

TABLE OF CONTENTS

A	Results 1 - Application of ball milling technology for production of co-crystals (Chapter 4)	4
A.1	Caffeine/oxalic acid	4
A.2	2,4,6-trinitrotoluene/naphthalene	11
A.3	2,4,6-trinitrotoluene/anthracene	18
A.4	2,4,6-trinitrotoluene/1,4-dimethoxybenzene	24
B	Results 2 – Investigation of co-crystallisation potential in electron deficient ring systems (Chapter 5)	31
B.1	1,3-dinitrobenzene/2,4-dinitroaniline	31
B.2	1,3-dinitrobenzene/2,4-dinitroanisole	36
B.3	1,3-dinitrobenzene/1,3,5-trichloro-,2,4,6-trinitrobenzene	41
B.4	1,3-dinitrobenzene/2,4,6-trinitroaniline	45
B.5	2,4-dinitrotoluene/2,4-dinitroaniline	47
B.6	2,4-dinitrotoluene/2,4-dinitroanisole	52
B.7	2,4-dinitrotoluene/1,3-dinitrobenzene	61
B.8	2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene	66
B.9	2,4-dinitrotoluene/2,4,6-trinitroaniline	71
B.10	2,4-dinitrotoluene/2,4,6-trinitrotoluene	72
B.11	2,4,6-trinitrotoluene/2,4-dinitroaniline	77
B.12	2,4,6-trinitrotoluene/2,4-dinitroanisole	81
B.13	2,4,6-trinitrotoluene/1,3-dinitrobenzene	86
B.14	2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene	91
B.15	2,4,6-trinitrotoluene/2,4,6-trinitroaniline	96
B.16	Molecular electrostatic potential	97
C	Results 3 – Manipulation of electrostatic potential and its effect on co-crystal formation	101
C.1	2-naphthol/pyrrolidine	101
C.2	2-naphthol/3-pyrroline	102
C.3	2-naphthol/pyrrole	103
C.4	2-naphthol/2-nitropyrrole	104
C.5	2-naphthol/2-methylpyrrole	105
C.6	2-naphthol/3-methylpyrrole	106
C.7	2-naphthol/2,4-dimethylpyrrole	107
C.8	2-naphthol/2,5-dimethylpyrrole	108
C.9	2-naphthol/pyrazole	109
C.10	2-naphthol/3-nitropyrazole	110
C.11	2-naphthol/4-nitropyrazole	111
C.12	2-naphthol/5-methylpyrazole	112
C.13	2-naphthol/pyrazol-4-amine	113

C.14	2-naphthol/3-bromopyrazole.....	114
C.15	2-naphthol/4-bromopyrazole.....	115
C.16	2-naphthol/3,4-dimethylpyrazole	116
C.17	2-naphthol/3,5-dimethylpyrazole	117
C.18	2-naphthol/3,4,5-tribromopyrazole.....	119
C.19	2-naphthol/3-methyl-5-nitropyrazole	120
C.20	2-naphthol/5-methylpyrazol-3-amine	121
C.21	2-naphthol/4-bromopyrazol-3-amine.....	122
C.22	2-naphthol/3-bromopyrazol-5-amine.....	123
C.23	2-naphthol/3,5-dimethylpyrazol-4-amine	124
C.24	2-naphthol/3,4-dimethylpyrazol-5-amine	125
C.25	2-naphthol/3-methyl-4-bromopyrazole.....	126
C.26	2-naphthol/3-bromo-5-methylpyrazole.....	127
C.27	2-naphthol/4-bromo-3,5-dimethylpyrazole	128
C.28	2-naphthol/imidazole	129
C.29	2-naphthol/2-nitroimidazole	130
C.30	2-naphthol/2-methylimidazole.....	131
C.31	2-naphthol/4-methylimidazole.....	132
C.32	2-naphthol/imidazol-2-amine	133
C.33	2-naphthol/2-bromoimidazole	134
C.34	2-naphthol/4-bromoimidazole	135
C.35	2-naphthol/2,4-dimethylimidazole.....	136
C.36	2-naphthol/4,5-dinitroimidazole	137
C.37	2-naphthol/4,5-dichloroimidazole	138
C.38	2-naphthol/2,4,5-tribromoimidazole	139
C.39	2-naphthol/2-methyl-5-nitroimidazole	140
C.40	2-naphthol/4-methyl-5-nitroimidazole	141
C.41	2-naphthol/2-bromo-5-nitroimidazole.....	142
C.42	2-naphthol/4-bromo-2-methylimidazole	143
C.43	2-naphthol/5-bromo-4-methylimidazole	144
C.44	2-naphthol/4,5-dibromo-2-methylimidazole	145
C.45	2-naphthol/2,5-dibromo-4-methylimidazole	146
C.46	2-naphthol/1,2,3-triazole.....	147
C.47	2-naphthol/5-nitro-1,2,3-triazole	148
C.48	2-naphthol/1,2,4-triazole.....	149
C.49	2-naphthol/3-methyl-1,2,4-triazole	150
C.50	2-naphthol/1,2,4-triazol-3-amine.....	151
C.51	2-naphthol/5-bromo-1,2,4-triazole	152
C.52	2-naphthol/1,2,4-triazol-3,5-diamine	153
C.53	2-naphthol/3,5-dimethyl-1,2,4-triazole	154
C.54	2-naphthol/3,5-dibromo-1,2,4-triazole.....	155

C.55	2-naphthol/1,2,3,4-tetrazole.....	156
C.56	2-naphthol/1,2,3,4-tetrazol-5-amine.....	157
C.57	2-naphthol/5-methyl-1,2,3,4-tetrazole.....	158
C.58	2-naphthol/3-nitro-1,2,4-triazol-5-one	159
C.59	Molecular Electrostatic Potentials.....	160

A Results 1 - Application of ball milling technology for production of co-crystals (Chapter 4)

A.1 Caffeine/oxalic acid

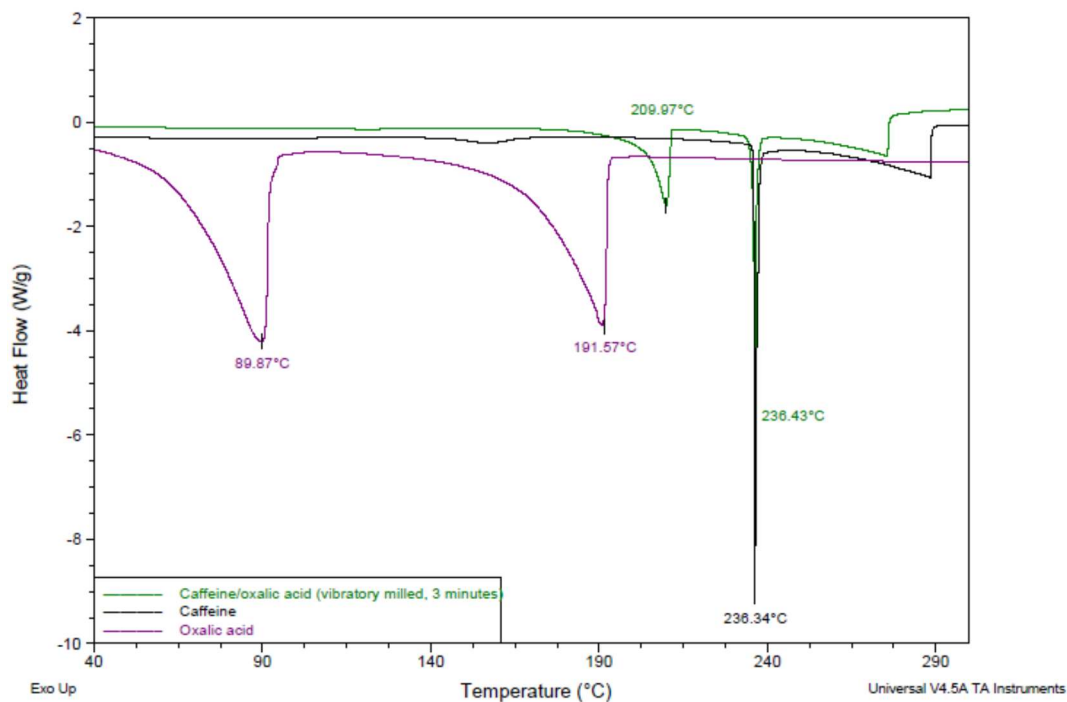


Figure A.1 - Thermal analysis of caffeine/oxalic acid produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

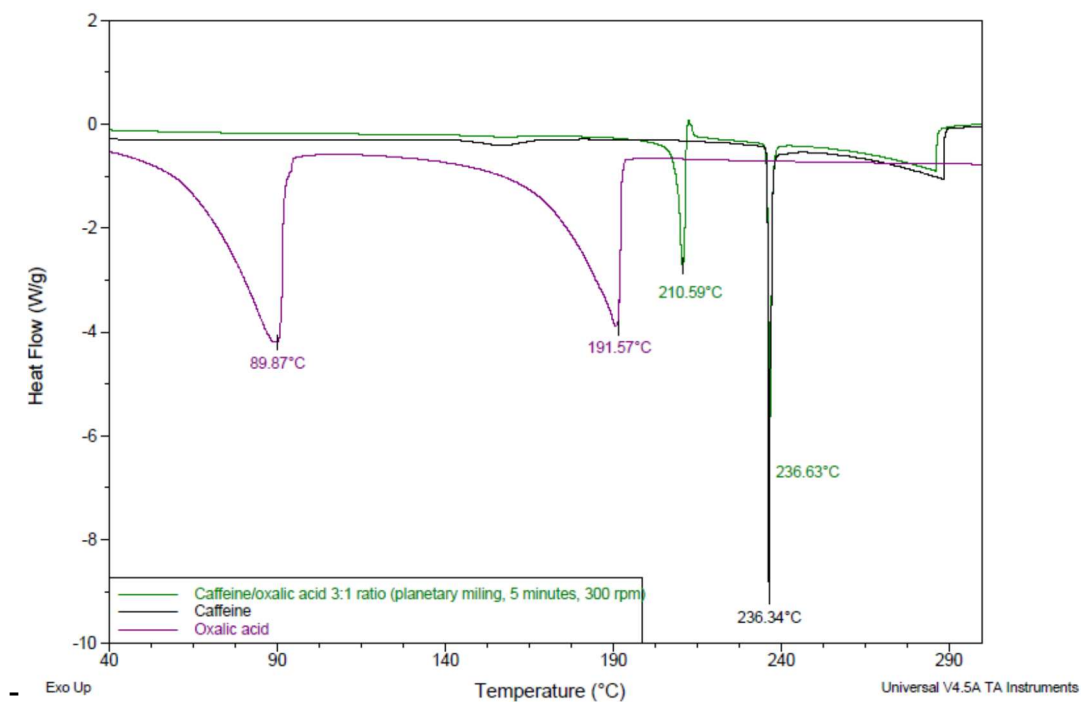


Figure A.2 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

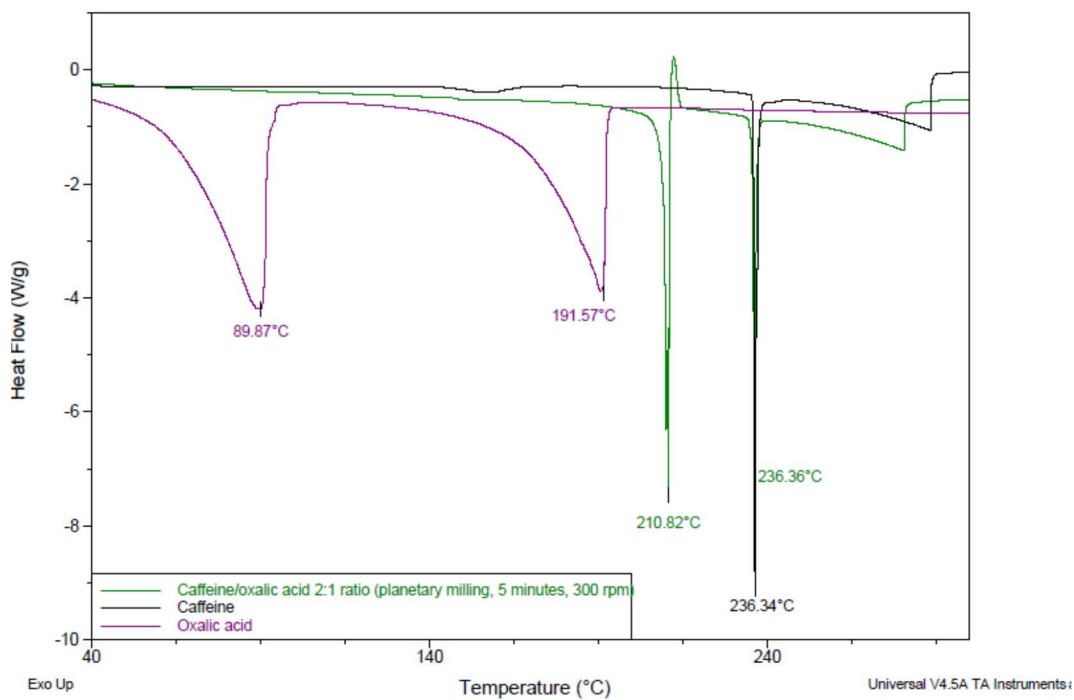


Figure A.3 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

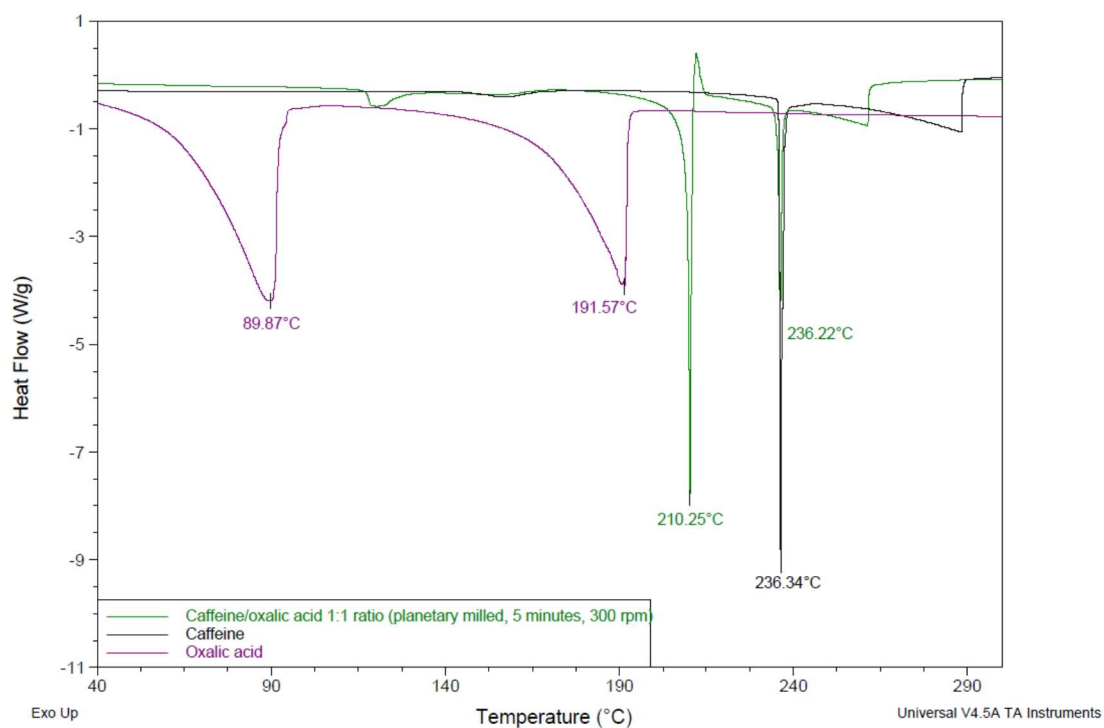


Figure A.4 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

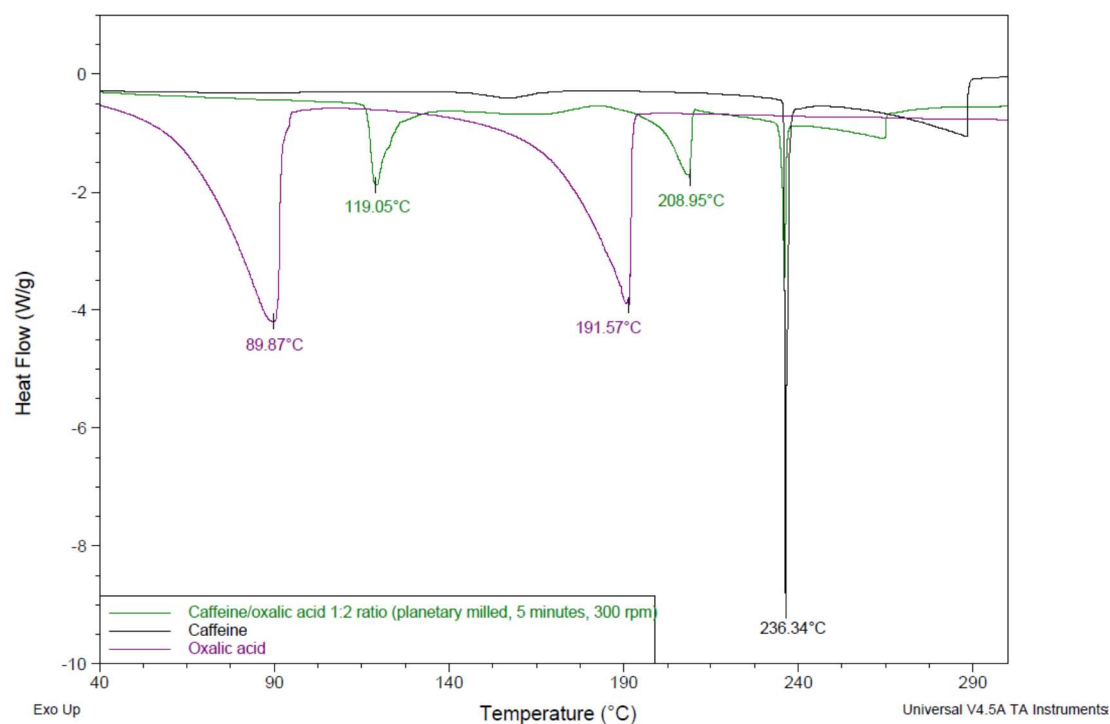


Figure A.5 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

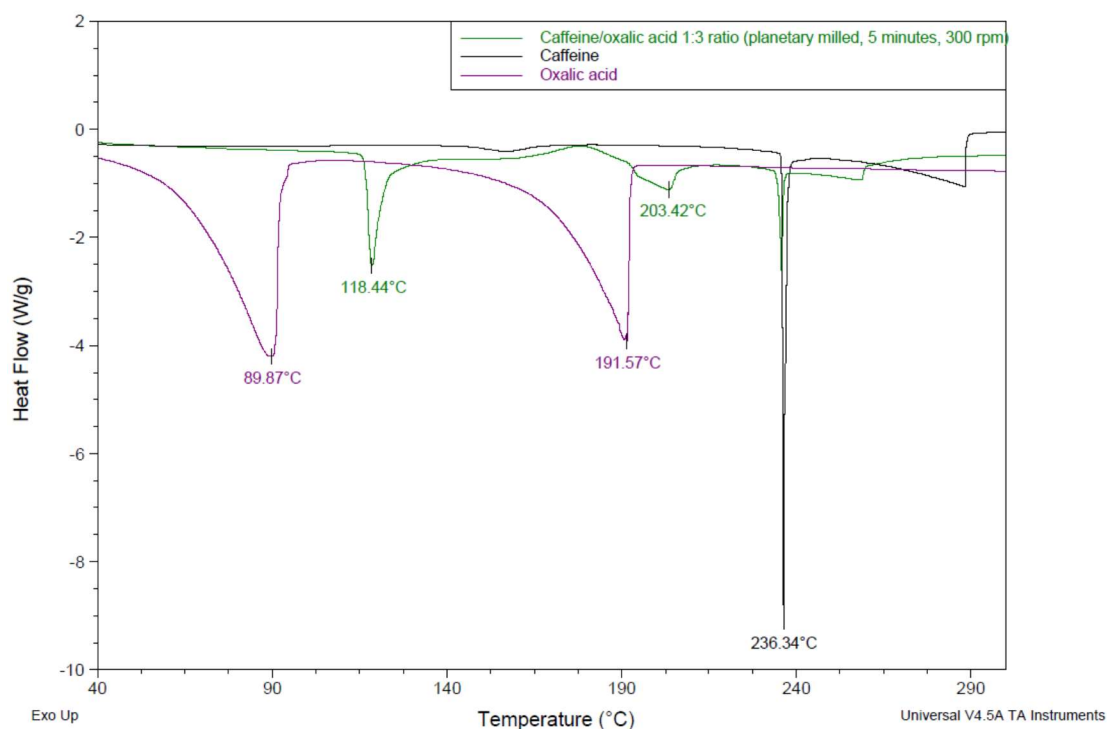


Figure A.6 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

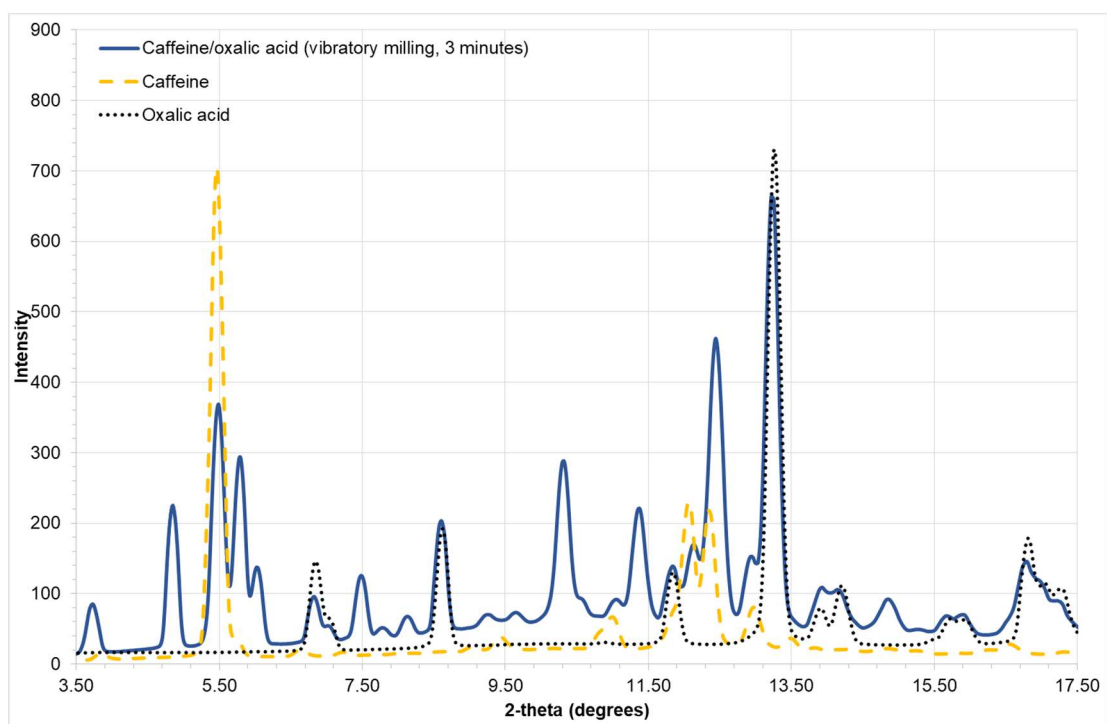


Figure A.7 - Powder x-ray pattern of caffeine/oxalic acid produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

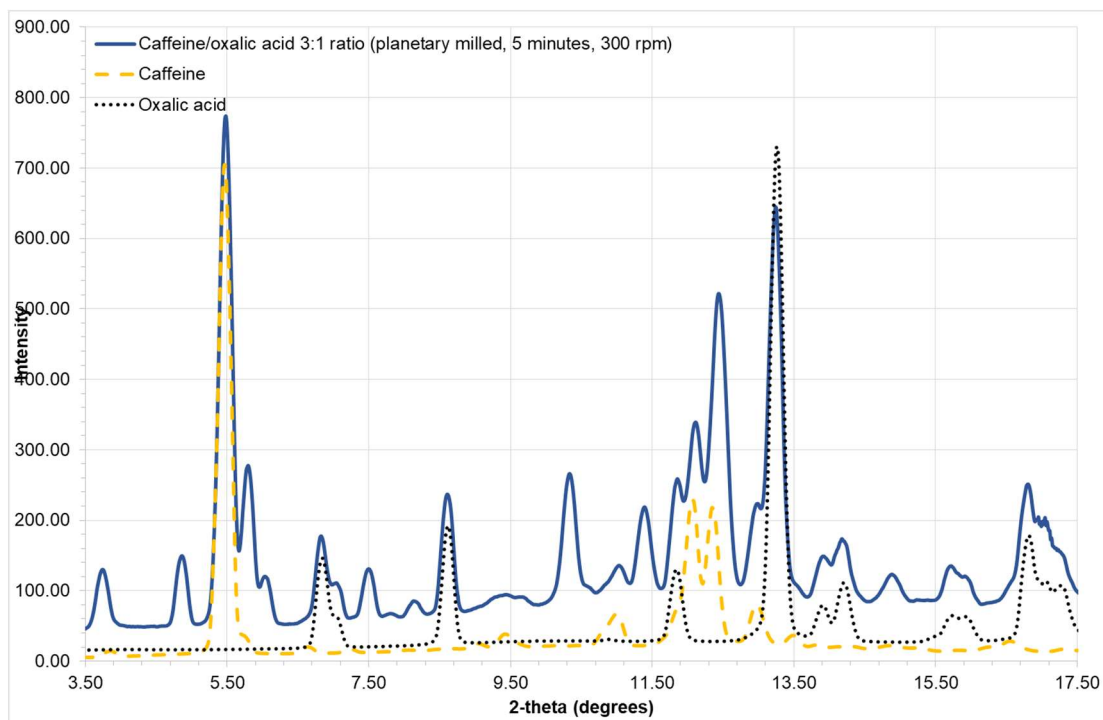


Figure A.8 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 3:1 stoichiometry.

