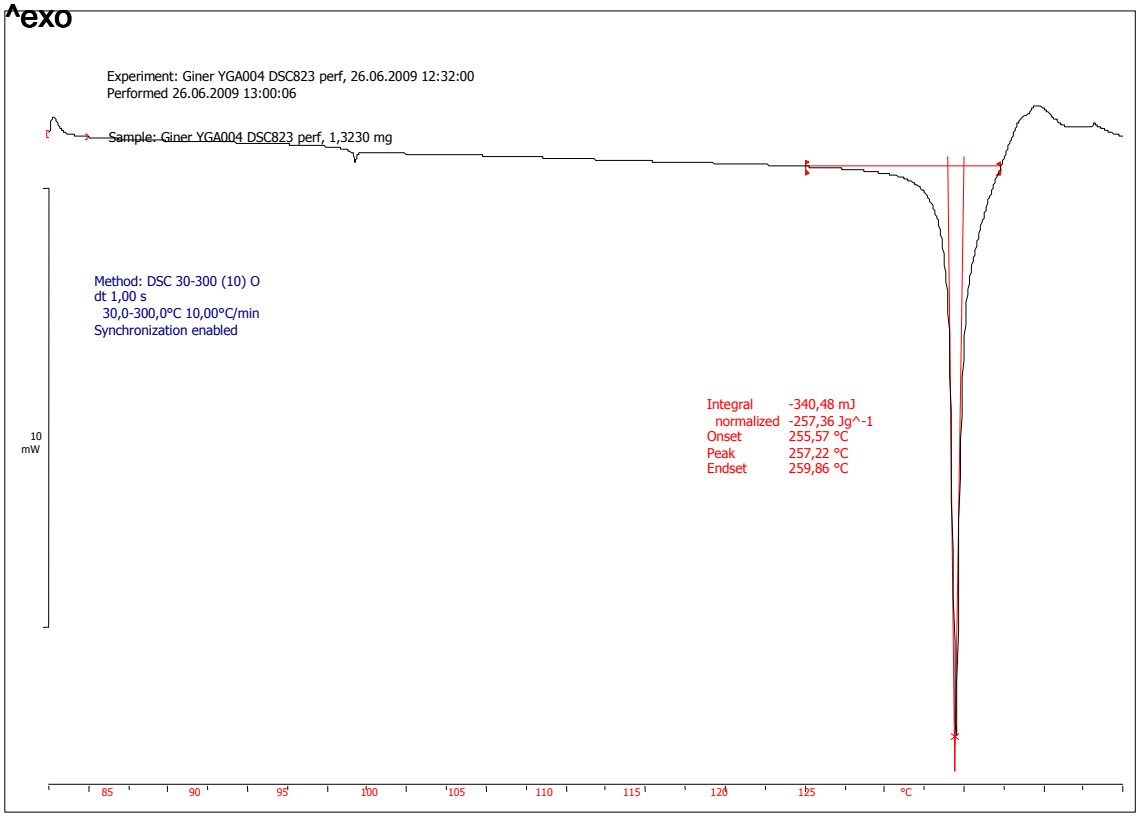


Lab: IQAC STARe SW 9.20

TGA and DSC for compound (4)