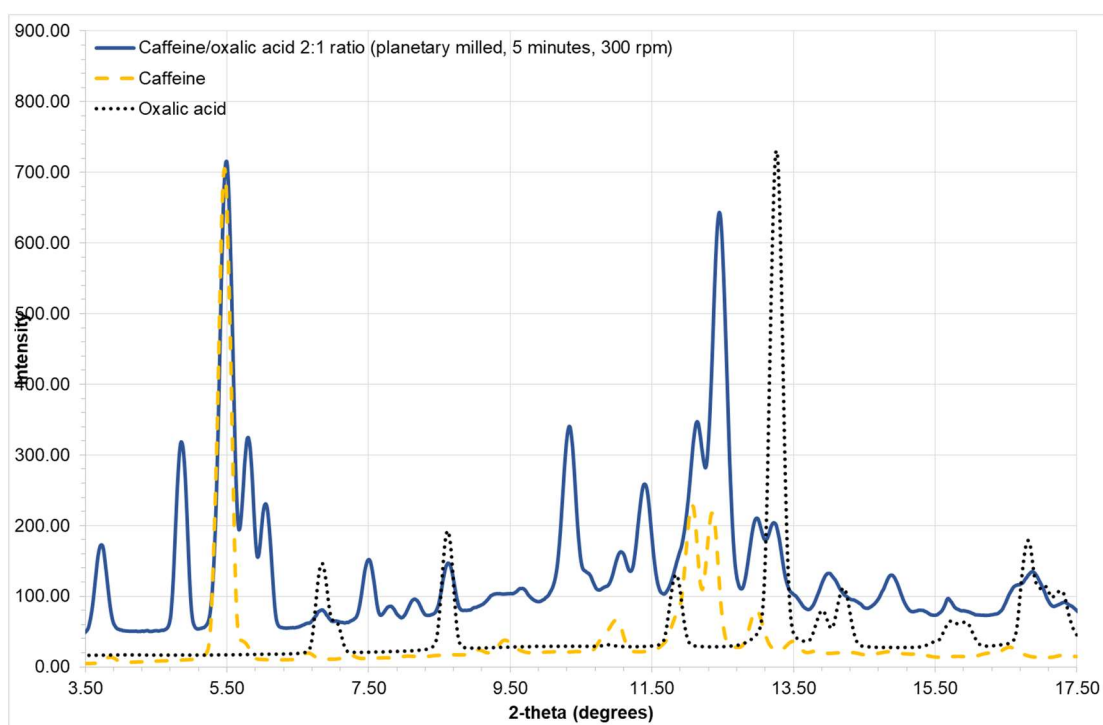


Figure A.9 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 2:1 stoichiometry.

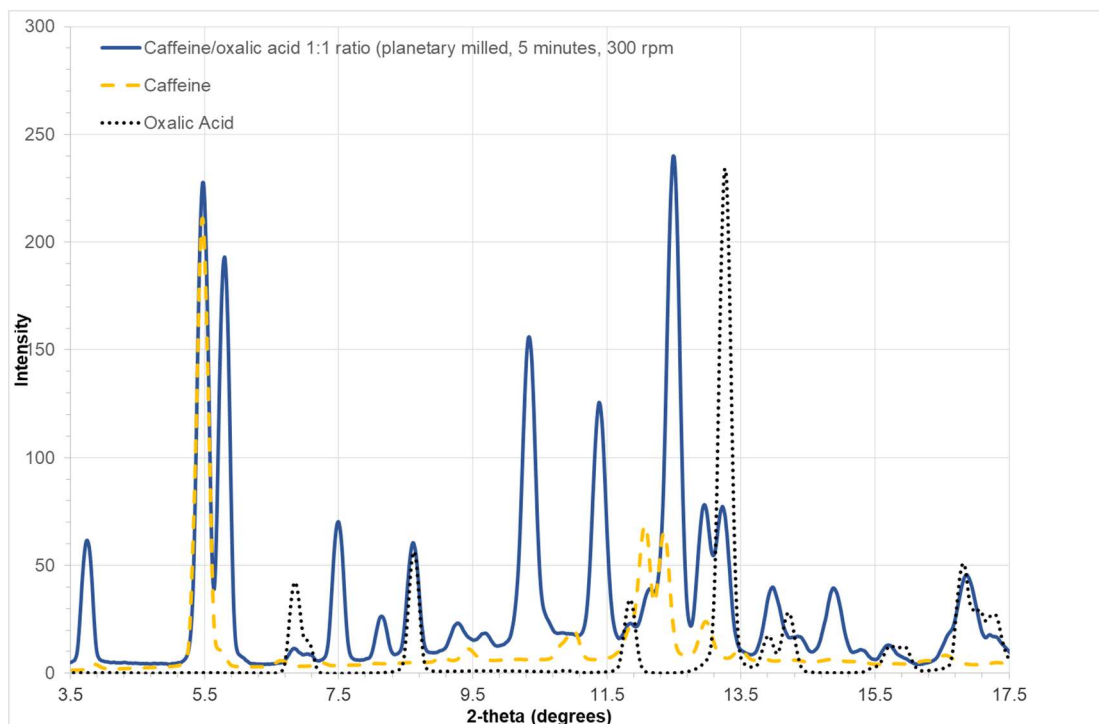


Figure A.10 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

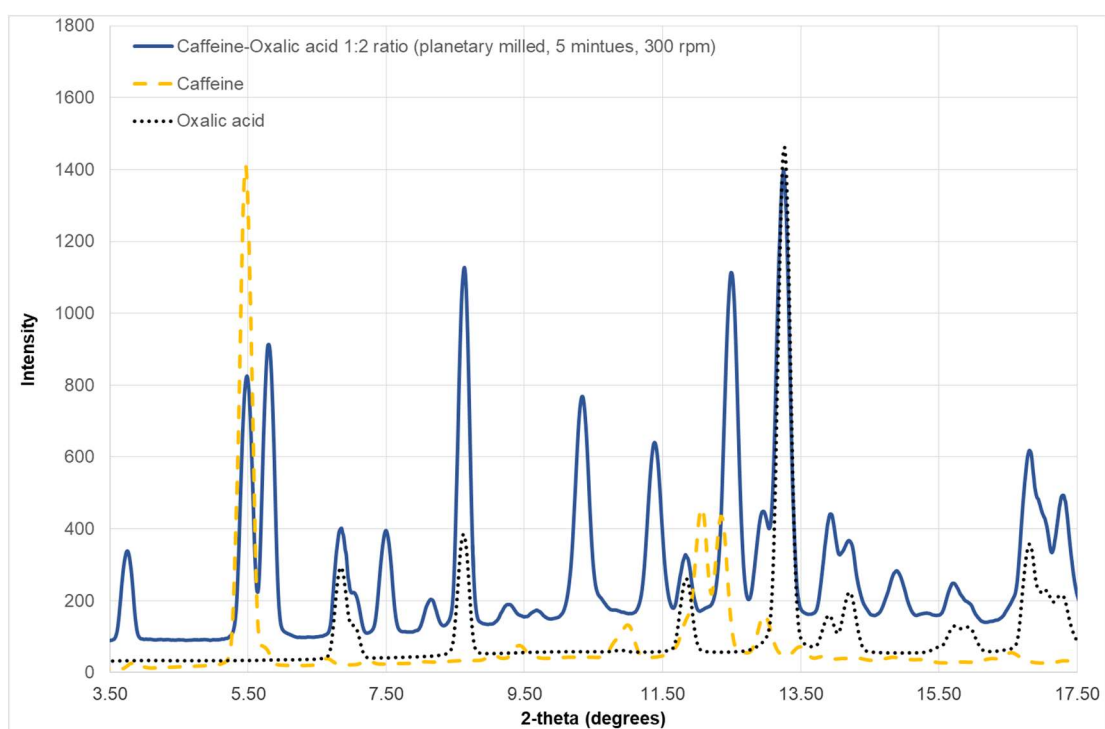


Figure A.11 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:2 stoichiometry.

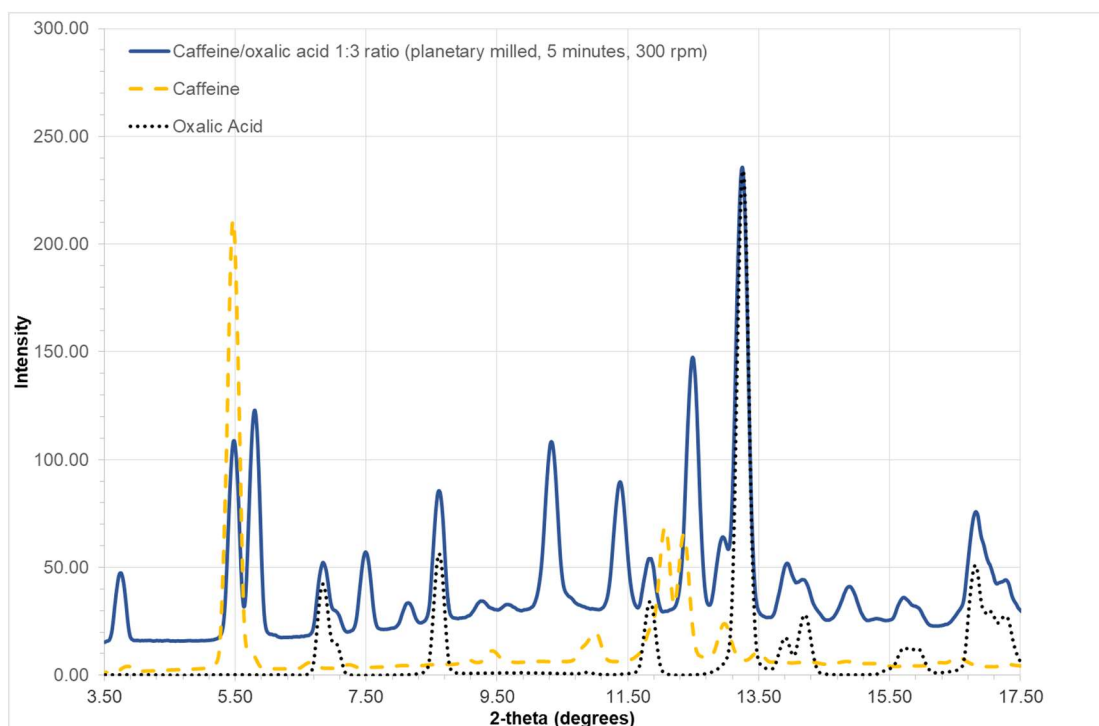


Figure A.12 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:3 stoichiometry.

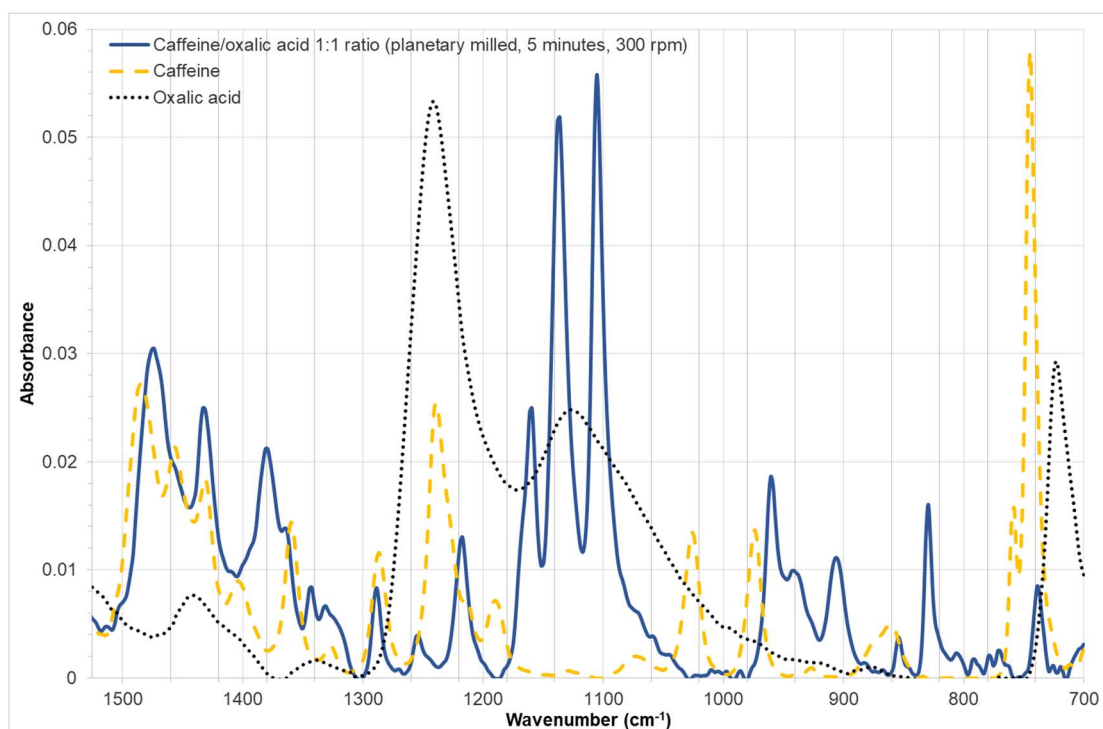


Figure A.13 - Infra-red spectra of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

A.2 2,4,6-trinitrotoluene/naphthalene

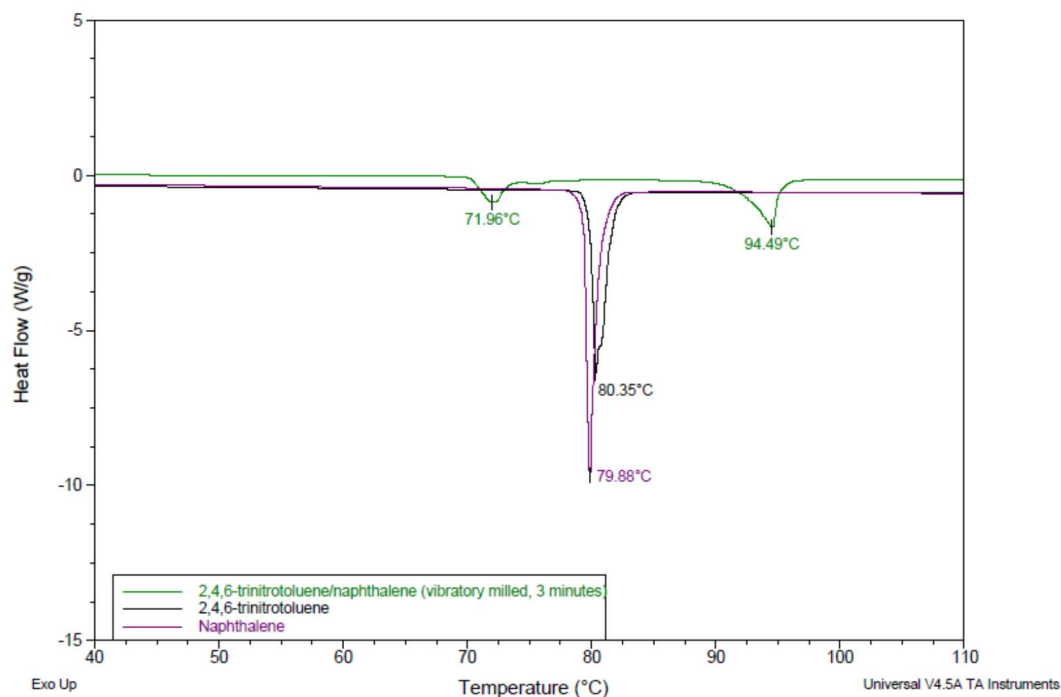


Figure A.14 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

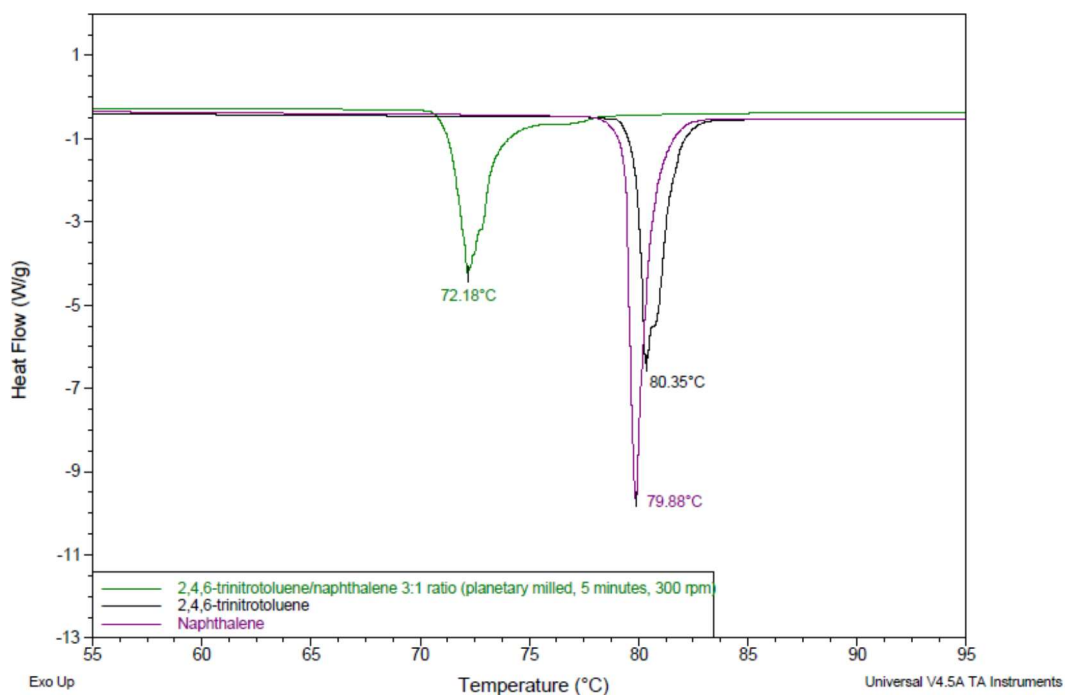


Figure A.15 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 3:1 stoichiometry.

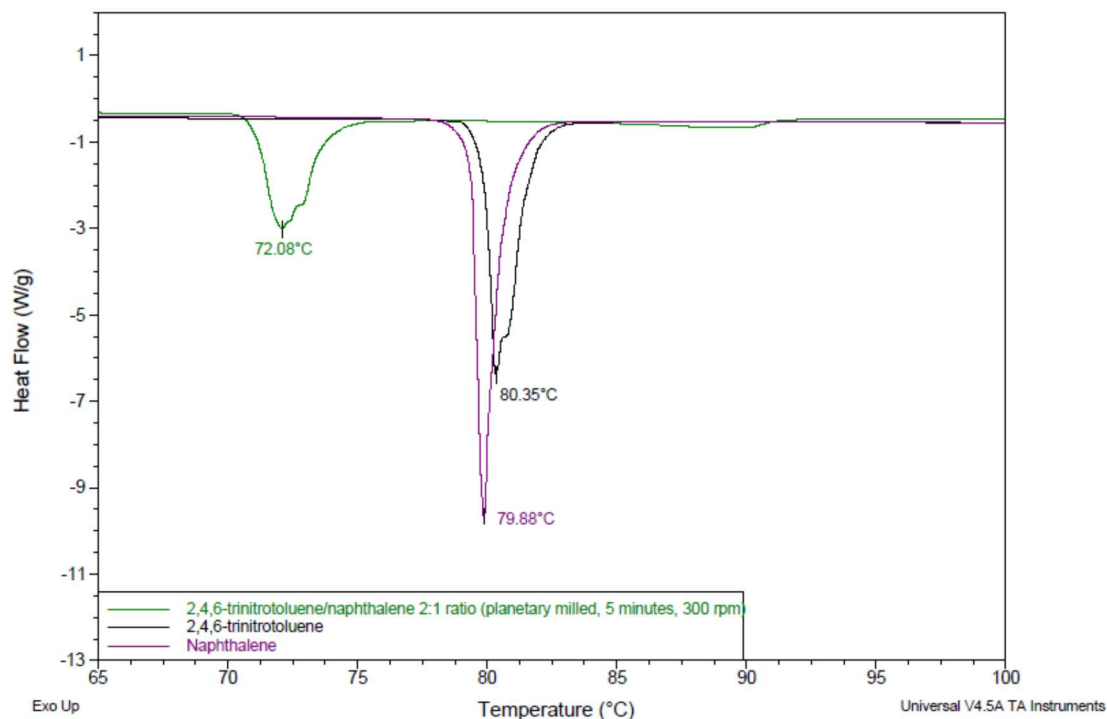


Figure A.16 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 2:1 stoichiometry.

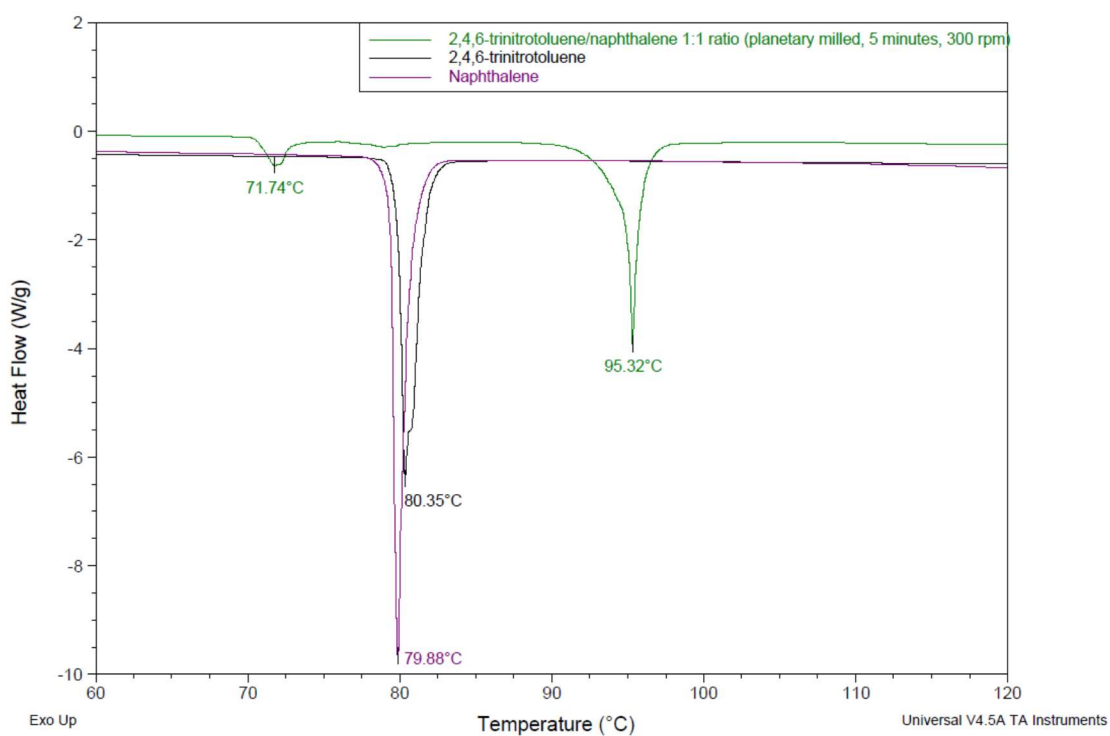


Figure A.17 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

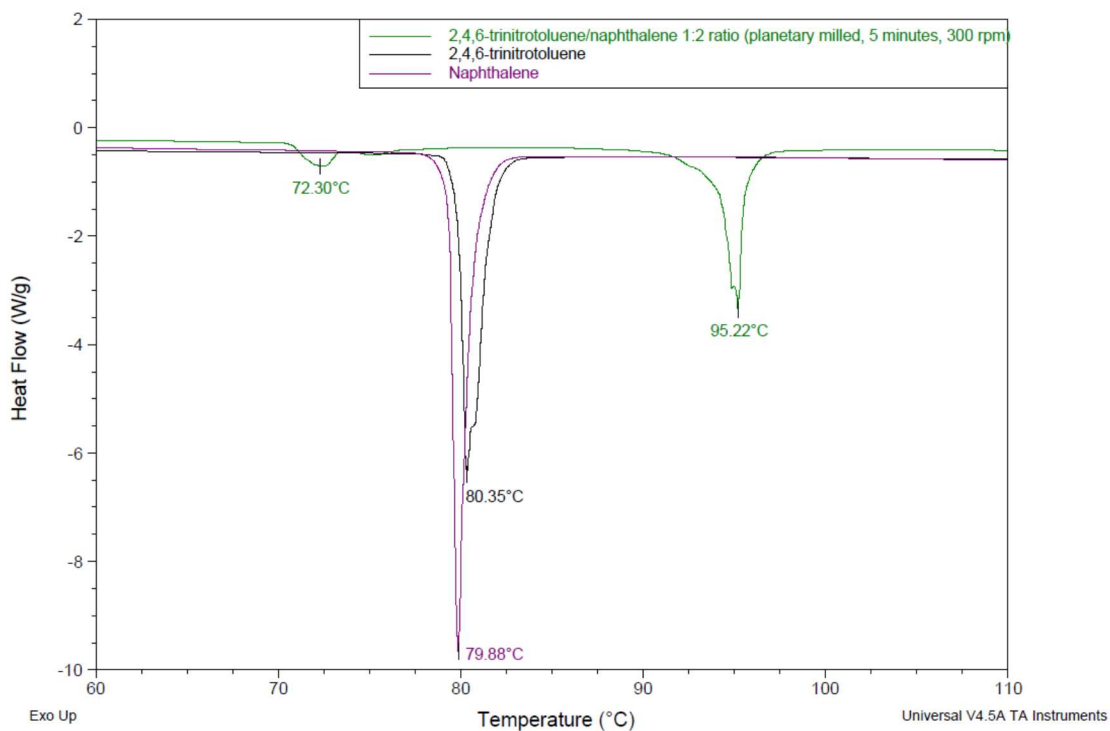


Figure A.18 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:2 stoichiometry.

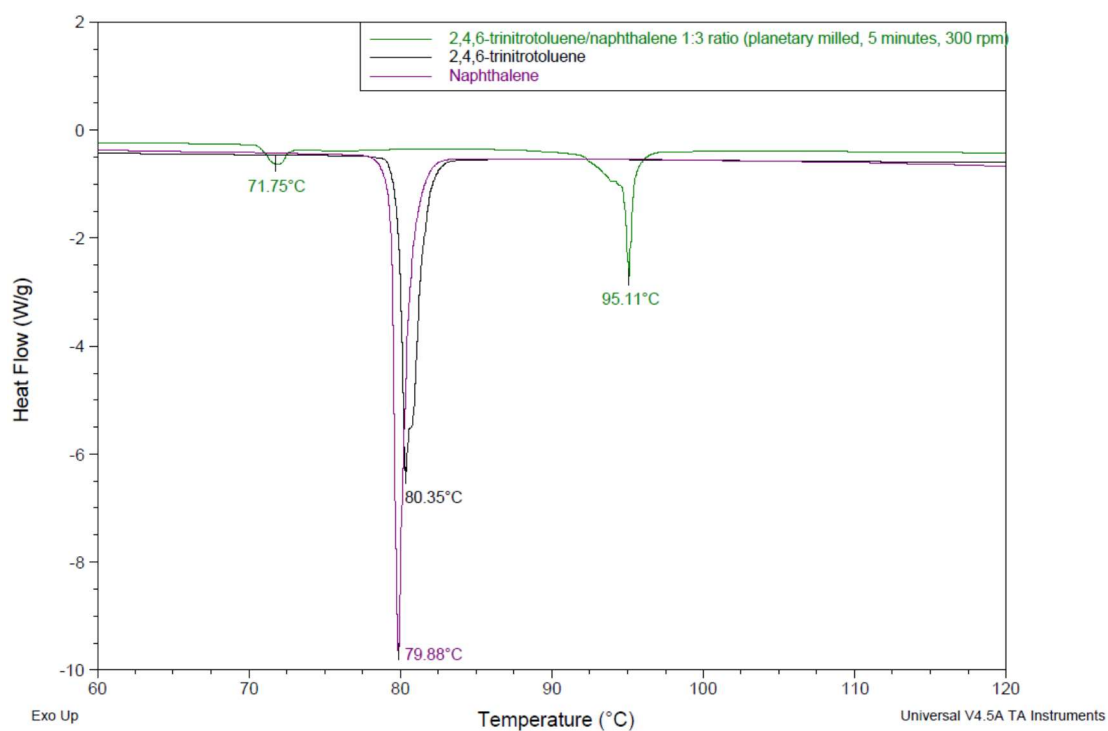


Figure A.19 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:3 stoichiometry.