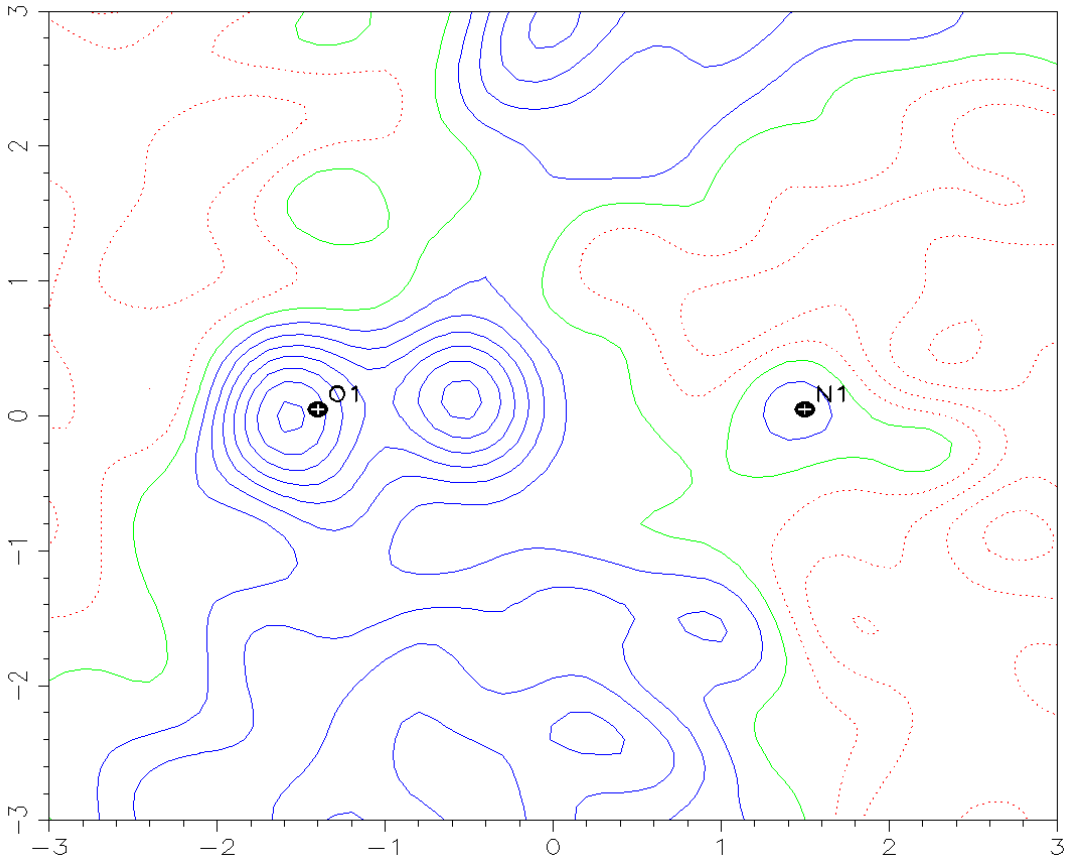


Lab: IQAC STARe SW 9.20



Lab: IQAC STARe SW 9.20

Electron density difference map showing the clear discrete position of the hydrogen peak between the donor (O1) and the acceptor (N1) in **3**.



O1–H1···N1

	D–H	H···A	D···A	D>H>A
Fixed	0.840	2.196	2.900	141.37
Refined	0.904	2.156	2.900	138.97

Computational details. Total energies computed at the B3LYP/6-311+G** level of calculation (in a.u.) and cartesian coordinates (in Å) of the energy minima for the monomer and dimer species.

A comparison between the interaction energies between X-ray and optimitzed structures has been done with the same level of theory.

	E_{int} (Kcal/mol)	
Compound	X-ray	Optimitzed
1	2.34	5.22
4	6.65	8.53

$1_{monomer}$
E= -717.15205

O	-0.70450200	1.98777700	-1.29607700
H	-1.54402700	2.45572300	-1.37001100
C	0.49054800	0.26387500	-0.11523000
C	1.92983200	0.97928000	0.37078400
C	1.93569000	2.46406600	0.70136000
H	1.36094300	3.03105300	-0.03112300
H	2.96550600	2.82093300	0.67673500
H	1.53632800	2.65050800	1.69898200
C	-0.75970900	1.18122500	-0.12164000
H	-0.66641400	1.82265800	0.76161300
C	-2.08623500	0.44724600	-0.00210000
C	-2.69478300	-0.13315100	-1.11998600
H	-2.20480800	-0.08324500	-2.08452300
C	-3.92464600	-0.77446700	-0.99545300
H	-4.38625500	-1.22379700	-1.86743700
C	-4.55982400	-0.84287800	0.24404000
H	-5.51641400	-1.34408900	0.33827900
C	-3.96372700	-0.25794800	1.35925200
H	-4.45549800	-0.29857300	2.32446600
C	-2.73587800	0.38843200	1.23366200
H	-2.27794900	0.84563300	2.10476300
B	1.94309000	-1.63658700	1.29951500
H	1.99143400	-2.36947300	2.22556100
B	1.74266100	0.54295900	-1.28926300
H	1.60050200	1.40742000	-2.06748100
B	0.80007700	-0.96338000	-1.26275800
H	0.00665400	-1.14265400	-2.11486600
B	0.42124700	-1.36306900	0.42854200
H	-0.63279900	-1.79992300	0.71523300