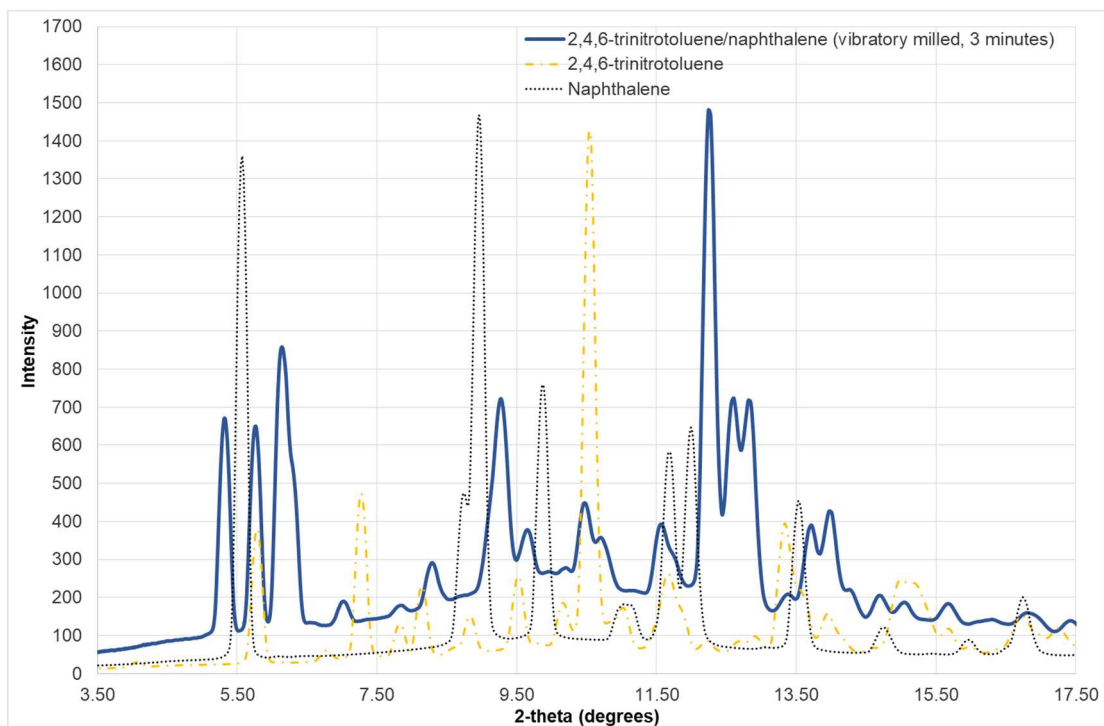


Figure A.20 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

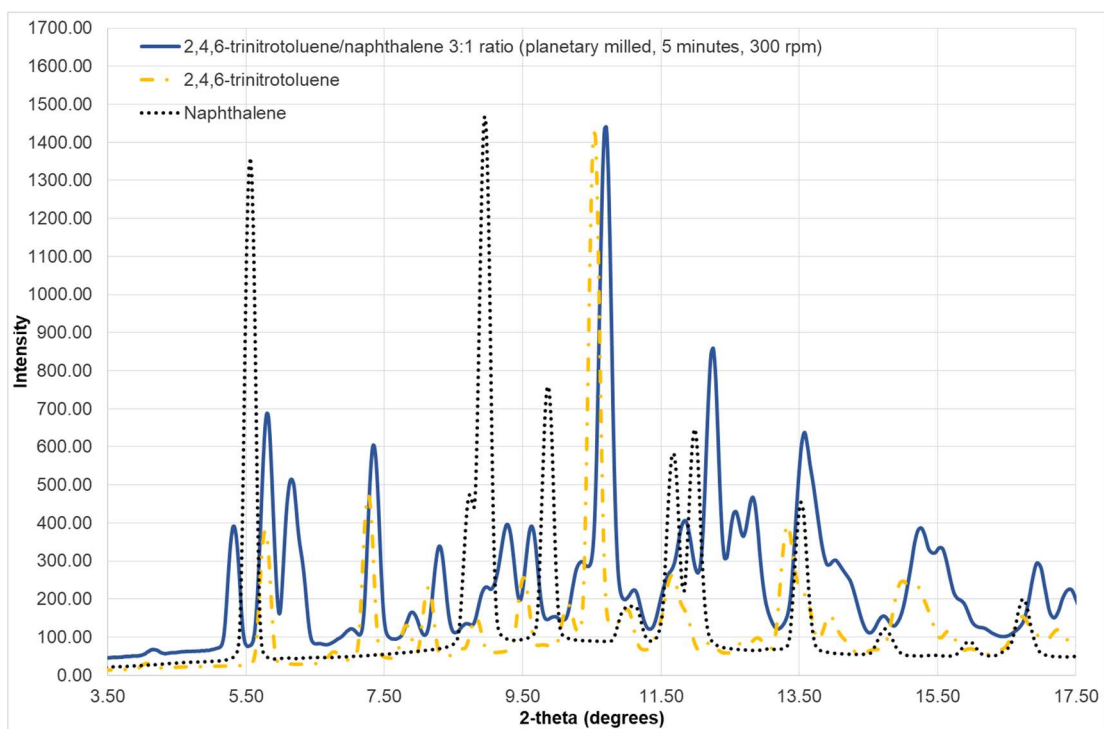


Figure A.21 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 3:1 stoichiometry.

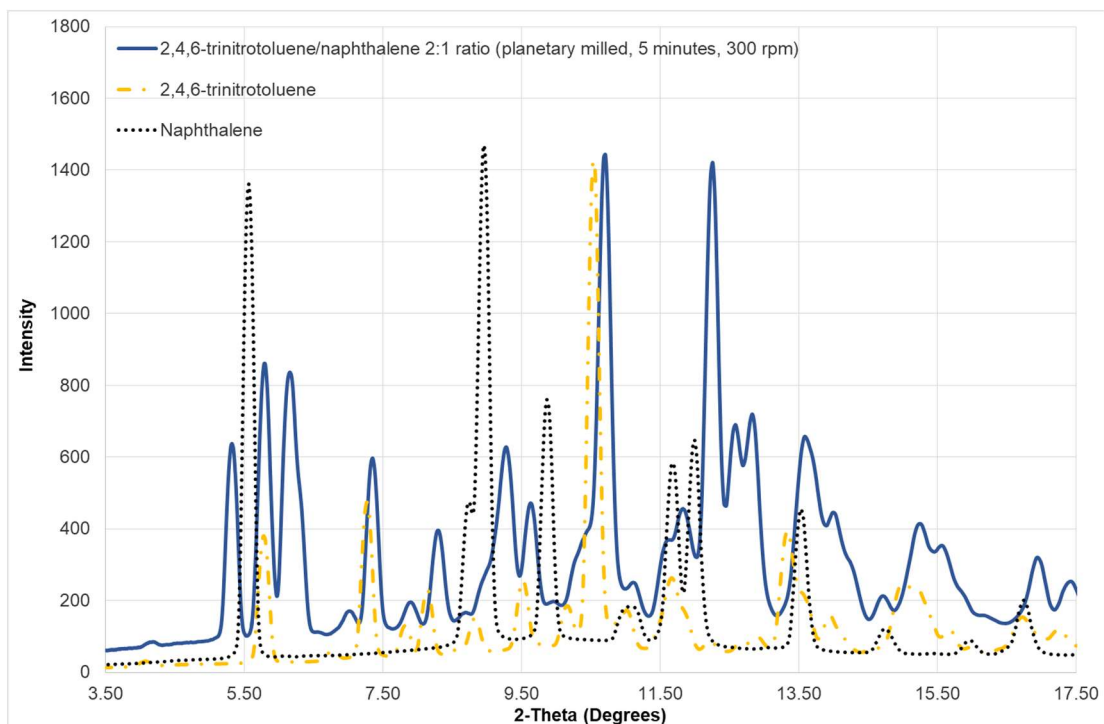


Figure A.22 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 2:1 stoichiometry.

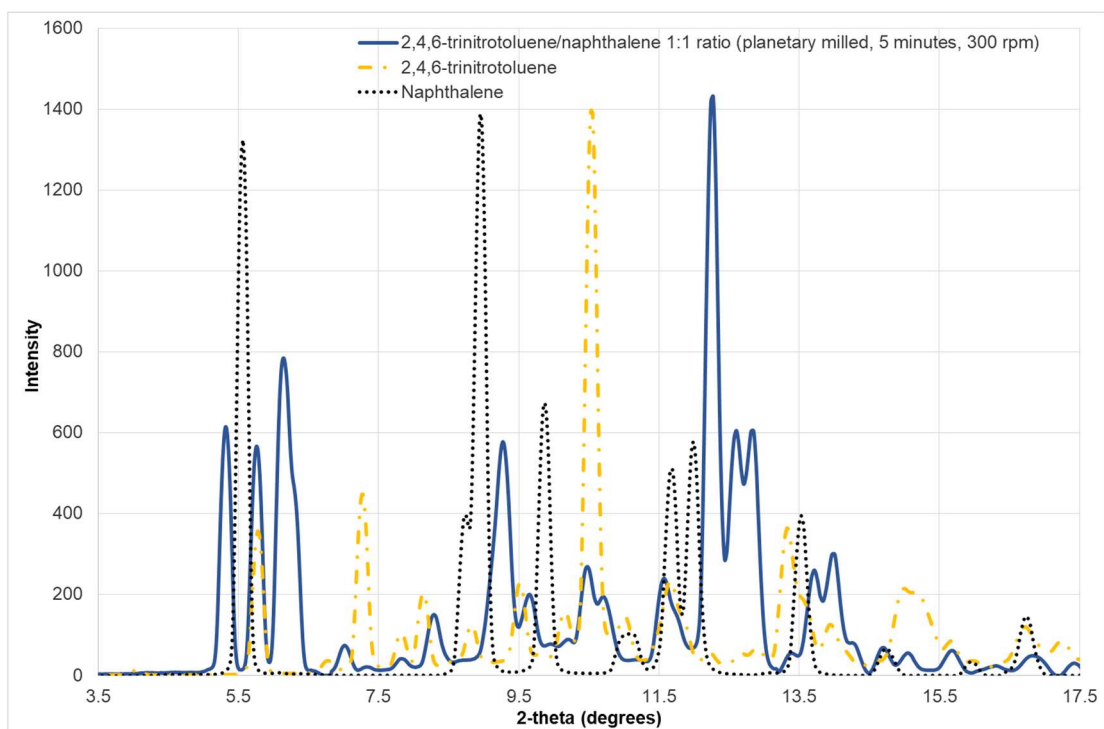


Figure A.23 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

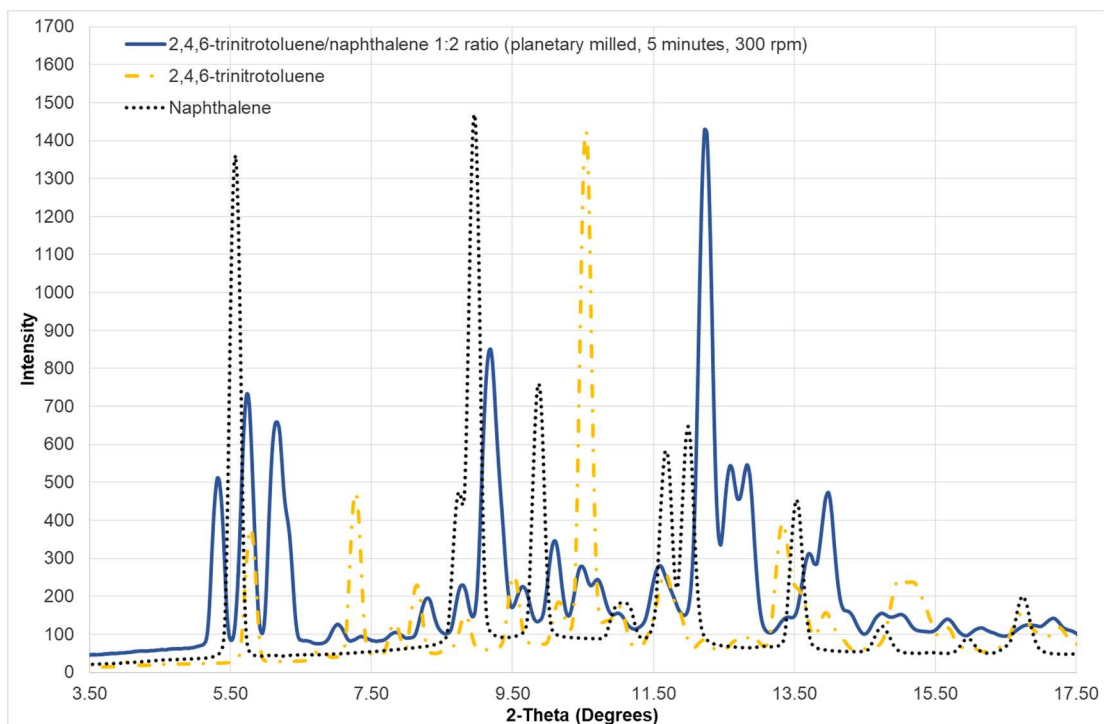


Figure A.24 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:2 stoichiometry.

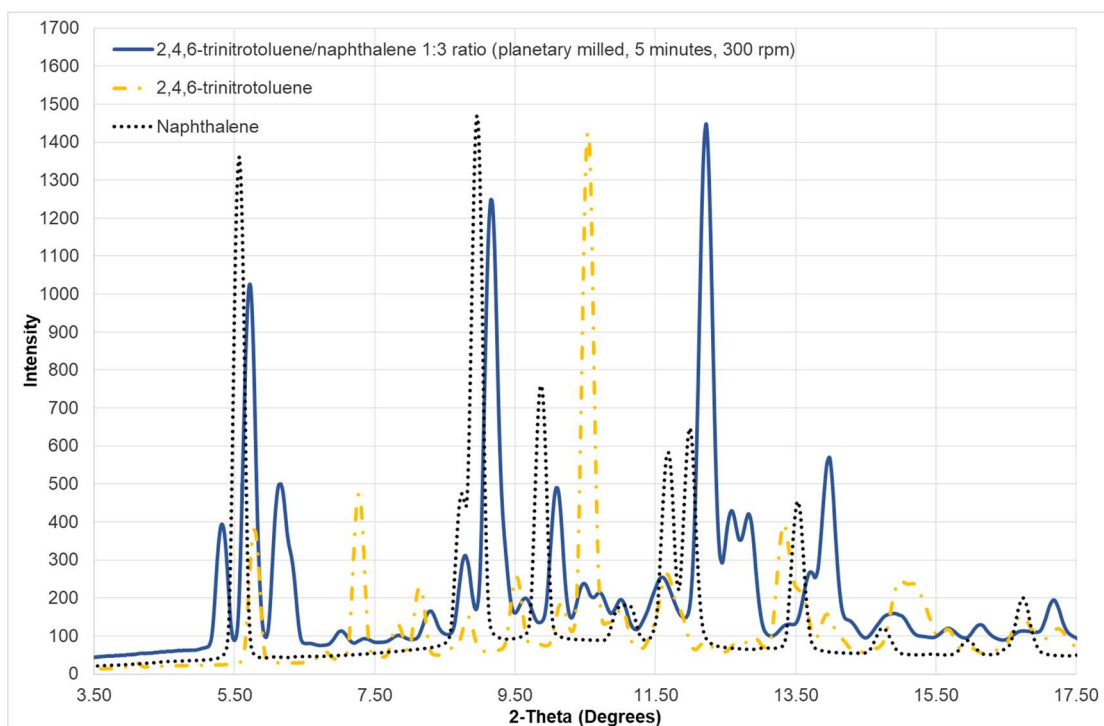


Figure A.25 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:3 stoichiometry.

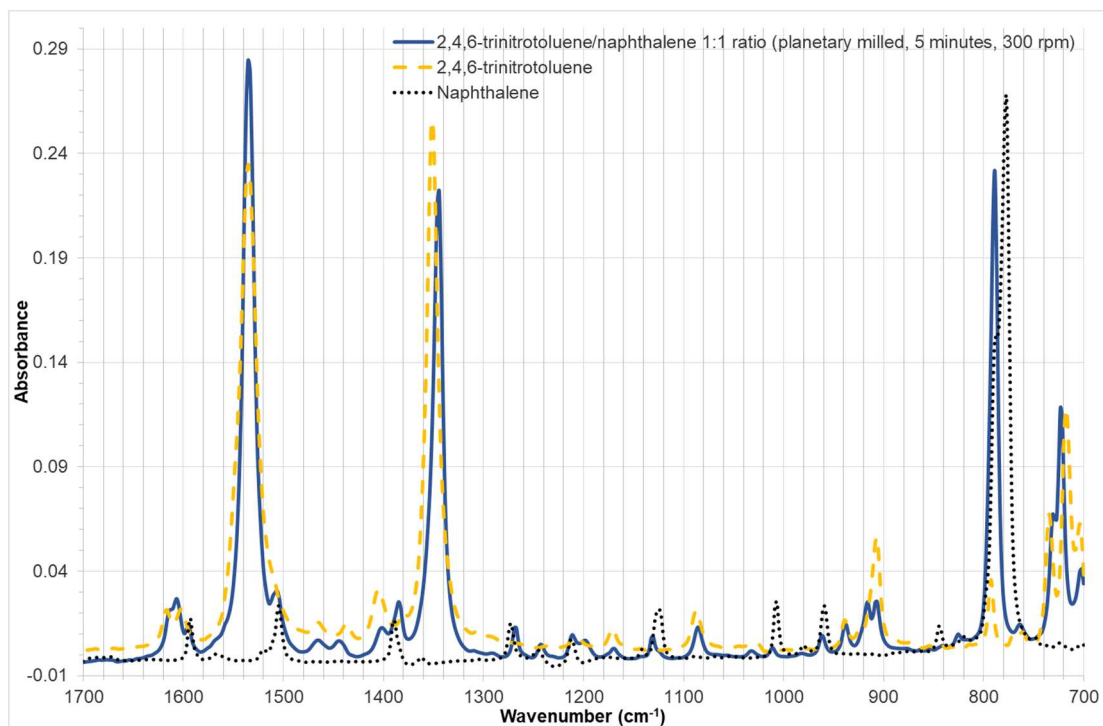


Figure A.26 - Infra-red spectra of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