B	1.11202100	-0.09352200	1.45200100
H	0.56180100	0.39511500	2.37252700
B	3.25967600	0.25827600	-0.41892000
H	4.17251700	0.96263700	-0.67123300
B	2.56711000	-1.00534700	-1.45531600
H	3.06263300	-1.29239100	-2.48915800
B	1.75746200	-2.18858600	-0.39244800
H	1.66885600	-3.33317800	-0.67440600
B	2.87402100	-0.12405300	1.27044100
H	3.52684800	0.32164300	2.14738700
B	3.27879500	-1.42733900	0.13178600
H	4.29774400	-2.01905900	0.22727400

1_{dimer}
E= -1434.3124

O	1.07407300	-0.13416600	-0.44128300
H	0.21212100	0.04074900	-0.02673200
C	3.44758500	-0.32982400	-0.08842900
C	3.77217200	-1.93182100	-0.47374100
C	2.69770900	-2.97942200	-0.22542400
H	2.72268800	-3.33373900	0.80556800
H	2.88214600	-3.82966600	-0.88237500
H	1.70730000	-2.58513700	-0.45090400
C	2.06791100	-0.05653900	0.56680700
H	1.91879400	-0.86390200	1.29339200
C	1.98834500	1.25405200	1.34118200
C	1.71328500	2.46061300	0.68784900
H	1.59585200	2.46945000	-0.38877900
C	1.59255600	3.64371700	1.41495800
H	1.38680000	4.57399300	0.89714500
C	1.74476500	3.63525300	2.80188200
H	1.65325700	4.55672600	3.36562700
C	2.01362200	2.43625000	3.45859700
H	2.12802100	2.41947200	4.53657500
C	2.12906100	1.25295100	2.73102100
H	2.33215300	0.32170200	3.24962400
B	4.54955200	-1.21814500	0.89587300
H	4.16905200	-1.55289100	1.96000500
B	4.88040600	0.45791100	0.43275600
H	4.77977300	1.29631300	1.25268700
B	4.22445800	0.71177100	-1.19983000
H	3.69061600	1.72385000	-1.48156600
B	3.49965400	-0.81066800	-1.75910100
H	2.49326400	-0.89221000	-2.35333800
B	5.42313600	-2.28874600	-0.21313600
H	5.68200000	-3.37805300	0.16142500
B	6.15905700	-0.77105300	0.34455400
H	7.06020200	-0.76857600	1.10947900
B	5.96854300	0.43182600	-0.96558000
H	6.74549900	1.30689200	-1.13429400