A.3 2,4,6-trinitrotoluene/anthracene

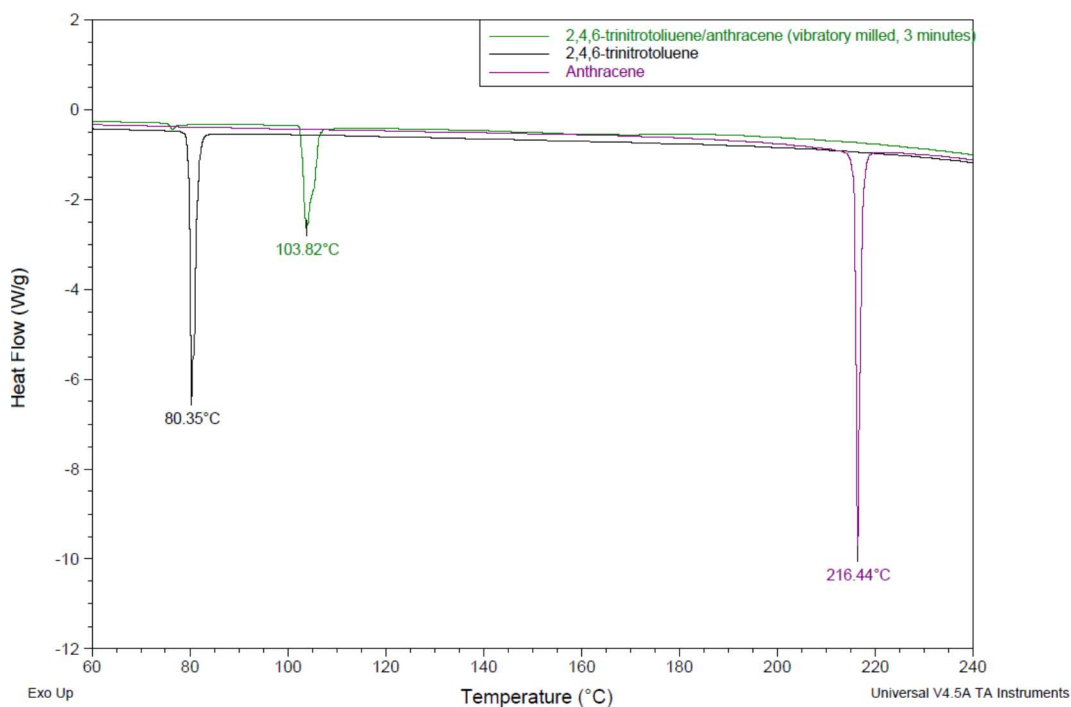


Figure A.27 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

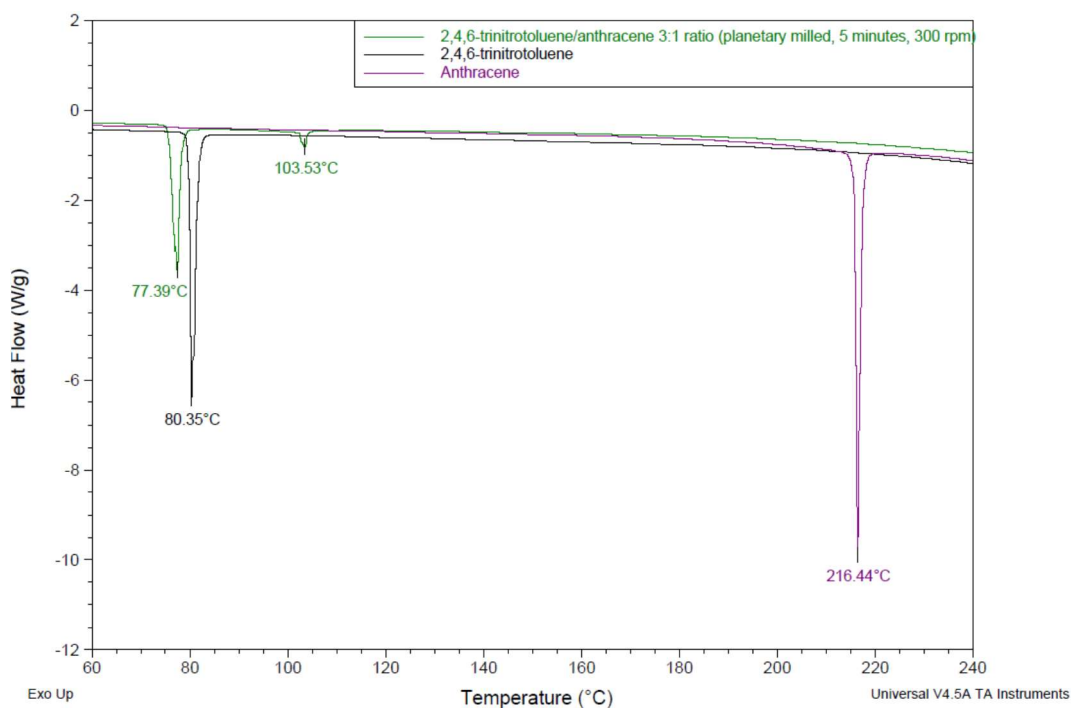


Figure A.28 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

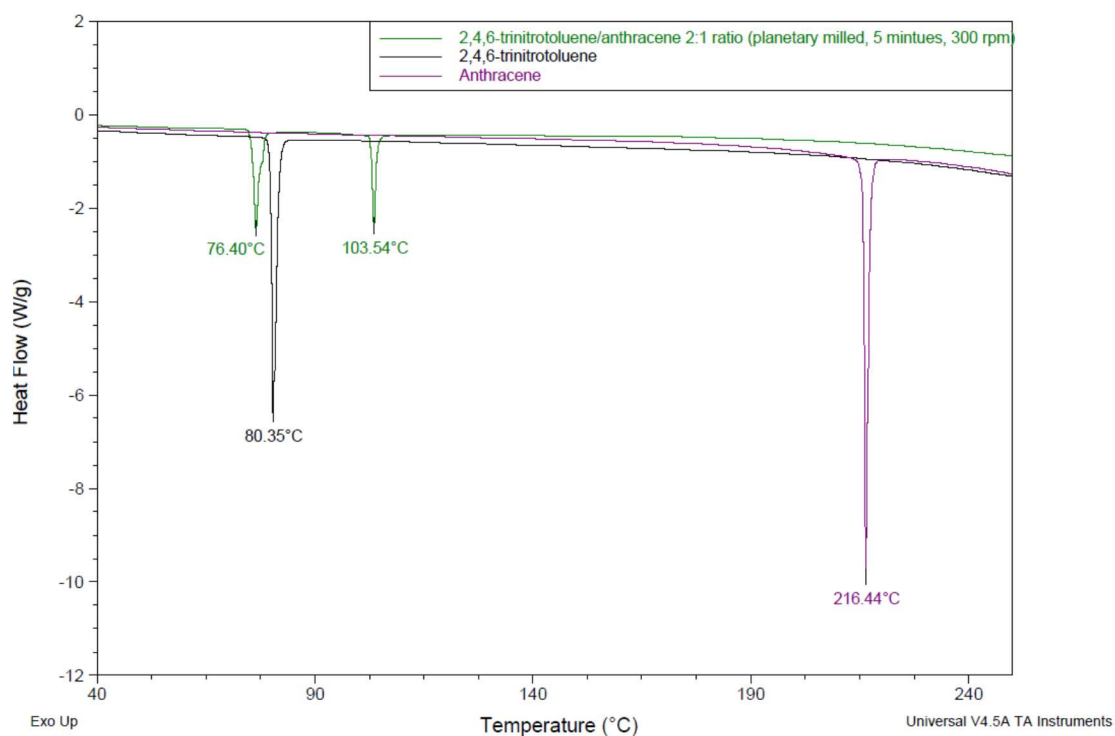


Figure A.29 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

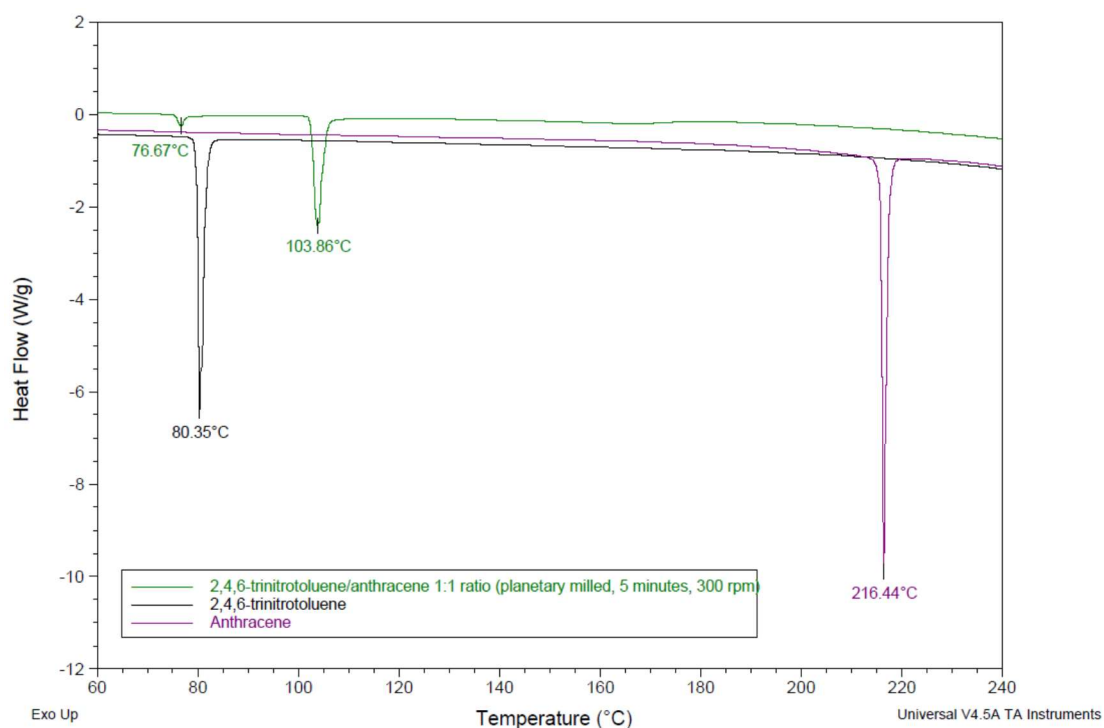


Figure A.30 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

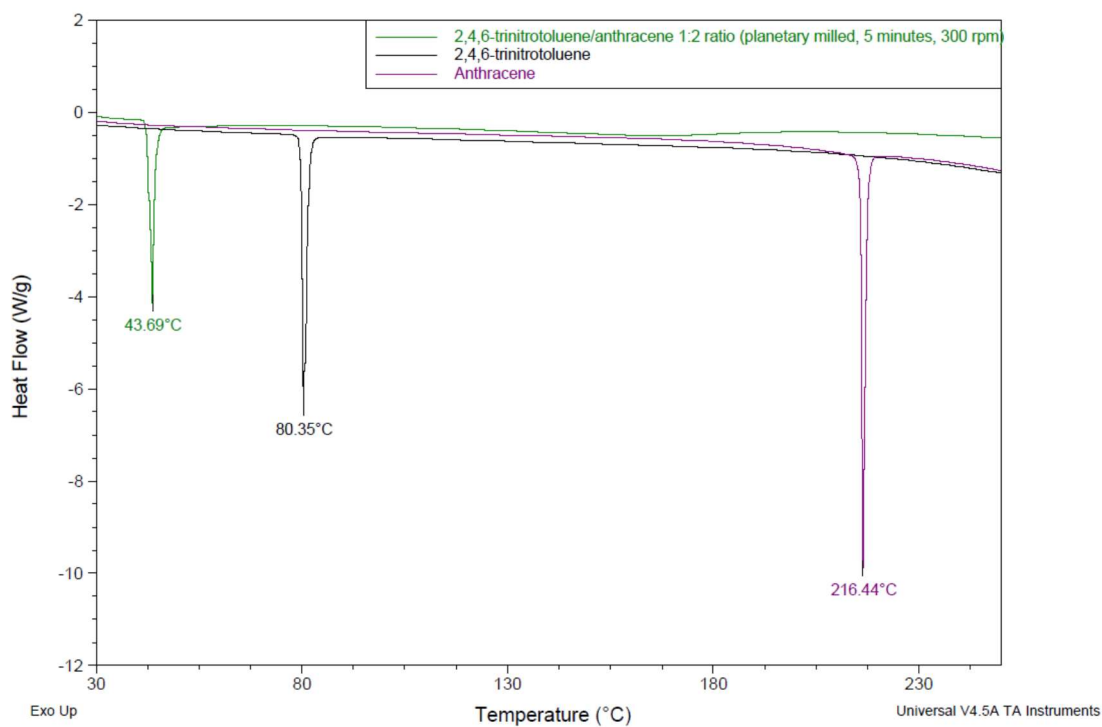


Figure A.31 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

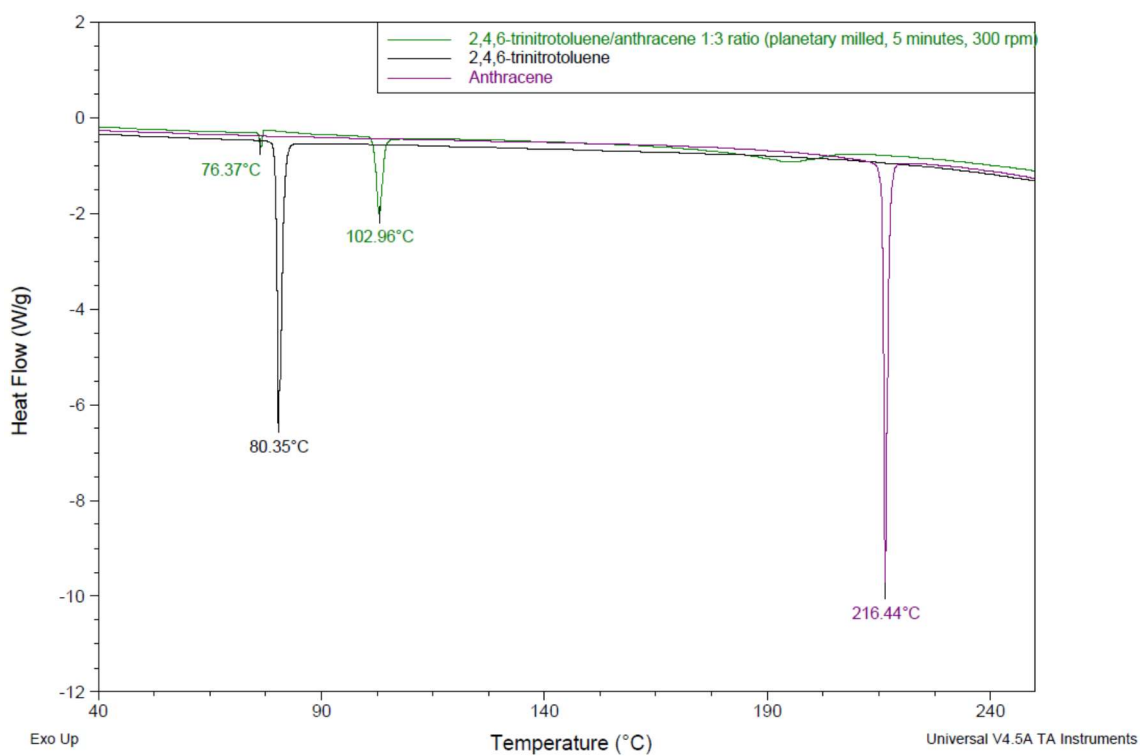


Figure A.32 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

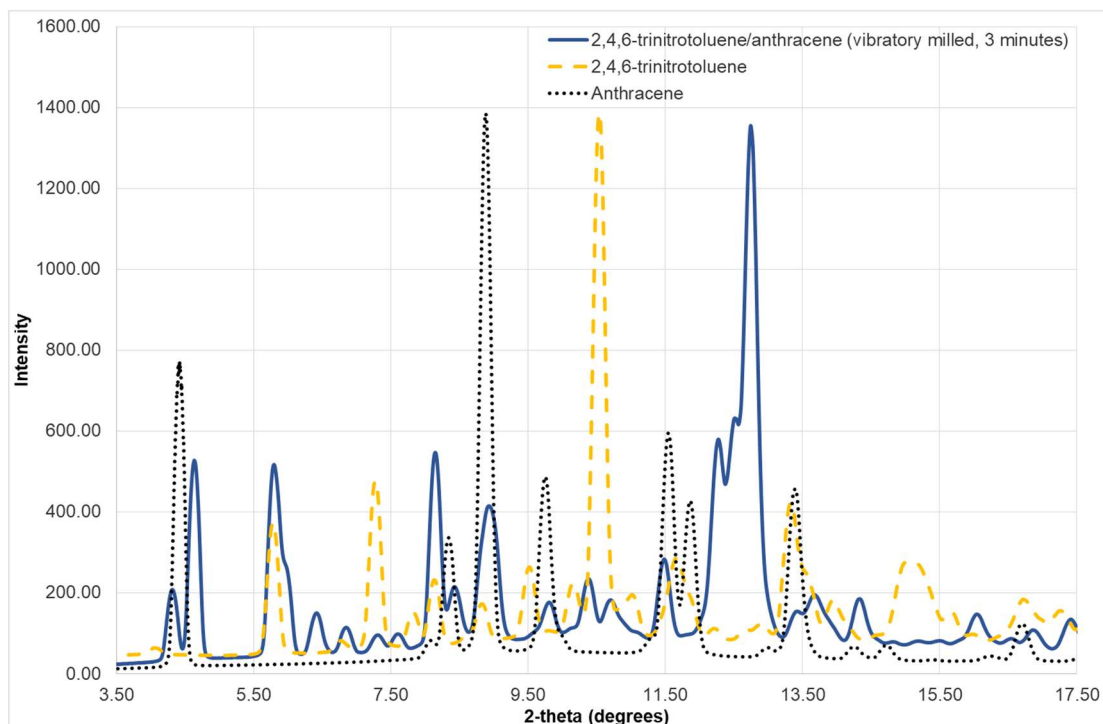


Figure A.33 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

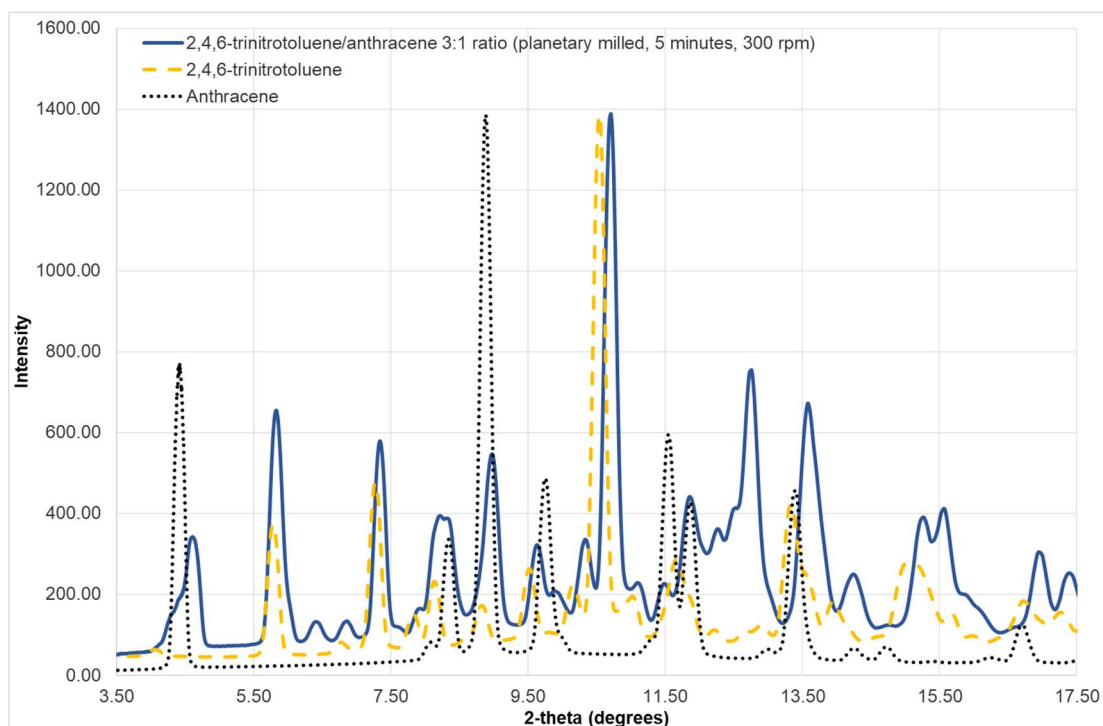


Figure A.34 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene 3:1 ratio produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

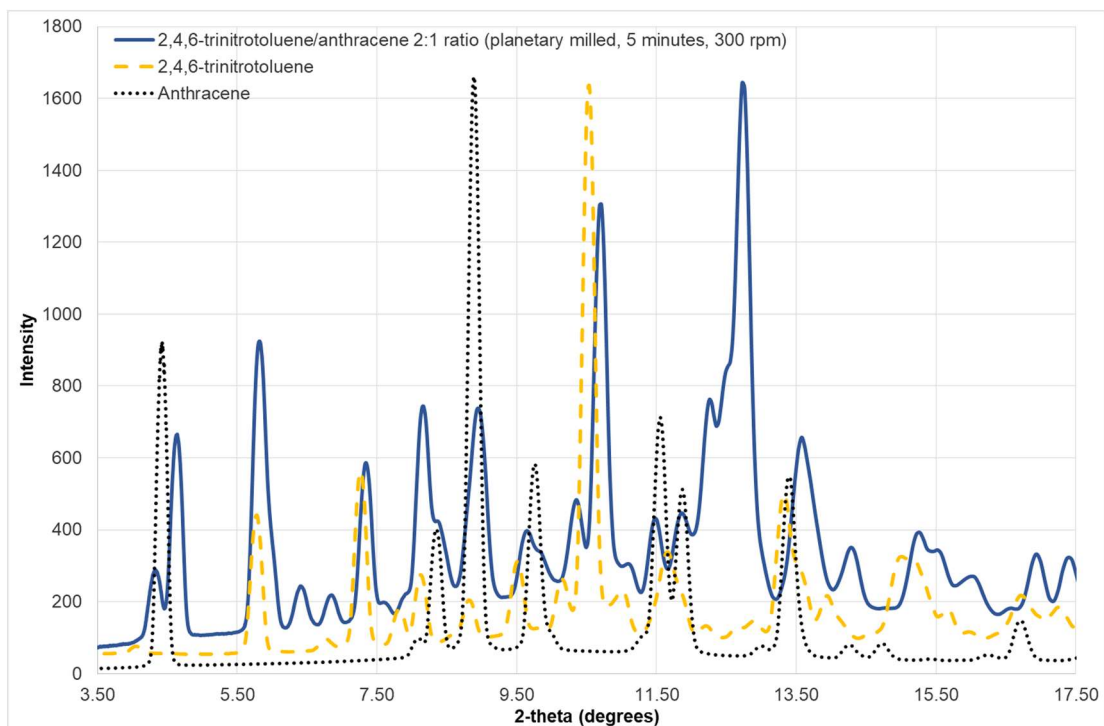


Figure A.35 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

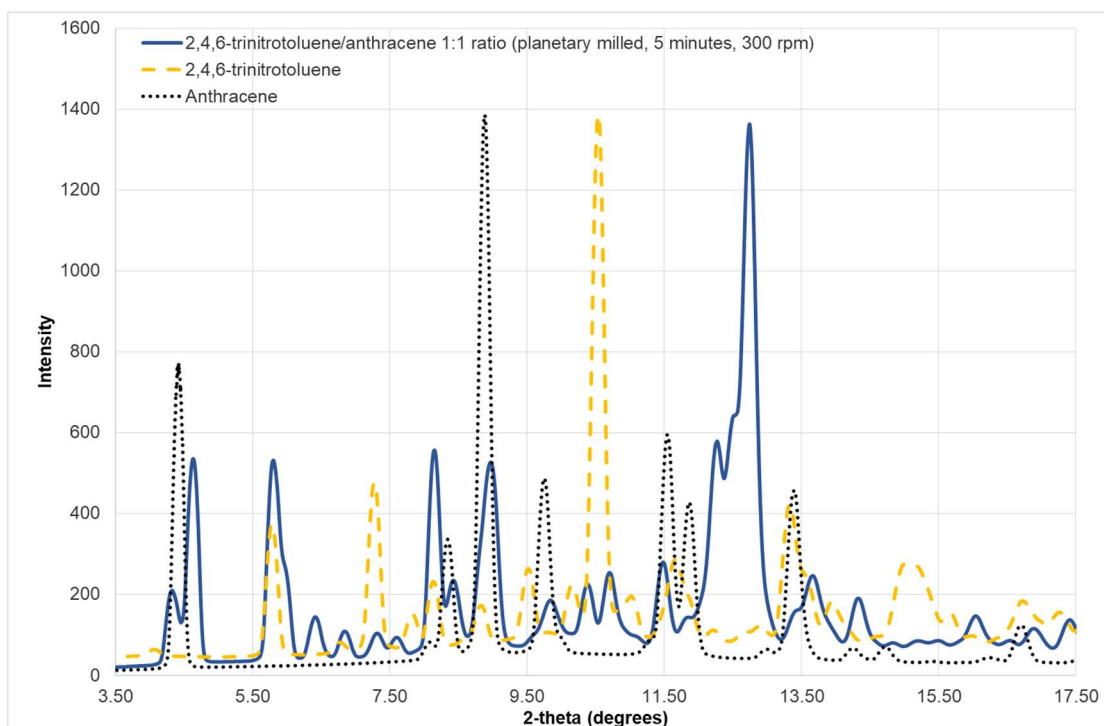


Figure A.36 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

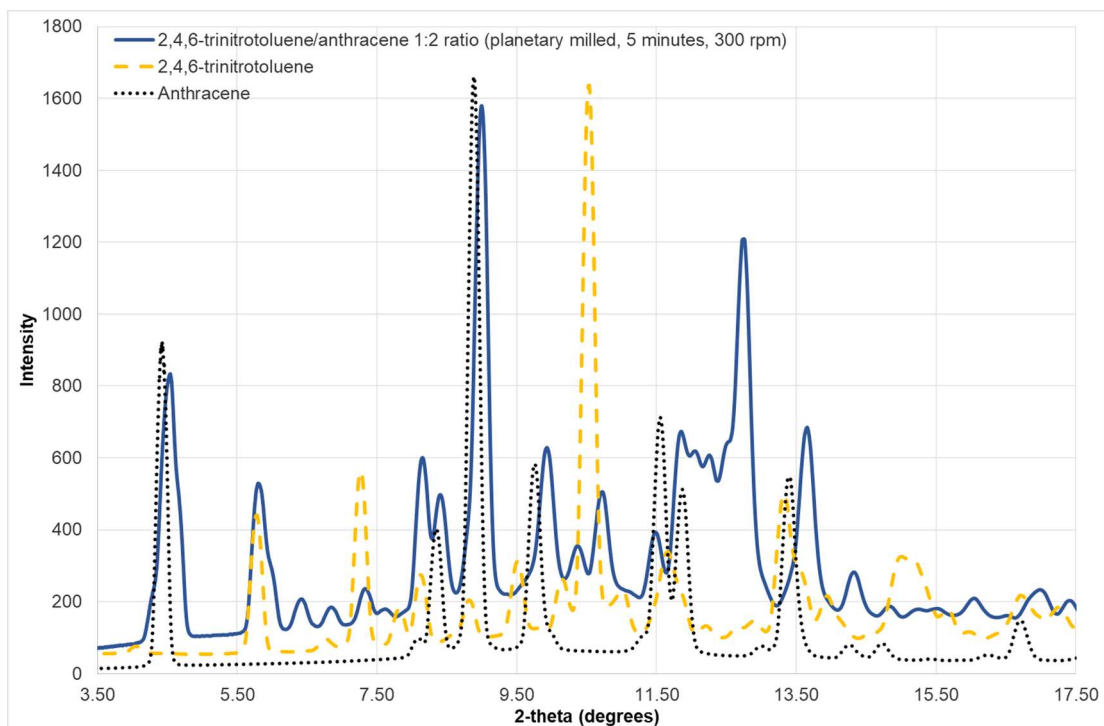


Figure A.37 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

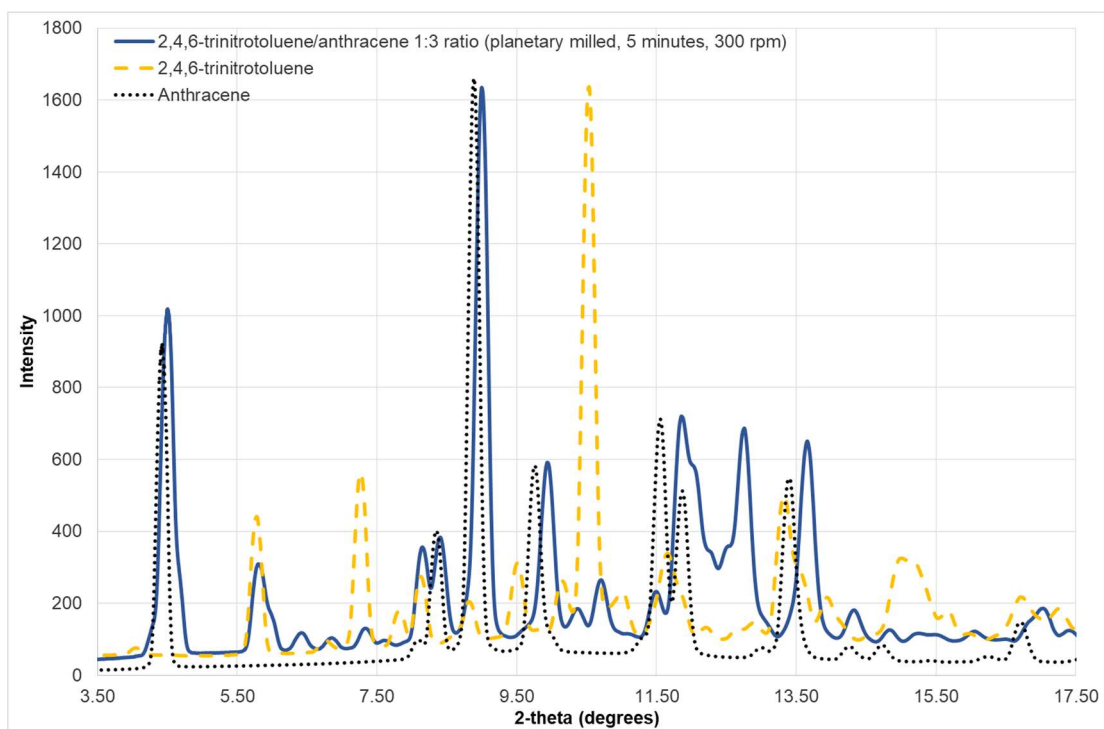


Figure A.38 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

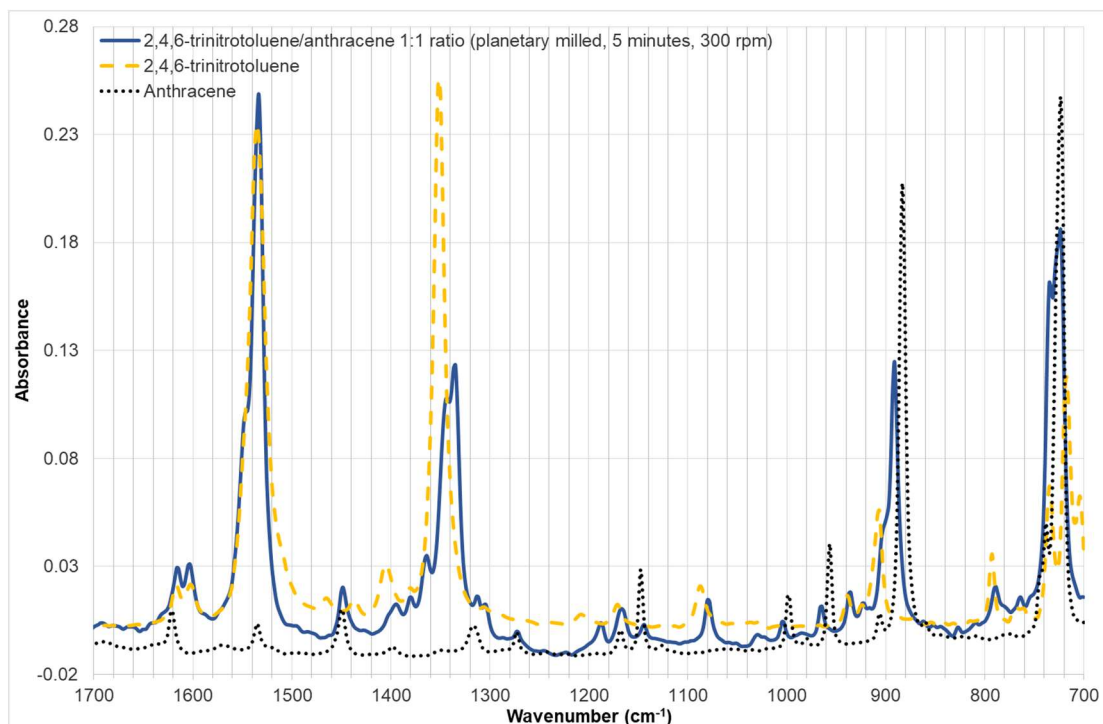


Figure A.39 - Infra-red spectra of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