B	5.10760900	-0.35044300	-2.31759400
H	5.26496900	-0.04906600	-3.44967200
B	4.78256100	-2.02969900	-1.84656100
H	4.61238300	-2.94945200	-2.56622800
B	6.30995200	-1.26888100	-1.36491200
H	7.33653300	-1.62920400	-1.82750600
O	-1.35169700	0.83372900	0.77605300
H	-1.00564800	1.72643400	0.91152000
C	-3.27912800	-0.49202700	0.17184700
C	-3.77134400	-1.30740500	1.56154400
C	-3.58222600	-0.63610700	2.91299300
H	-2.61638900	-0.13412000	2.97417000
H	-3.61371400	-1.40213700	3.68804200
H	-4.37744800	0.08234600	3.11419000
C	-2.72429300	0.94013700	0.37495900
H	-3.29288300	1.37225200	1.20364900
C	-2.89405600	1.86740100	-0.81747900
C	-2.01149600	1.83323200	-1.90213300
H	-1.19240600	1.12520500	-1.91477900
C	-2.18103900	2.71086000	-2.96973900
H	-1.49324000	2.67493500	-3.80679700
C	-3.22985200	3.63011700	-2.96597100
H	-3.35914300	4.31071500	-3.79970800
C	-4.10558700	3.67583500	-1.88376500
H	-4.91765100	4.39368600	-1.86876200
C	-3.93310300	2.80177600	-0.81256400
H	-4.61522300	2.84533100	0.03023700
B	-5.50328100	-2.02266800	-0.48677200
H	-6.61105600	-2.04667500	-0.89691700
B	-2.35493800	-1.84769500	0.74446000
H	-1.32133300	-1.64898200	1.26202000
B	-2.69098800	-1.60388600	-0.98408900
H	-1.80579000	-1.26255400	-1.68270200
B	-4.31056300	-0.88550300	-1.14357300
H	-4.51637500	-0.04961700	-1.94476300
B	-4.96336400	-0.65982500	0.48895000
H	-5.54018000	0.30064700	0.85356400
B	-3.54445600	-2.99018800	1.38531000
H	-3.25249100	-3.58955600	2.35909000
B	-2.87502900	-3.21037700	-0.24374400
H	-2.11261600	-4.08169700	-0.48061600
B	-4.09165600	-2.62250900	-1.41014200
H	-4.19583800	-3.07712200	-2.49583000
B	-5.15235600	-2.25515900	1.23907800
H	-5.94023000	-2.36373400	2.11120100
B	-4.61810300	-3.47603400	0.06102200
H	-5.10304600	-4.55356400	0.04370100

4$_{\textbf{monomer}}$
E= -733.18930

C	-0.48487100	0.25937000	0.24370900
C	-1.82200900	1.00095400	-0.49767300
C	0.78118700	1.14269400	0.47838800
H	0.68387300	2.00959800	-0.18378700
C	2.08511200	0.44574800	0.12660500
C	2.78751200	-0.29264100	1.07827500
H	2.41803100	-0.38195900	2.09100200
C	3.98357200	-0.89977300	0.70473900
H	4.54746600	-1.48067700	1.42881500
N	4.51060500	-0.81698200	-0.52120500
C	3.83805300	-0.09743700	-1.42209100
H	4.28259300	-0.02867500	-2.41087200
C	2.63533700	0.55180400	-1.14923800
H	2.14953900	1.13115400	-1.92573700
C	-1.73208700	2.46031700	-0.91647800
H	-1.43013100	3.10437200	-0.08971900
H	-2.72012200	2.78368500	-1.24440300
H	-1.04060300	2.59753800	-1.74795500
B	-1.88370600	0.64755800	1.18128700
H	-1.82745700	1.56122400	1.92768000
B	-1.01864100	-0.89098300	1.39268100
H	-0.36445400	-1.03241300	2.36193800
B	-0.41374600	-1.39753200	-0.19966800
H	0.64930000	-1.88771700	-0.30863600
B	-0.88792700	-0.15472200	-1.37633500
H	-0.19935200	0.25961000	-2.23621100
B	-3.27969800	0.37249400	0.13030300
H	-4.18654200	1.12287300	0.21367600
B	-2.79647600	-0.85196700	1.32436400
H	-3.44861300	-1.05400000	2.28833900
B	-1.89181900	-2.12359600	0.45419000
H	-1.89804400	-3.25111800	0.80704800
B	-1.80082500	-1.66187700	-1.27153800
H	-1.74771000	-2.44388200	-2.15520500
B	-2.66293200	-0.12157600	-1.46050300
H	-3.16024600	0.29117500	-2.44802000
B	-3.28496400	-1.34092800	-0.32682700
H	-4.30308400	-1.90043500	-0.54222800
O	0.89373100	1.57447200	1.82228600
H	0.04430800	1.91216700	2.12724100

4_{dimer}

E= -1466.39219

C	5.28365200	-0.22751400	0.26257200
C	6.55832100	-0.88400800	-0.64743000
C	4.27719600	-1.23417700	0.90080800
H	4.40984300	-2.18574000	0.37524200
C	2.82064300	-0.82954100	0.73951200
C	2.18581800	-0.03144500	1.69138800
H	2.72181600	0.32141000	2.56176800