A.4 2,4,6-trinitrotoluene/1,4-dimethoxybenzene

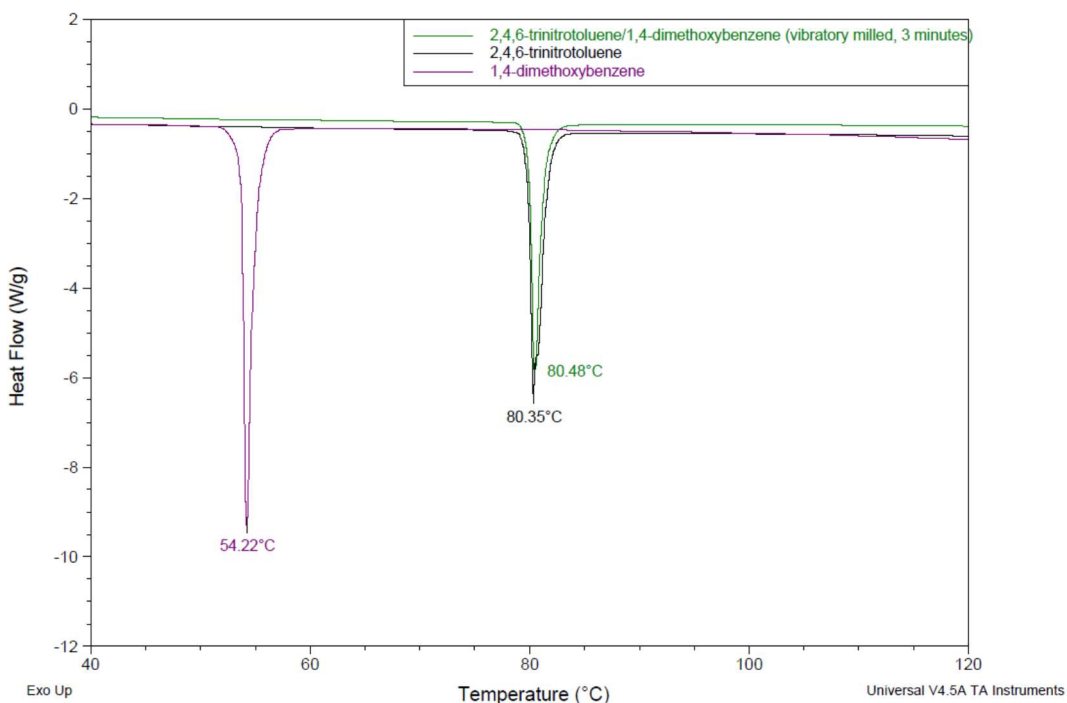


Figure A.40 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

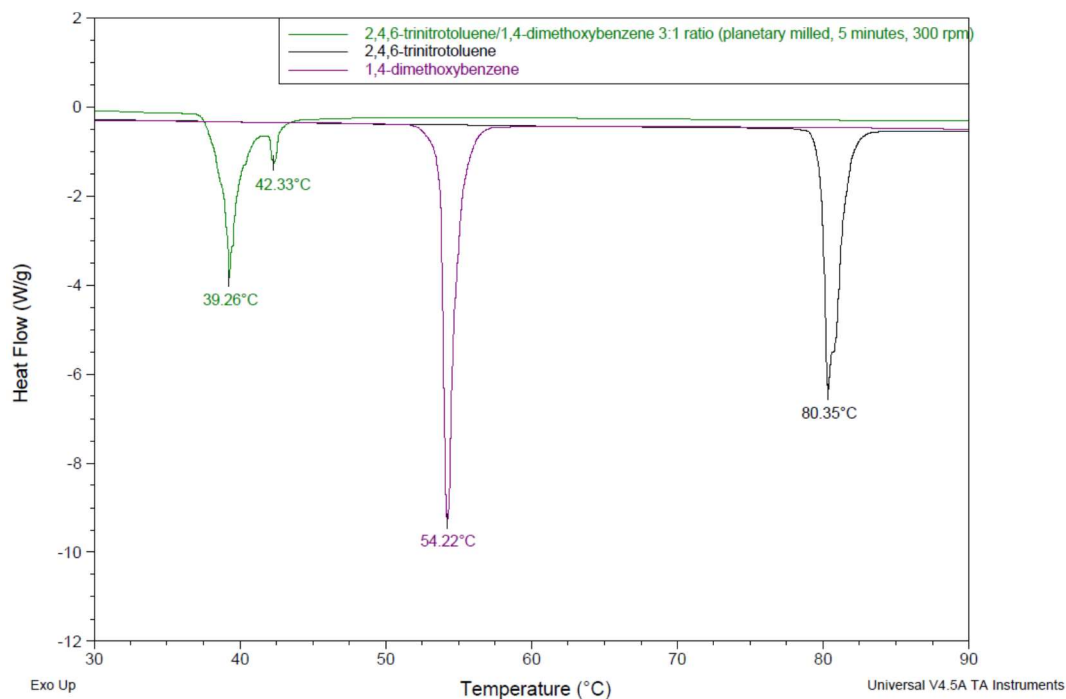


Figure A.41 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

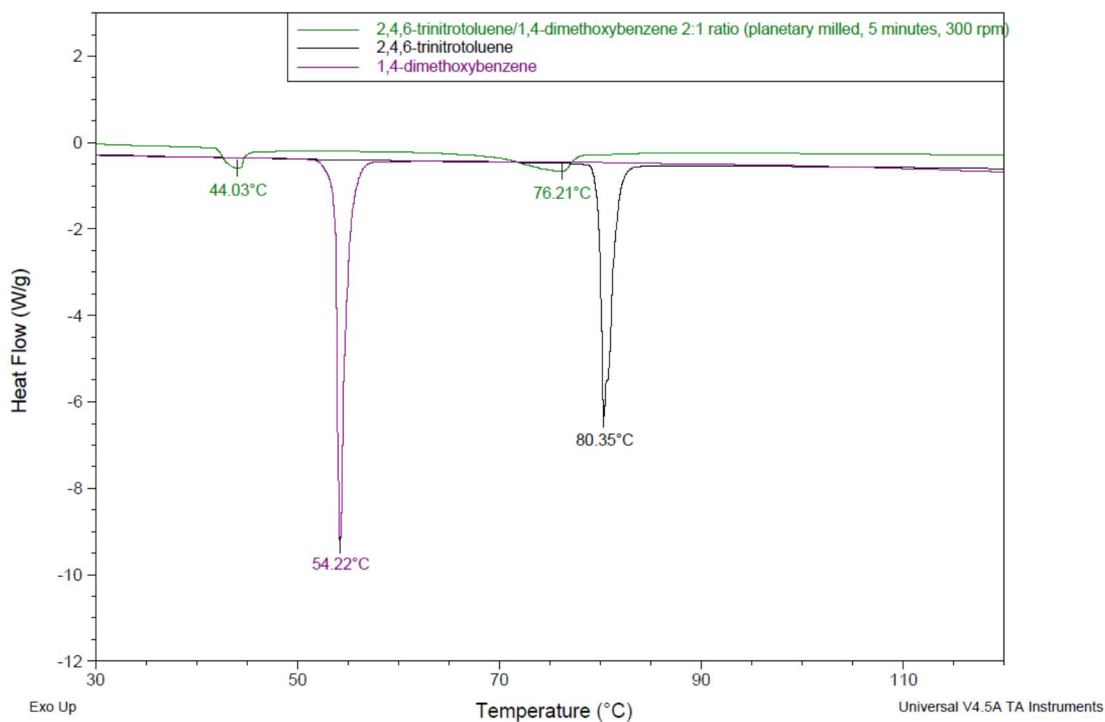


Figure A.42 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

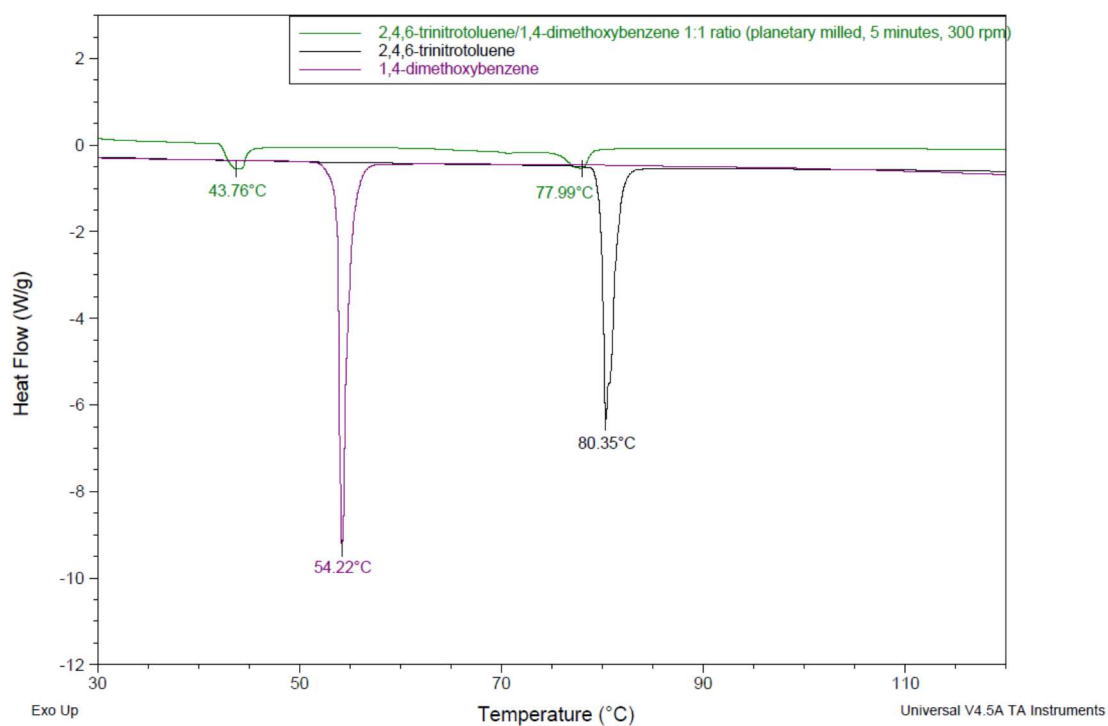


Figure A.43 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

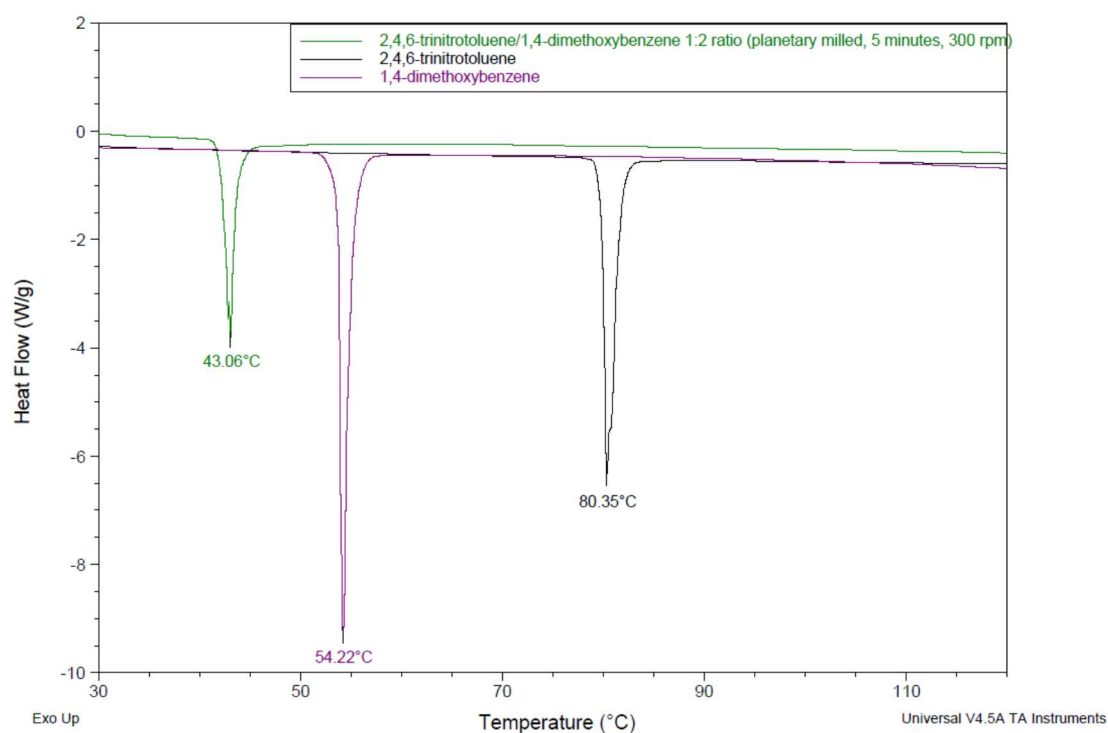


Figure A.44 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

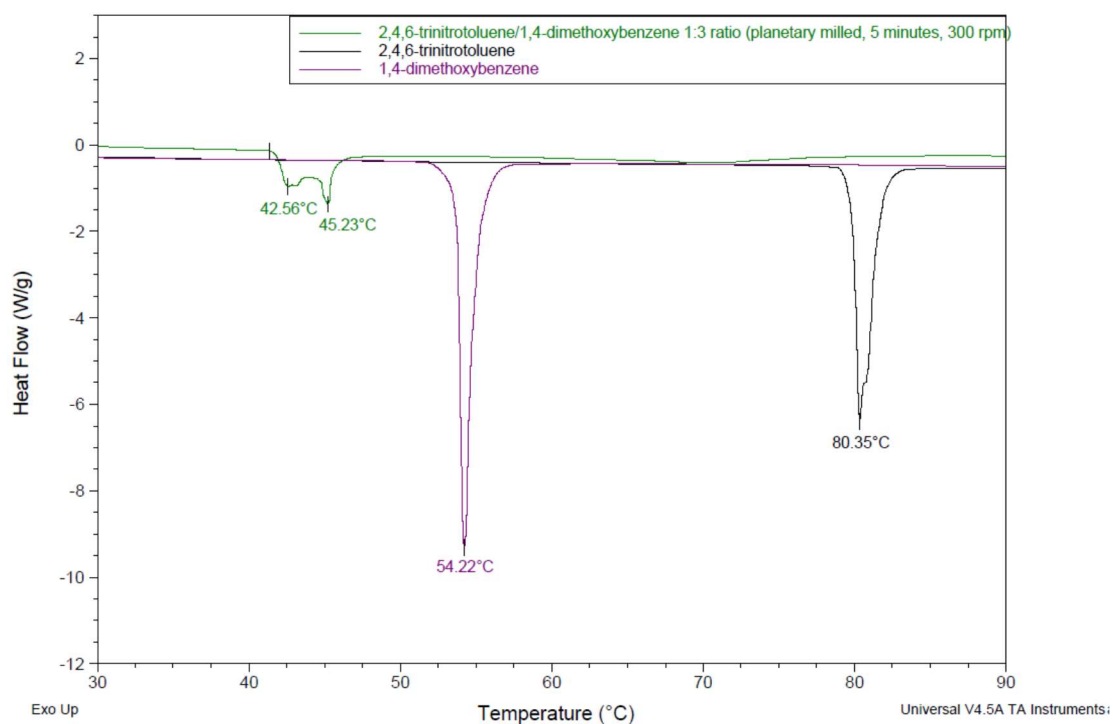


Figure A.45 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

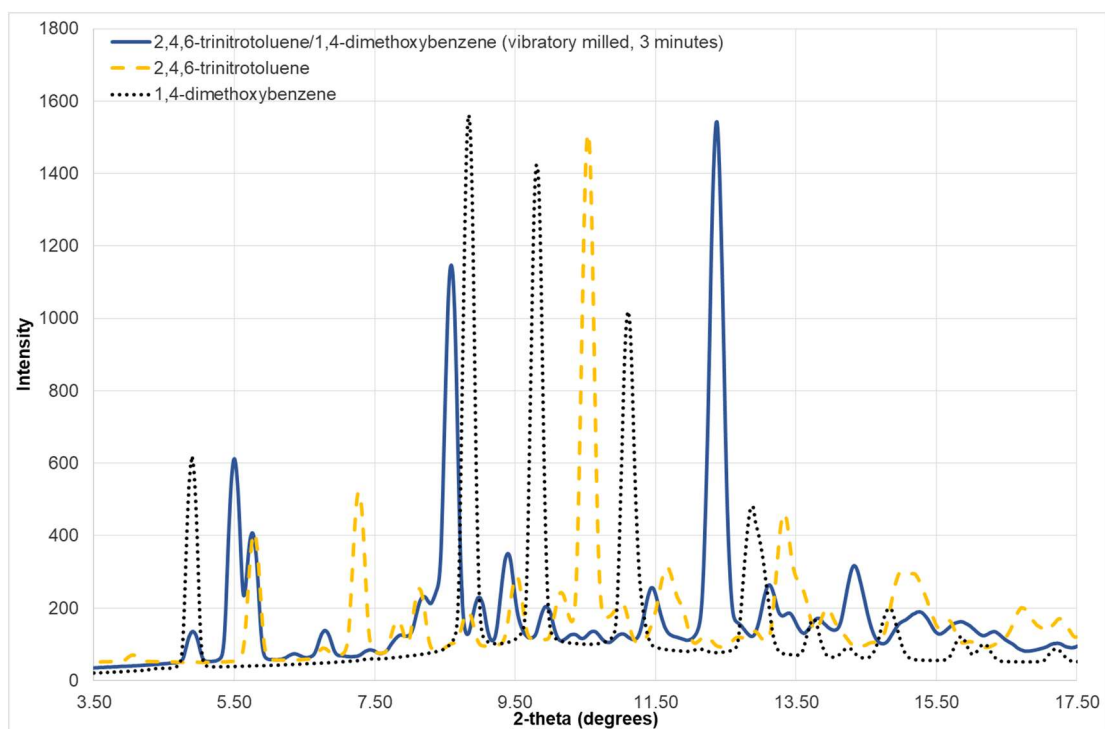


Figure A.46 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

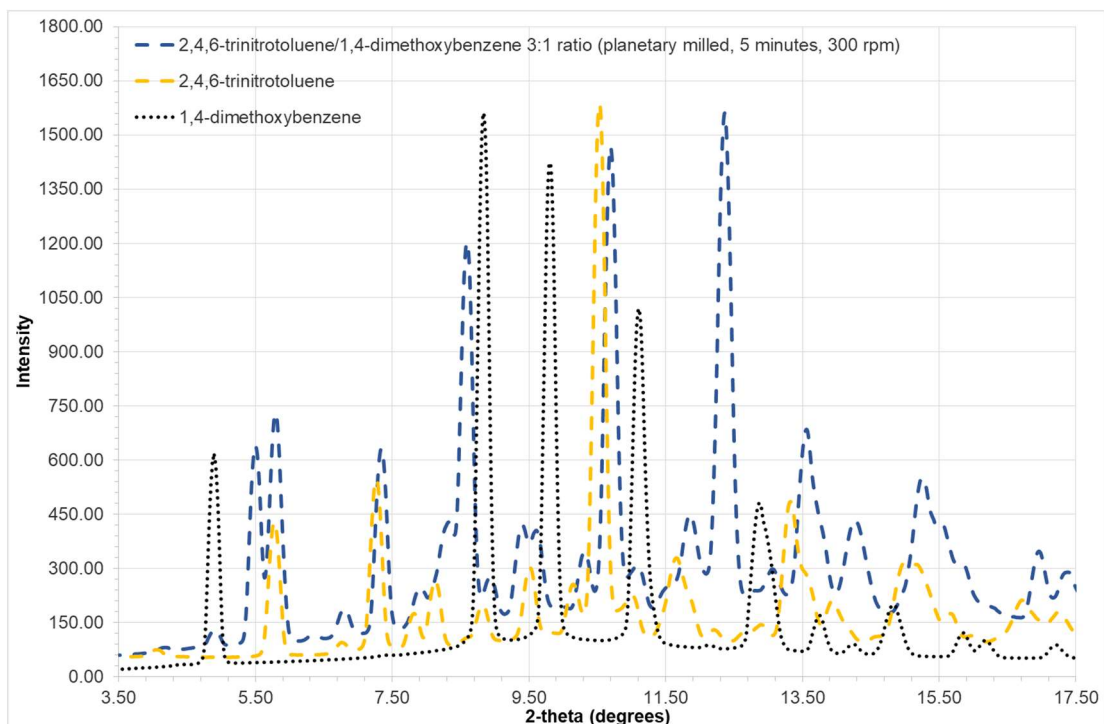


Figure A.47 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

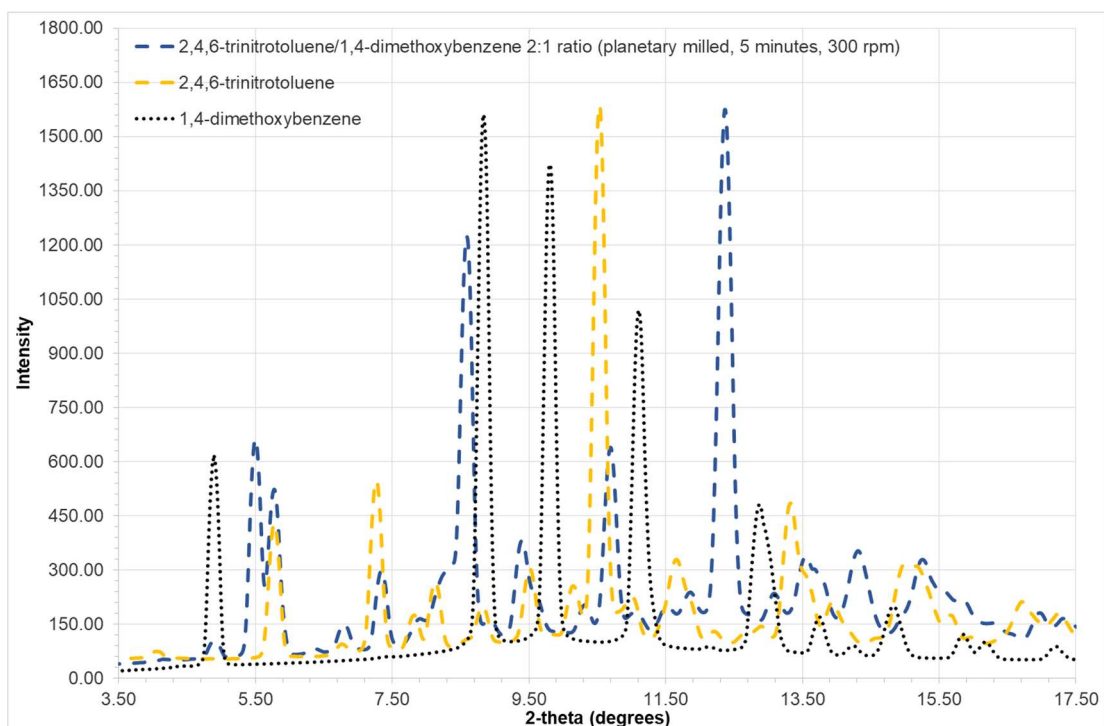


Figure A.48 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

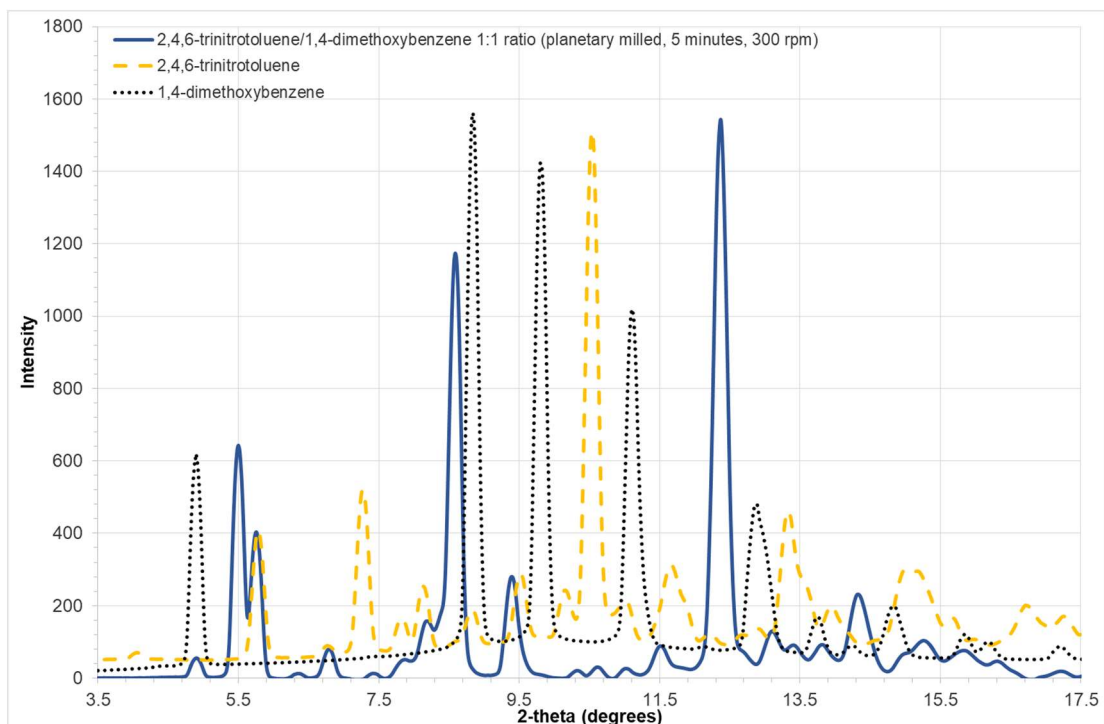


Figure A.49 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

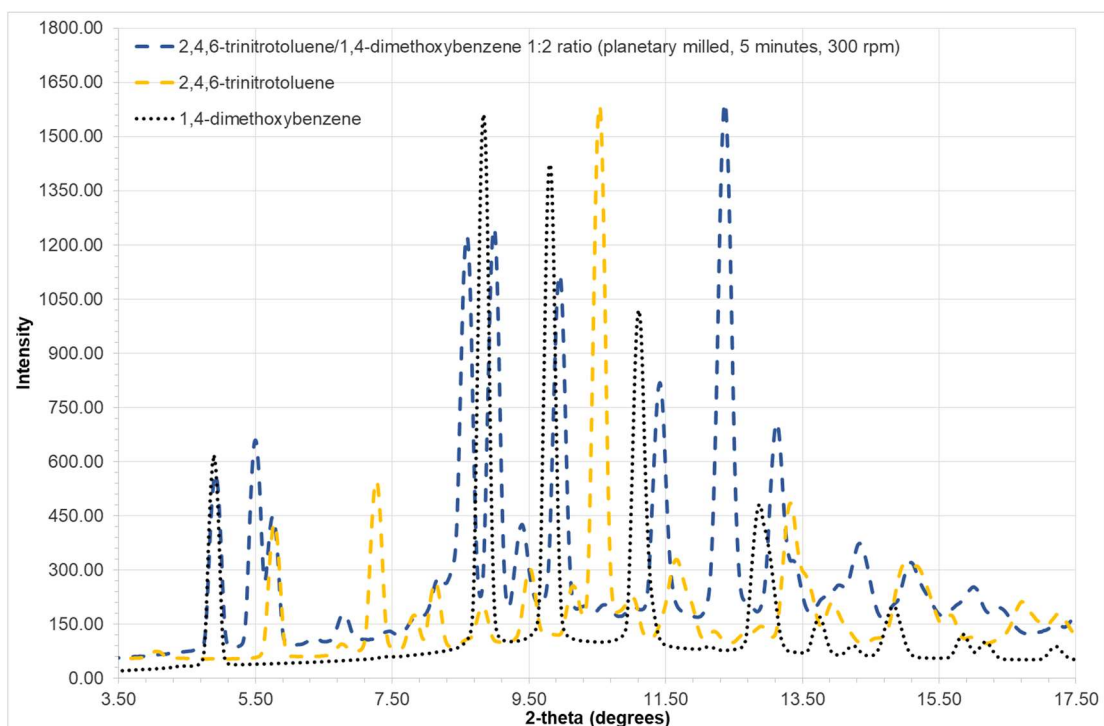


Figure A.50 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

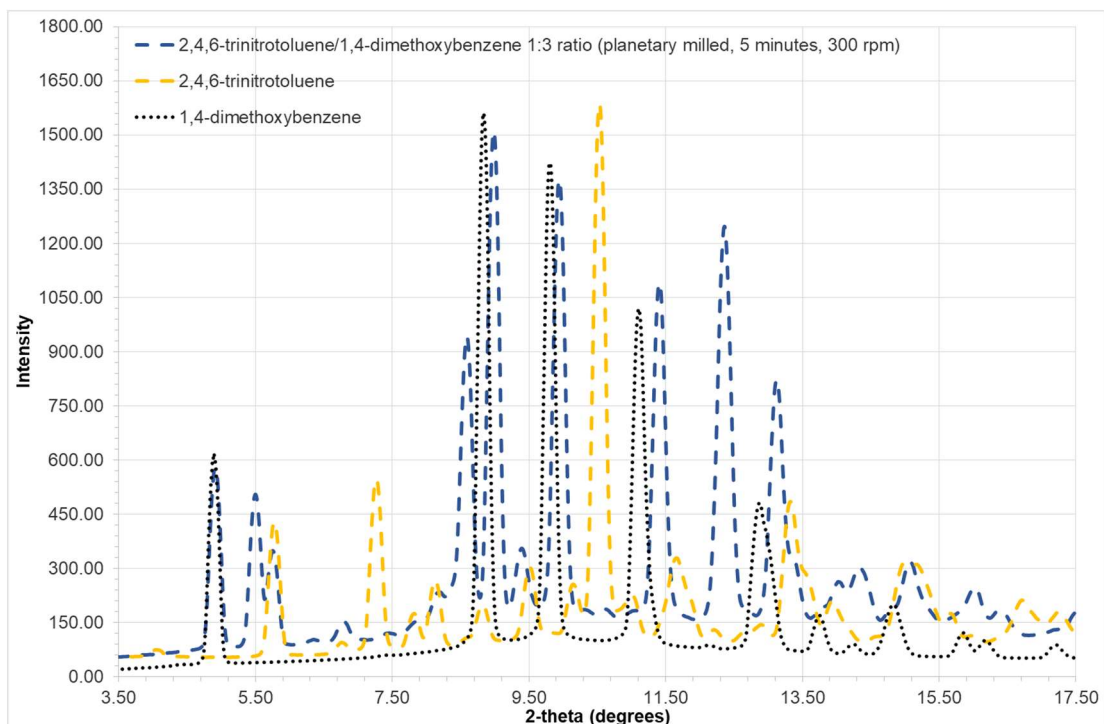


Figure A.51 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

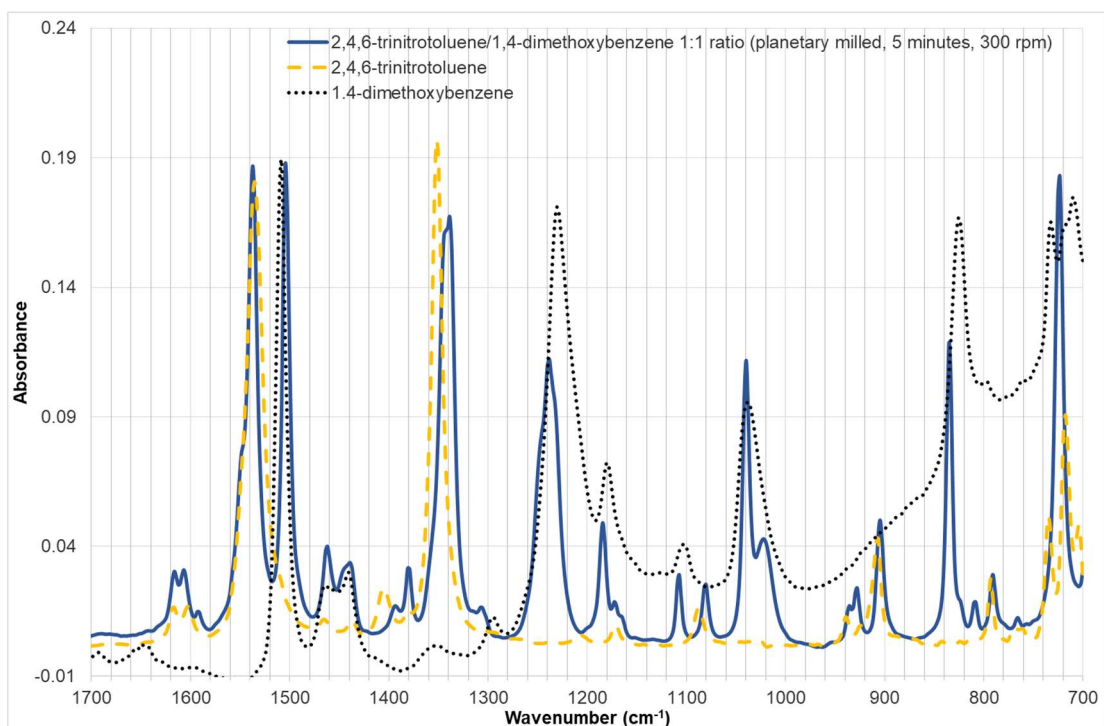