C	0.84724100	0.29382900	1.50823200
H	0.33212600	0.91999600	2.22978500
N	0.12253200	-0.12831000	0.46362800
C	0.73266100	-0.89962400	-0.44339600
H	0.12537200	-1.23102200	-1.27961100
C	2.06806100	-1.27684900	-0.34434100
H	2.50044600	-1.91479600	-1.10579400
C	6.65353400	-2.39127000	-0.82478900
H	6.64631800	-2.91644800	0.13119700
H	7.59828500	-2.61830000	-1.31919400
H	5.84732800	-2.77384700	-1.45106200
B	6.88610700	-0.23246500	0.90799000
H	7.14364500	-0.99852000	1.76951000
B	5.81437100	1.17378000	1.08930300
H	5.34895200	1.38492200	2.15084900
B	4.82587200	1.29574400	-0.38189900
H	3.69028200	1.59484100	-0.31703200
B	5.27460200	-0.05135100	-1.44759300
H	4.51423700	-0.70783500	-2.06134000
B	7.97108900	0.05376100	-0.45809700
H	8.99682900	-0.52881100	-0.47470900
B	7.52045700	1.38533200	0.62979900
H	8.30195000	1.84730400	1.38514500
B	6.24667700	2.33738400	-0.18519900
H	6.11553900	3.49734300	-0.00518600
B	5.90164000	1.56976000	-1.76470500
H	5.53125800	2.16496400	-2.71493700
B	6.97302400	0.16218200	-1.92346400
H	7.33066000	-0.34221100	-2.92828300
B	7.57633600	1.64131900	-1.14163000
H	8.41271200	2.29706500	-1.65710400
O	4.49711000	-1.41437300	2.28714800
H	5.43735200	-1.54604800	2.45279000
C	-4.41410700	-0.39600000	-0.13170800
C	-4.19715500	-1.85863300	0.68246600
C	-3.46943400	0.79246600	0.25683700
H	-3.19173000	0.63304300	1.30354400
C	-4.16910300	2.14377800	0.17973600
C	-4.12396700	2.90704900	-0.98627100
H	-3.59009300	2.54951100	-1.85654000
C	-4.76112900	4.14462300	-1.00301200
H	-4.74183800	4.75408600	-1.90223400
N	-5.41492300	4.66207100	0.04291000
C	-5.44143900	3.93085700	1.15963600
H	-5.96669600	4.36556300	2.00574800
C	-4.83906700	2.67974800	1.27824400
H	-4.89830500	2.14179600	2.21784000
C	-3.12013600	-1.96051300	1.75124700
H	-2.14657700	-1.64581800	1.37443700
H	-3.04084000	-3.00256900	2.06236300

H	-3.37391700	-1.36706100	2.63043400
B	-3.69225200	-1.73763400	-0.95848200
H	-2.53819500	-1.70926100	-1.16950600
B	-4.89146100	-0.69097900	-1.74414100
H	-4.51901200	0.06136300	-2.57067000
B	-6.07573200	-0.18301400	-0.52045200
H	-6.50277500	0.91233300	-0.52132300
B	-5.58539900	-0.89305600	1.02654500
H	-5.60109300	-0.33295600	2.06325000
B	-4.52319000	-3.17761100	-0.34841200
H	-3.87858800	-4.15301800	-0.18200200
B	-4.99071500	-2.46018200	-1.90326200
H	-4.74066900	-2.99900700	-2.92530300
B	-6.47277500	-1.50379300	-1.62993700
H	-7.28908400	-1.35307000	-2.47141900
B	-6.90085700	-1.62248400	0.10295000
H	-8.00852800	-1.56192800	0.51064900
B	-5.69123400	-2.65973800	0.88295600
H	-5.83155100	-3.28714900	1.87345800
B	-6.24208900	-3.03973300	-0.76239600
H	-6.88923600	-4.00637500	-0.97368300
O	-2.32718600	0.82396500	-0.56129900
H	-1.54075800	0.47041100	-0.09137600