Figure A.52 – Infra-red spectra of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

B Results 2 – Investigation of co-crystallisation potential in electron deficient ring systems (Chapter 5)

B.1 1,3-dinitrobenzene/2,4-dinitroaniline

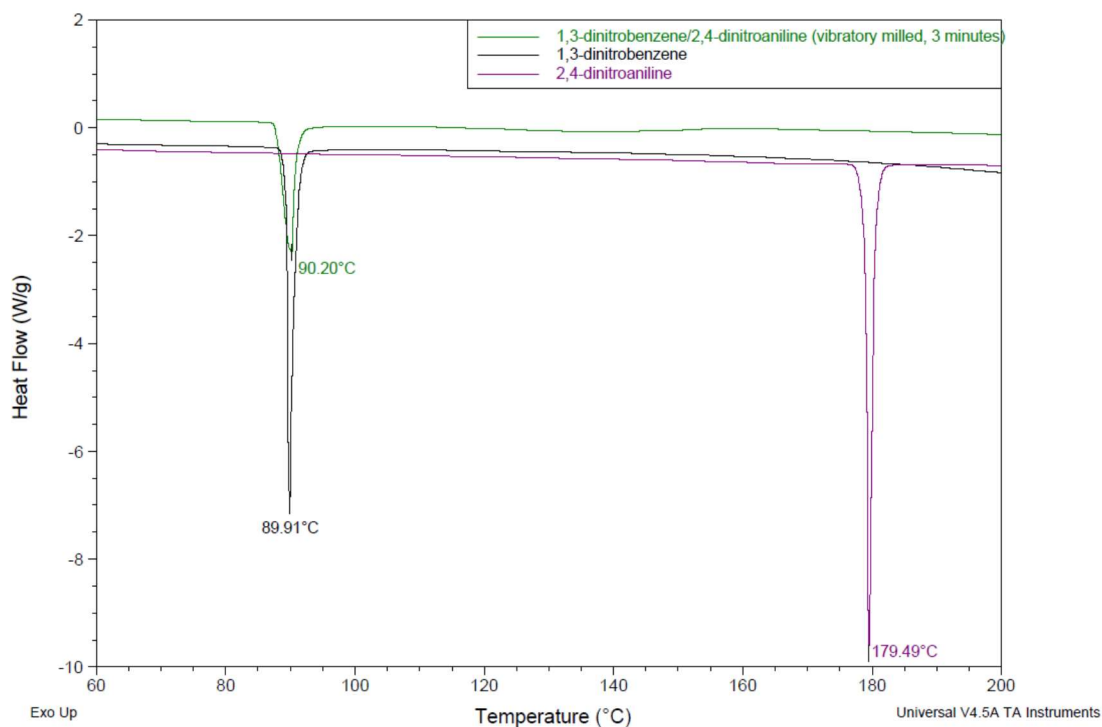


Figure B.1 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroaniline produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

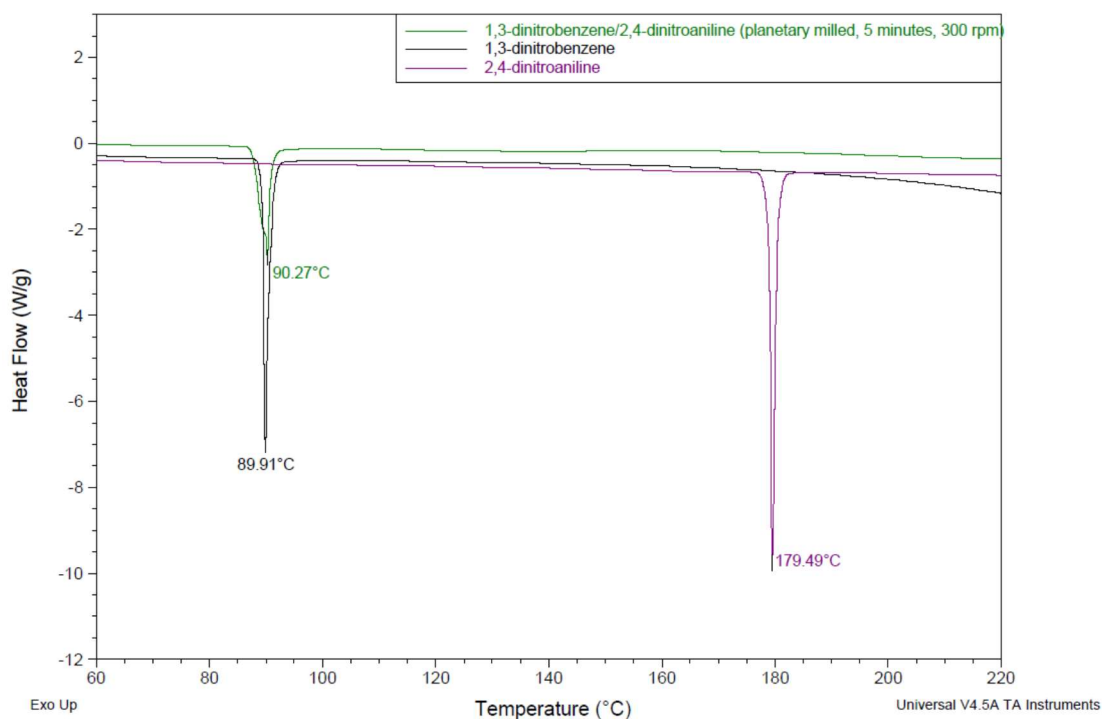


Figure B.2 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroaniline produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

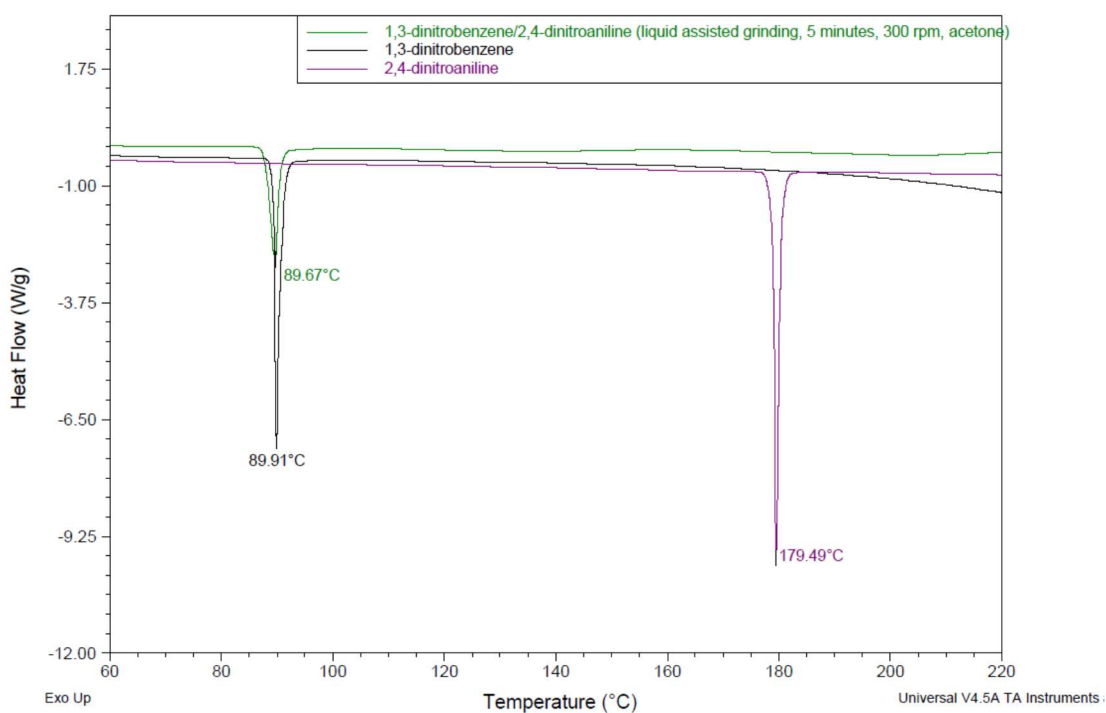


Figure B.3 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

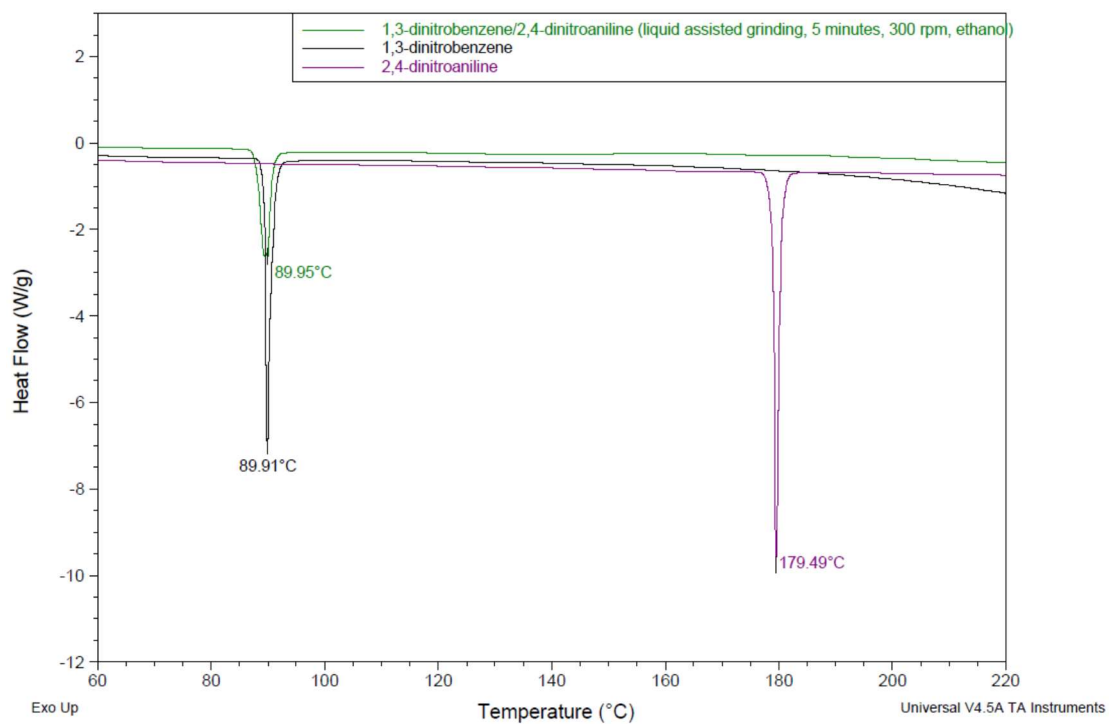


Figure B.4 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

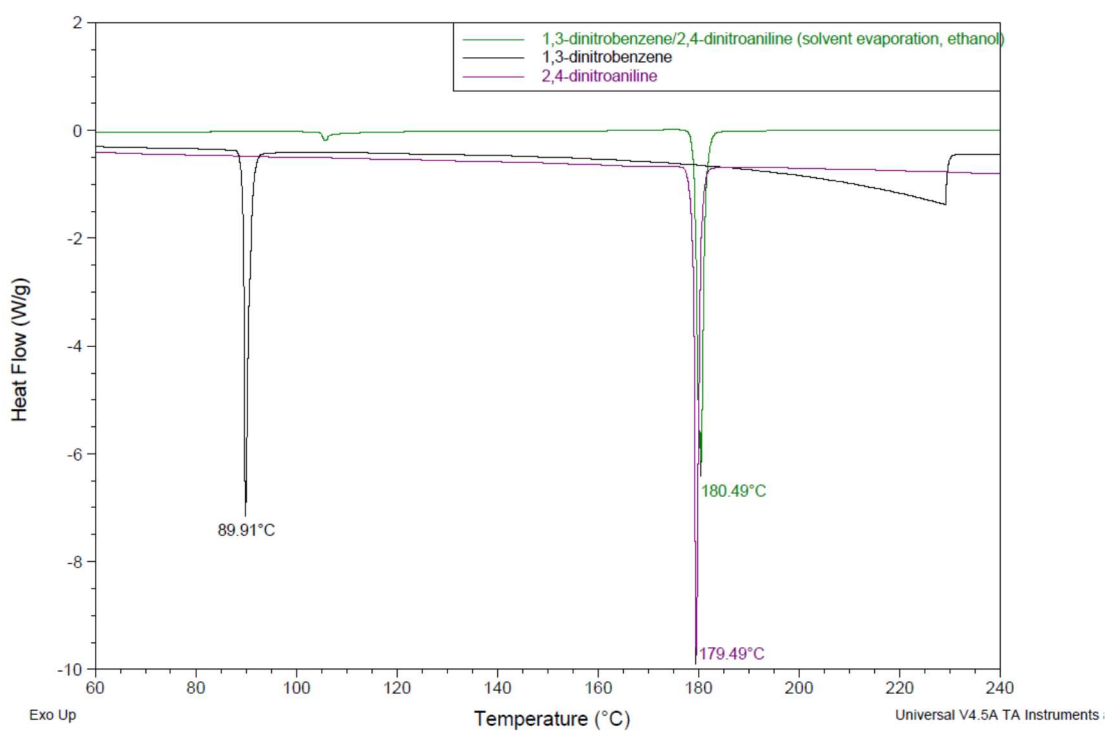


Figure B.5 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroaniline produced by solvent evaporation in ethanol.

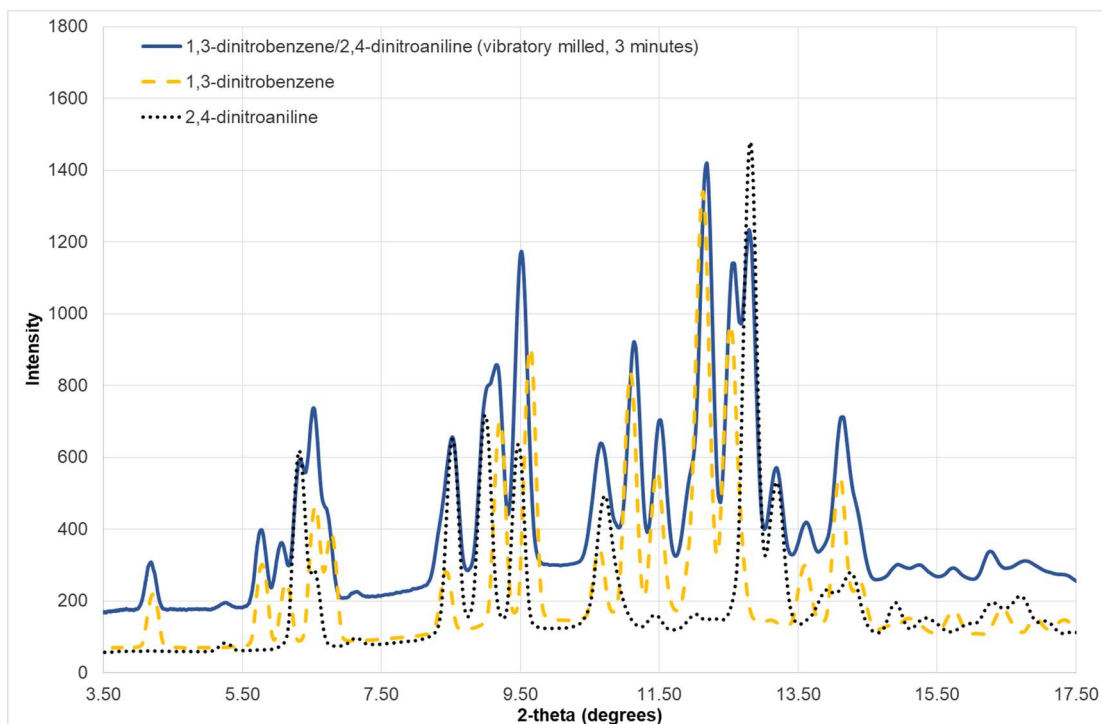


Figure B.6 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

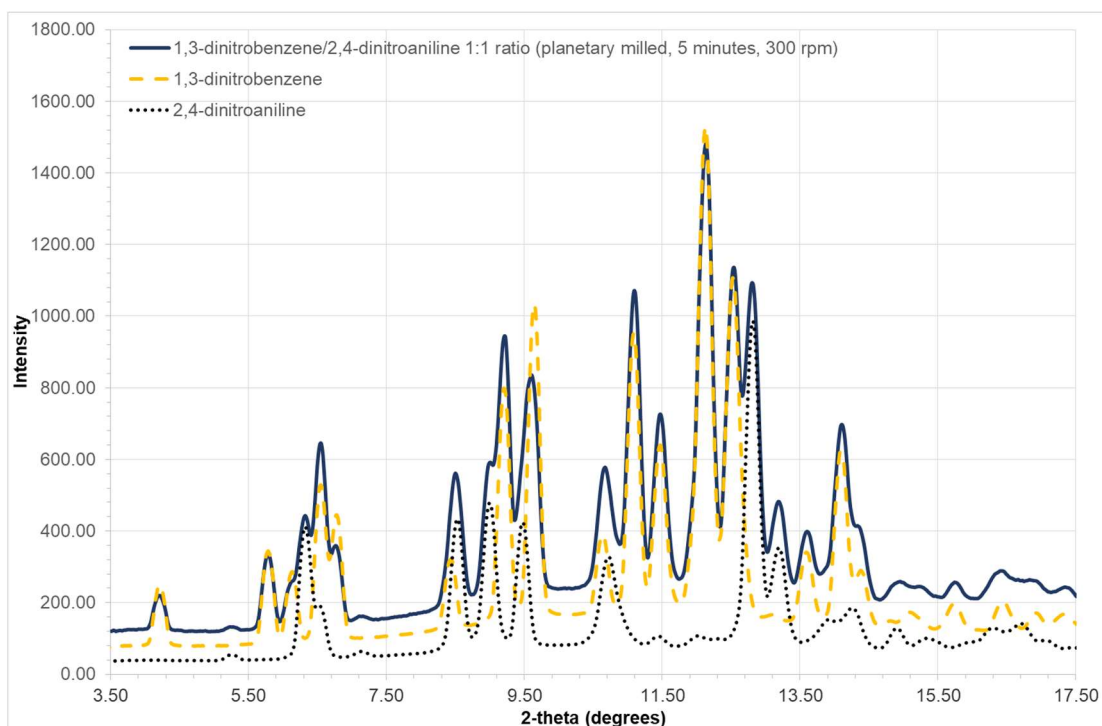


Figure B.7 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

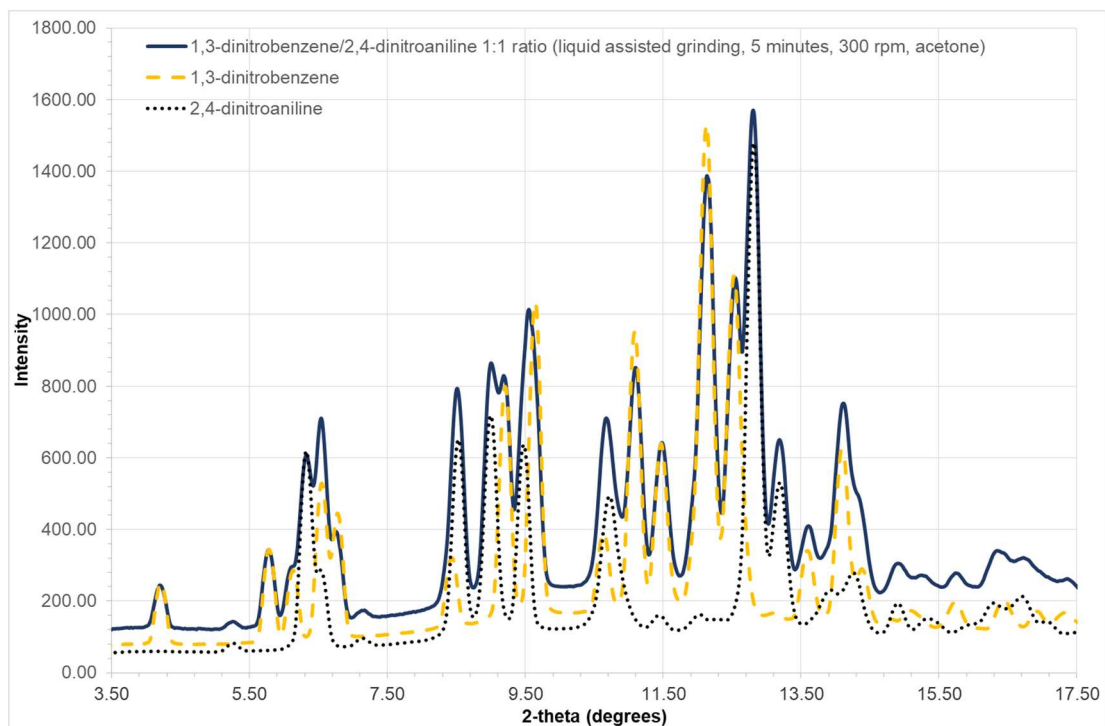


Figure B.8 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm in acetone.

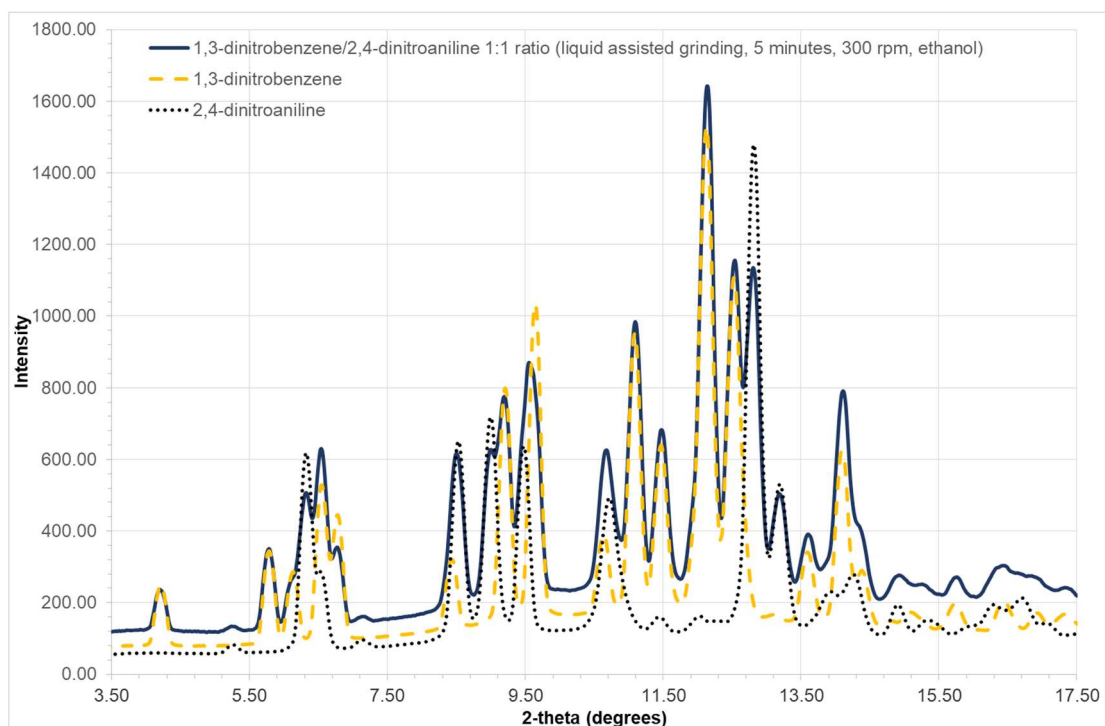


Figure B.9 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm in ethanol.

B.2 1,3-dinitrobenzene/2,4-dinitroanisole

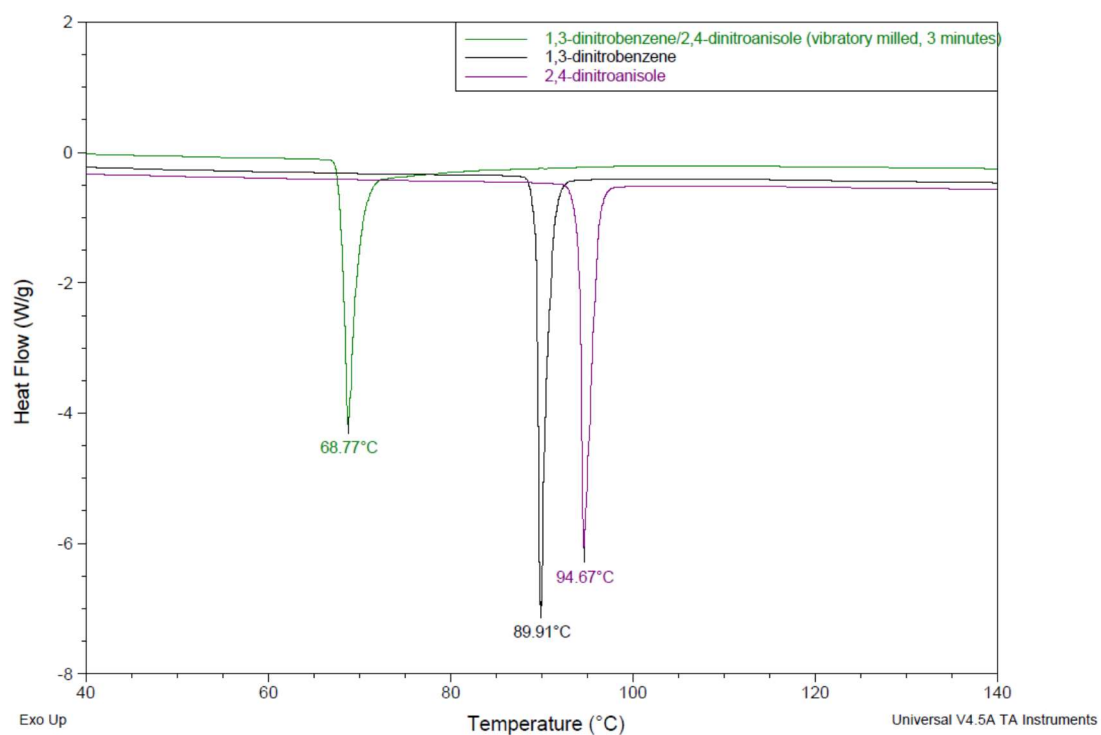


Figure B.10 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroanisole produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

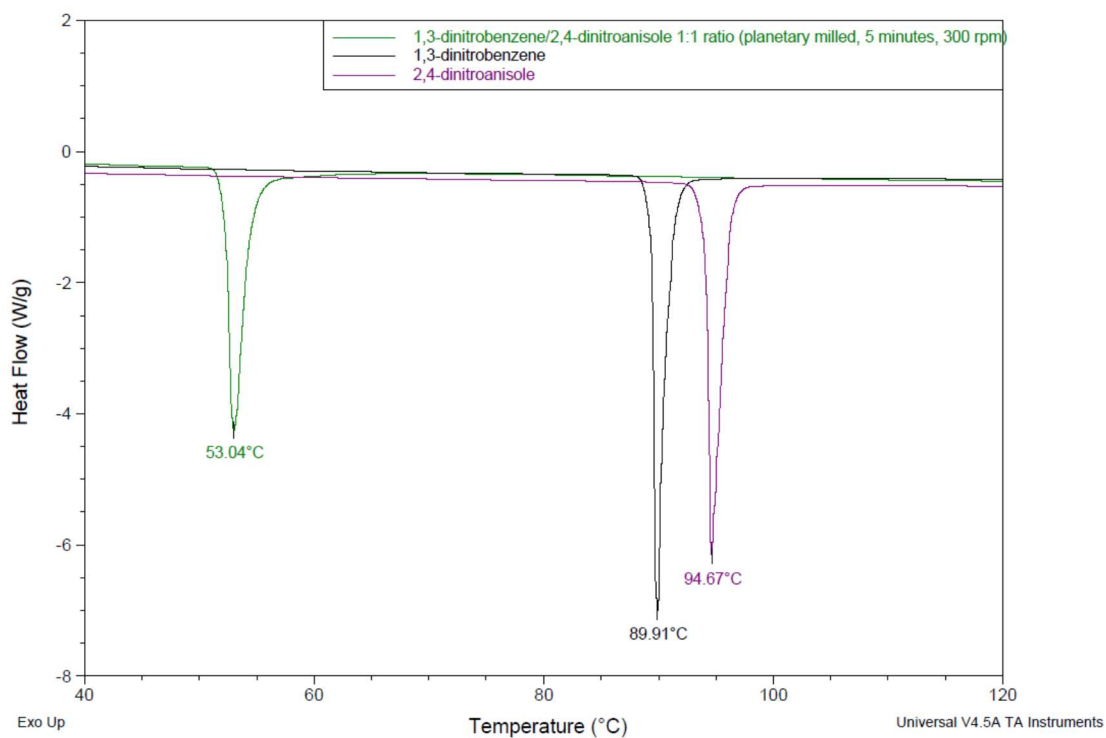


Figure B.11 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

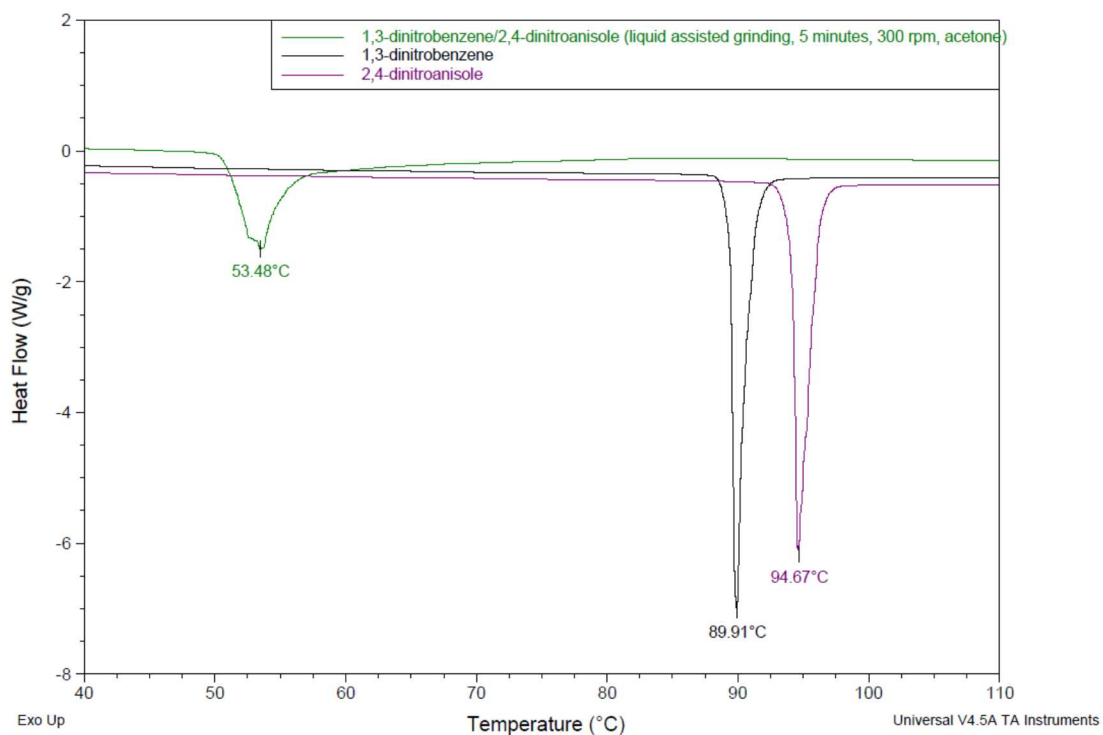


Figure B.12 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

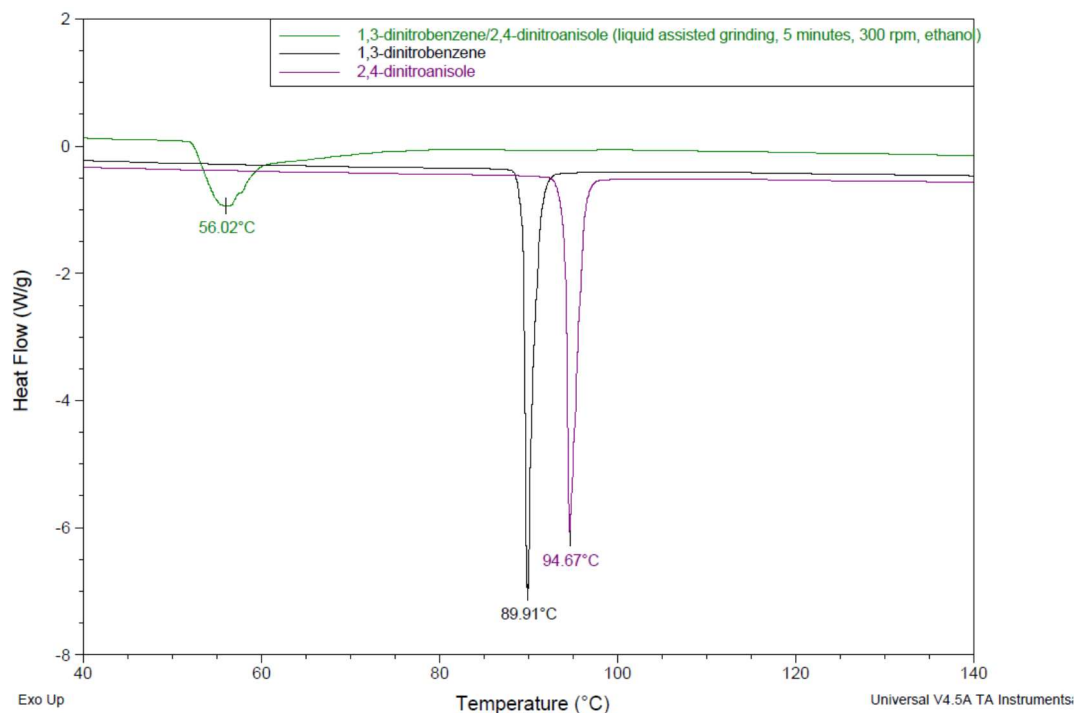


Figure B.13 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

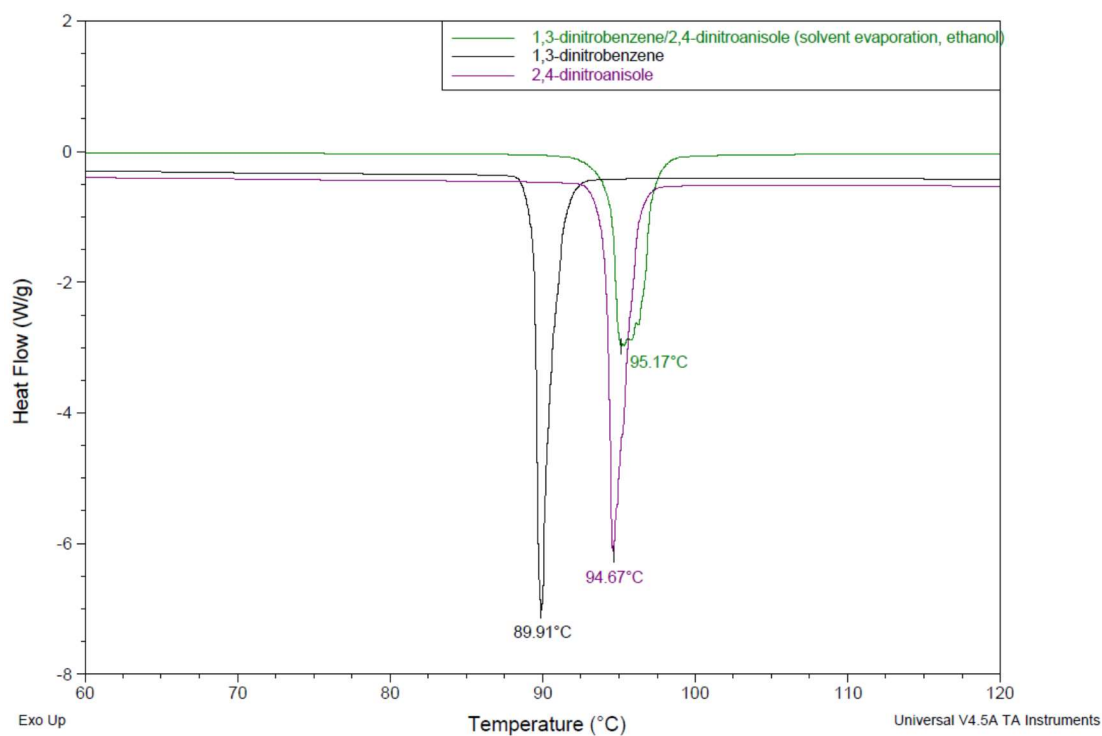


Figure B.14 - Thermal analysis of 1,3-dinitrobenzene/2,4-dinitroanisole produced by solvent evaporation from ethanol.

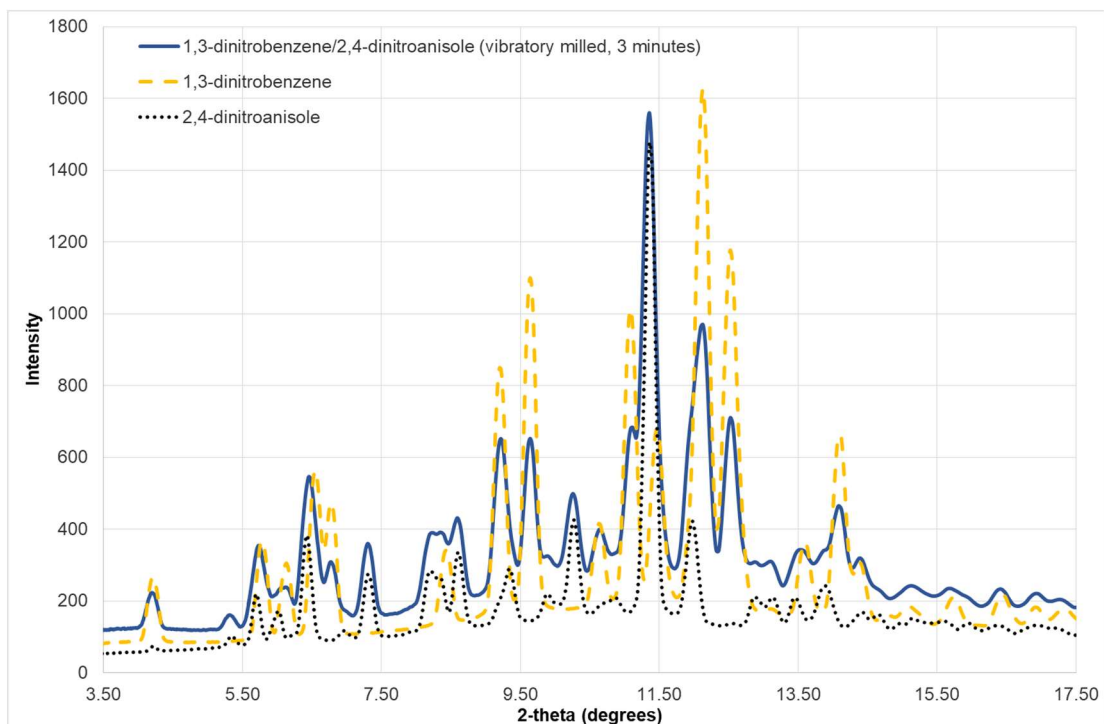


Figure B.15 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

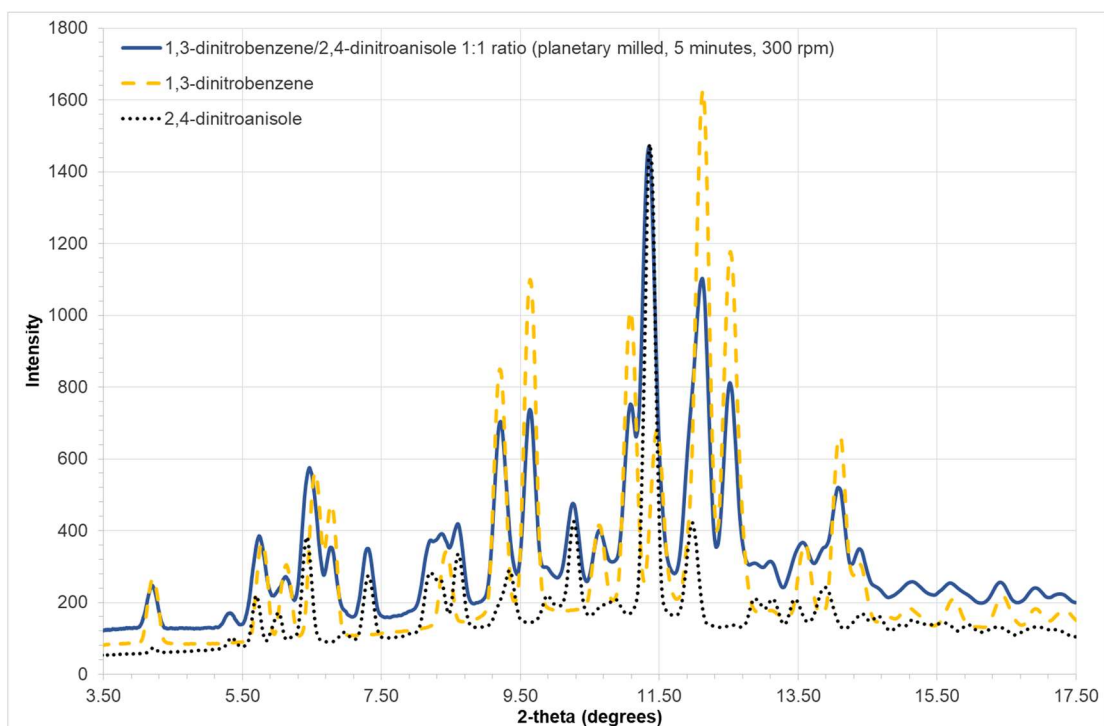


Figure B.16 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

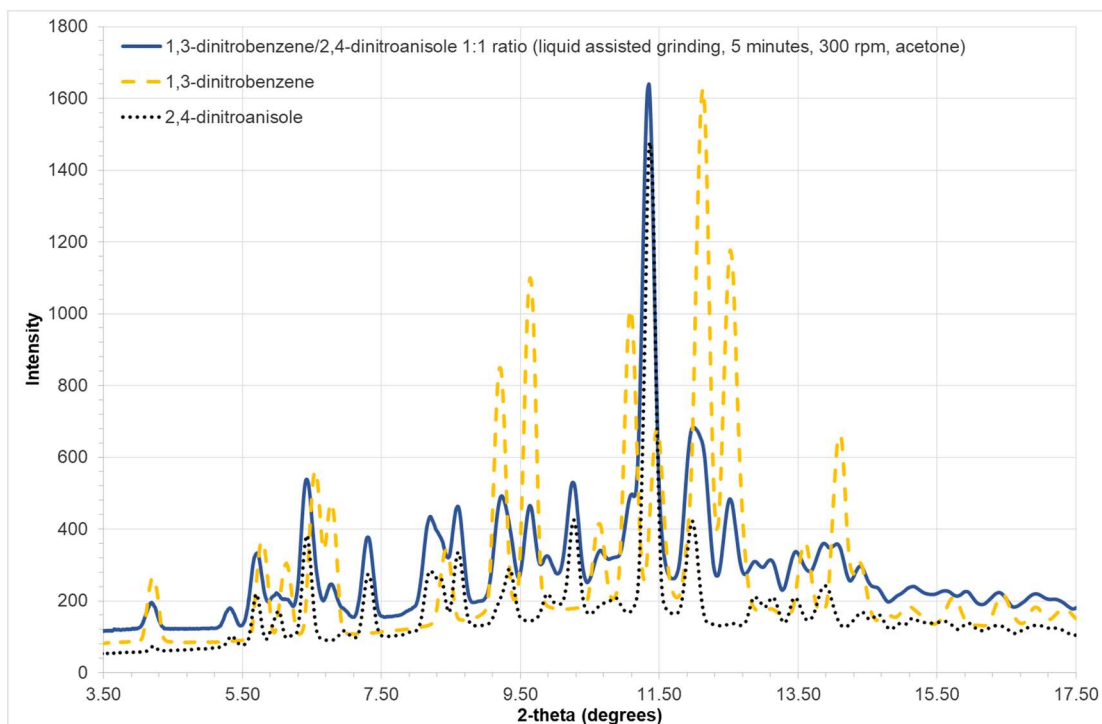


Figure B.17 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

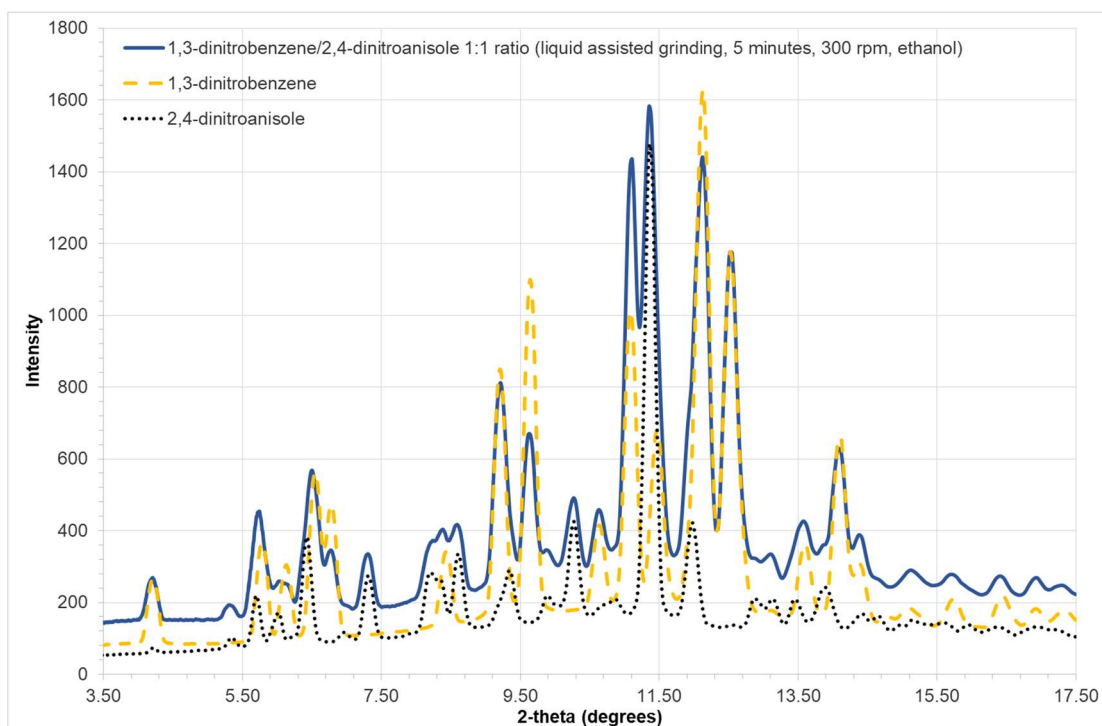


Figure B.18 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.3 1,3-dinitrobenzene/1,3,5-trichloro-,2,4,6-trinitrobenzene

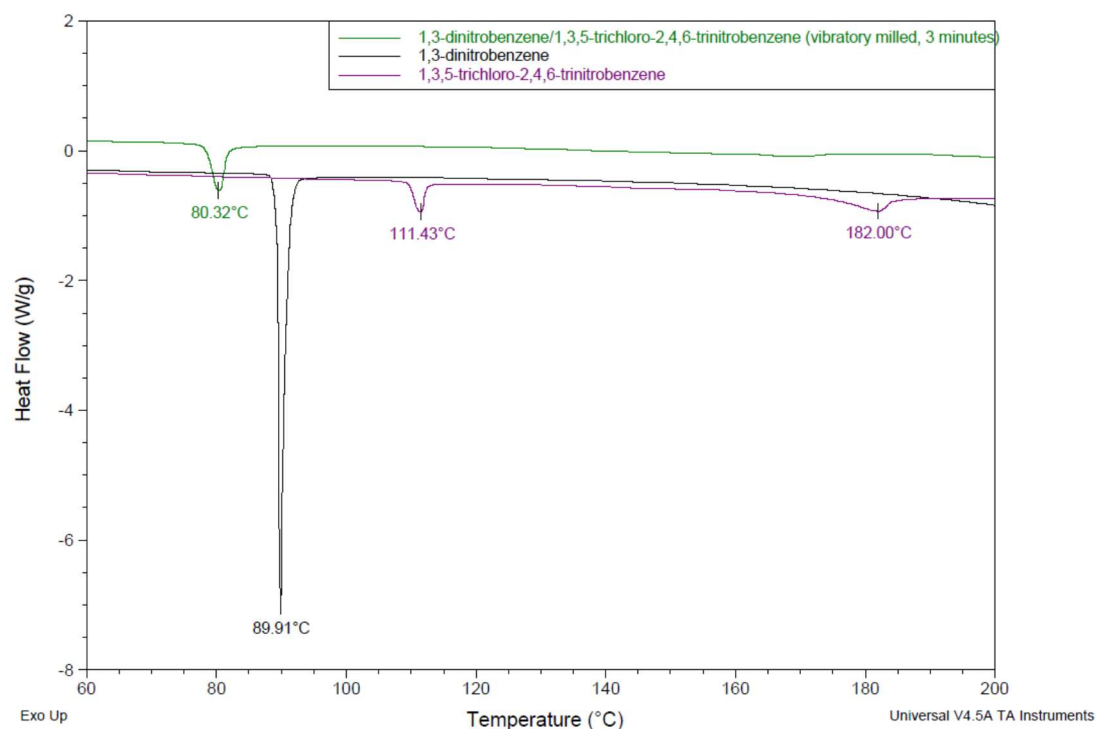


Figure B.19 – Thermal analysis of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by vibratory milling for 3 minutes.

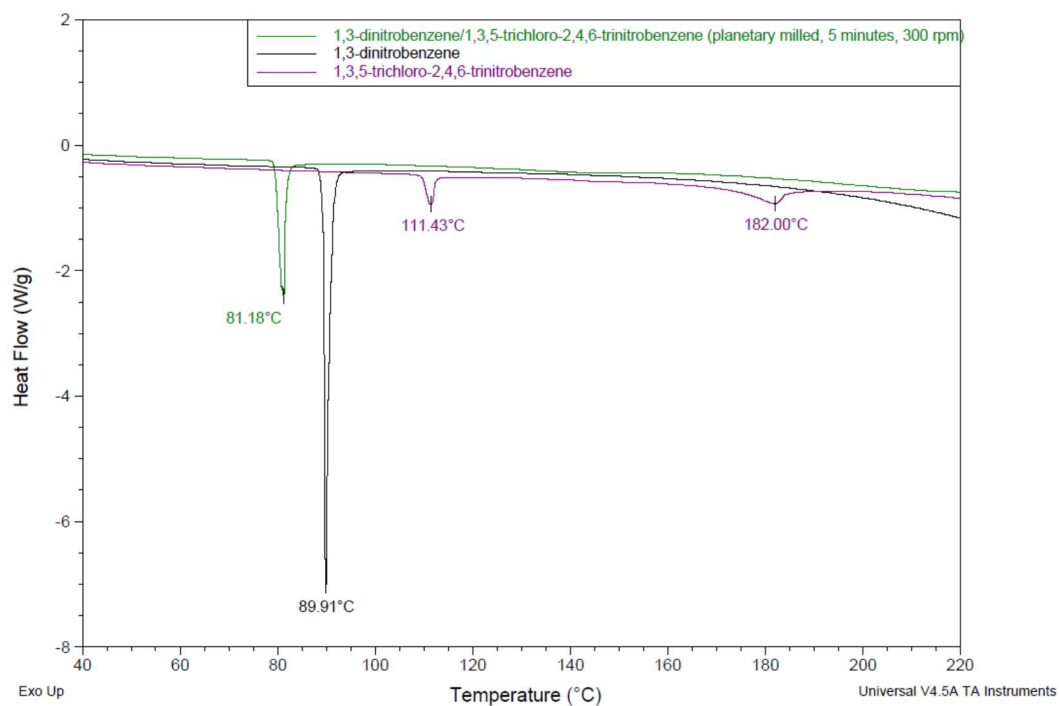


Figure B.20 - Thermal analysis of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

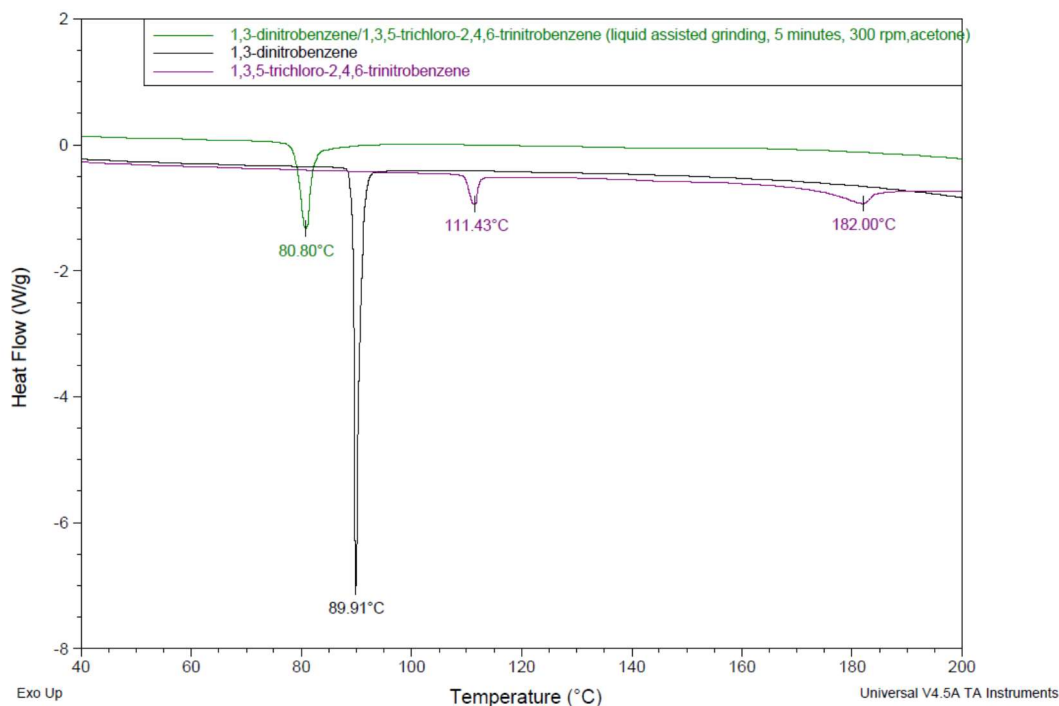


Figure B.21 - Thermal analysis of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

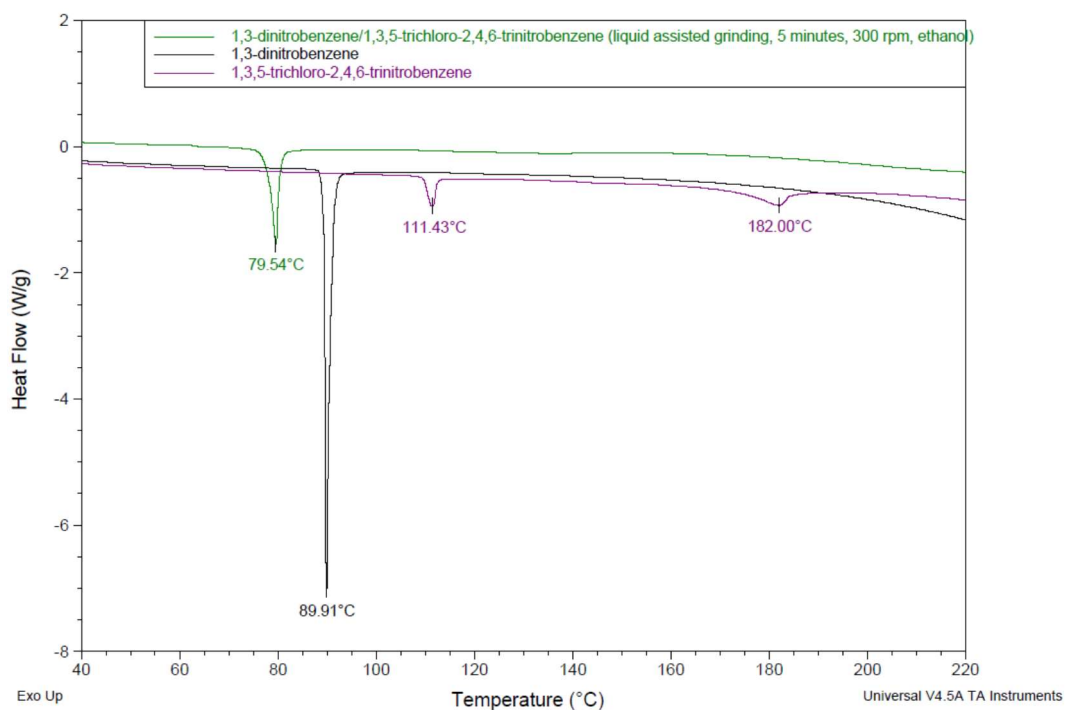


Figure B.22 - Thermal analysis of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

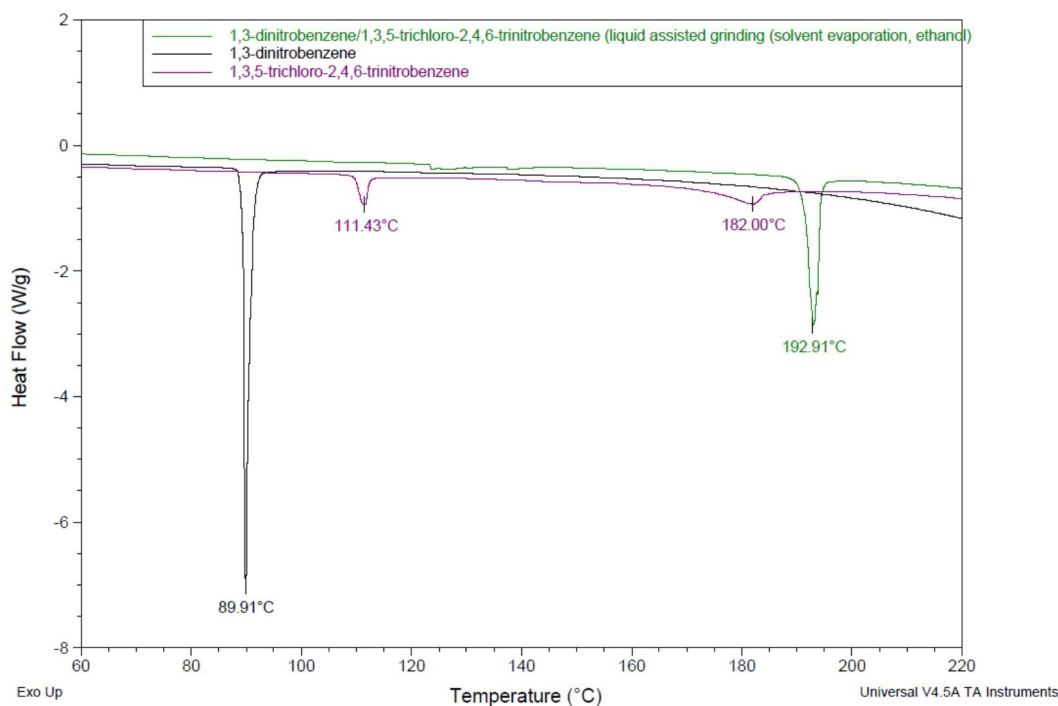


Figure B.23 - Thermal analysis of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by solvent evaporation with ethanol.

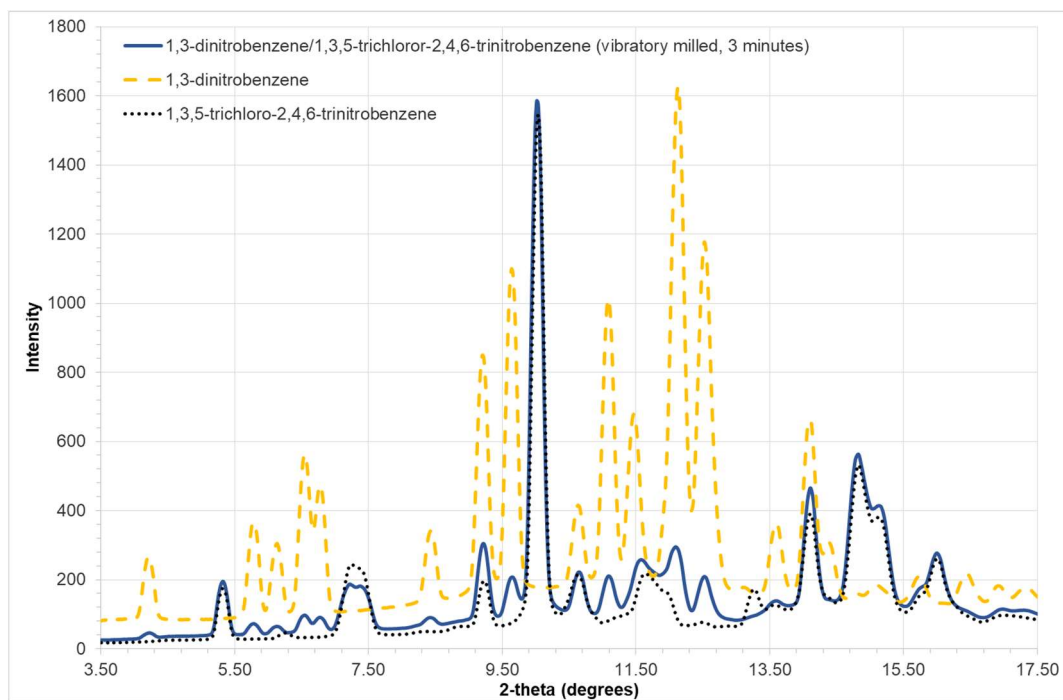


Figure B.24 - Powder x-ray pattern of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by vibratory milling for 3 minutes.

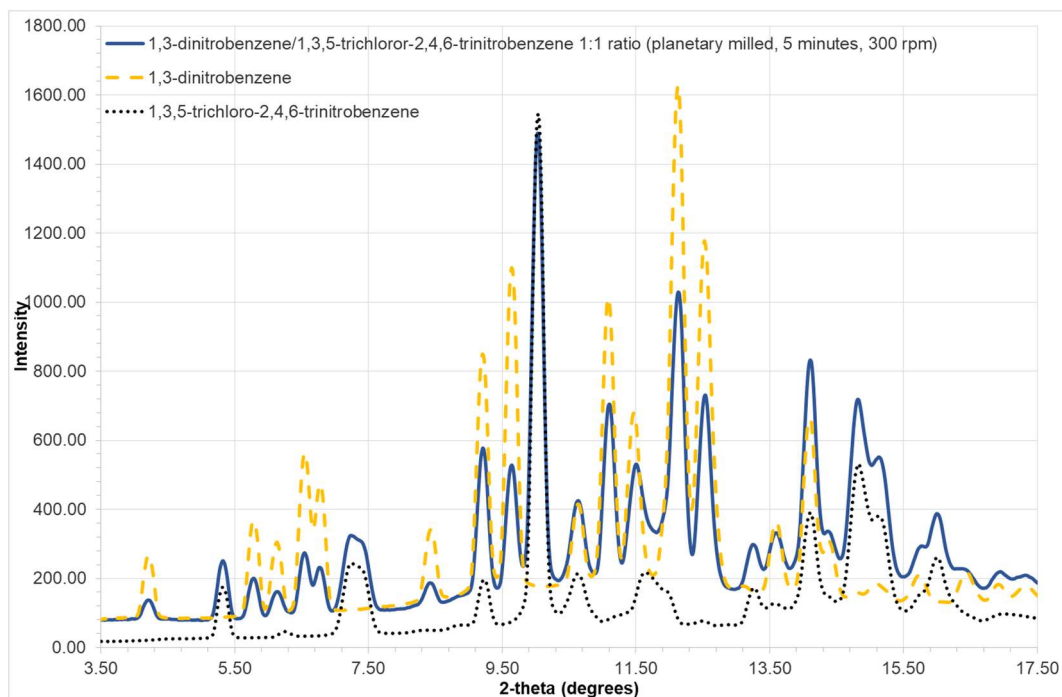


Figure B.25 - Powder x-ray pattern of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

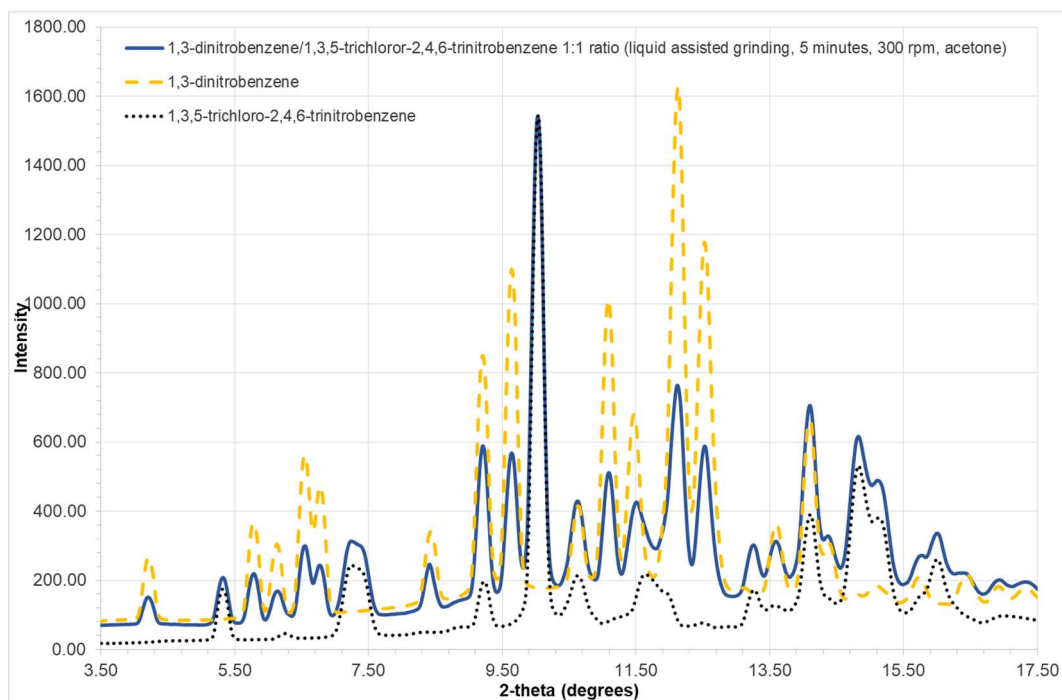


Figure B.26 - Powder x-ray pattern of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding, 5 minutes at 300 rpm with acetone.

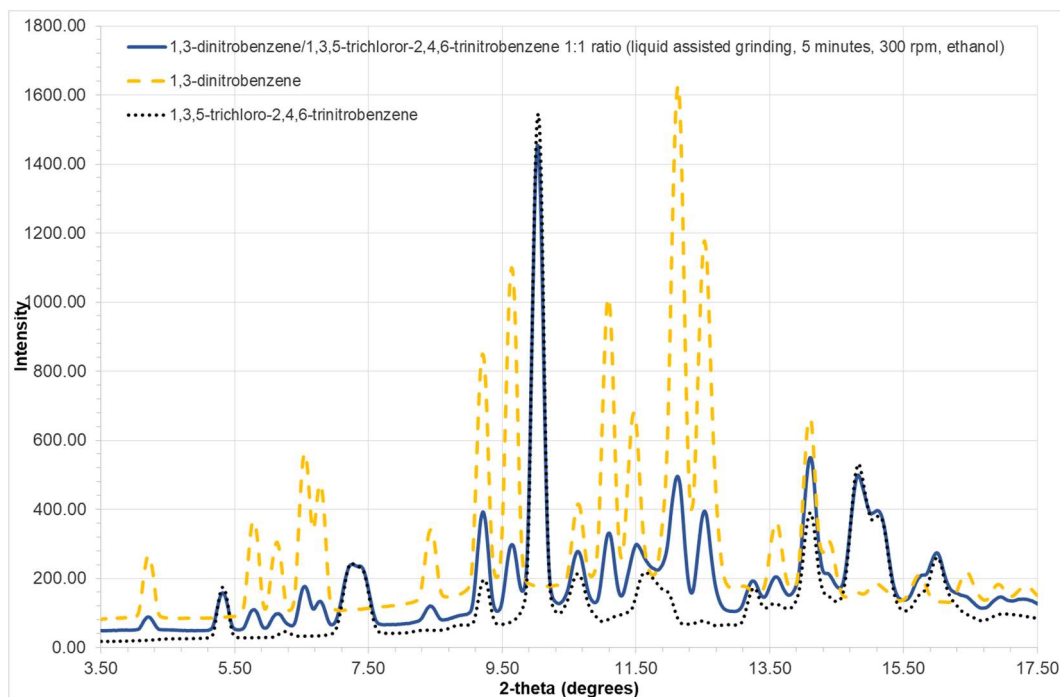


Figure B.27 - Powder x-ray pattern of 1,3-dinitrobenzene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding, 5 minutes at 300 rpm with ethanol.

B.4 1,3-dinitrobenzene/2,4,6-trinitroaniline

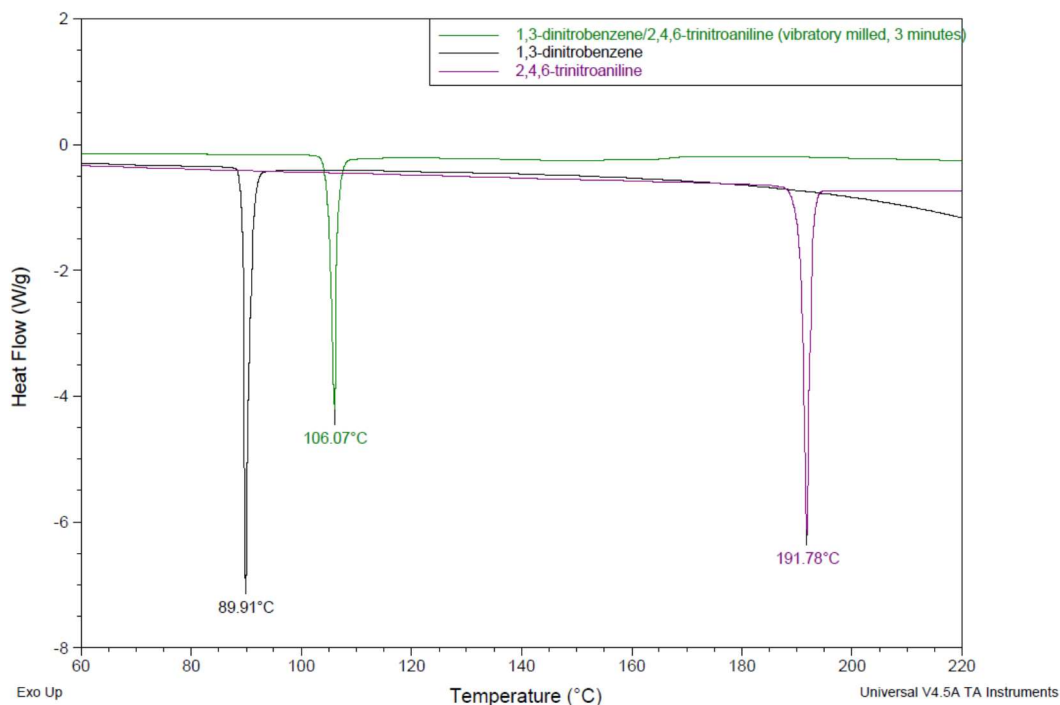


Figure B.28 – Thermal analysis of 1,3-dinitrobenzene/2,4,6-trinitroaniline produced by vibratory milling for 3 minutes.

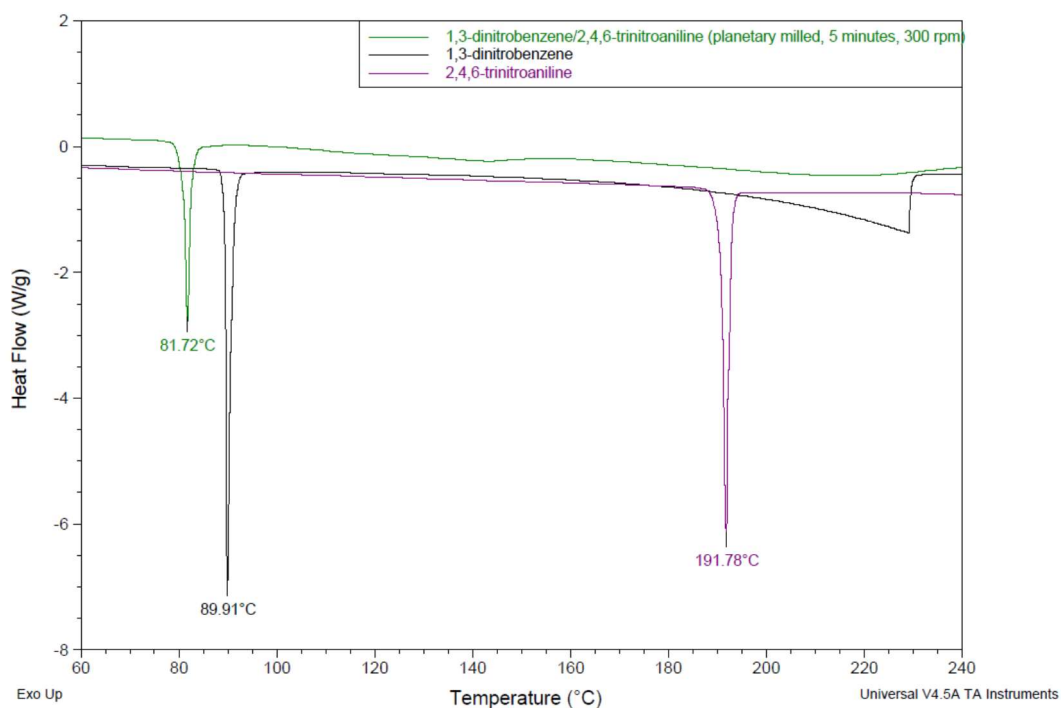


Figure B.29 - Thermal analysis of 1,3-dinitrobenzene/2,4,6-trinitroaniline produced by planetary milling for 5 minutes at 300 rpm.

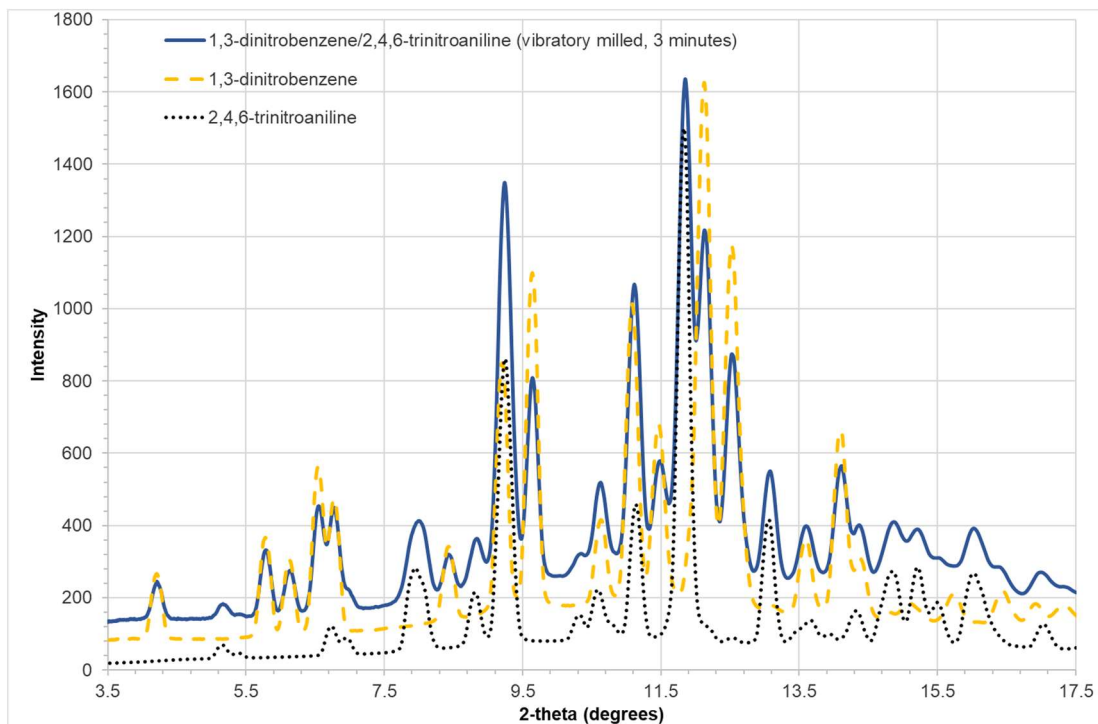


Figure B.30 – Powder x-ray pattern of 1,3-dinitrobenzene/2,4,6-trinitroaniline produced by vibratory milling for 3 minutes.

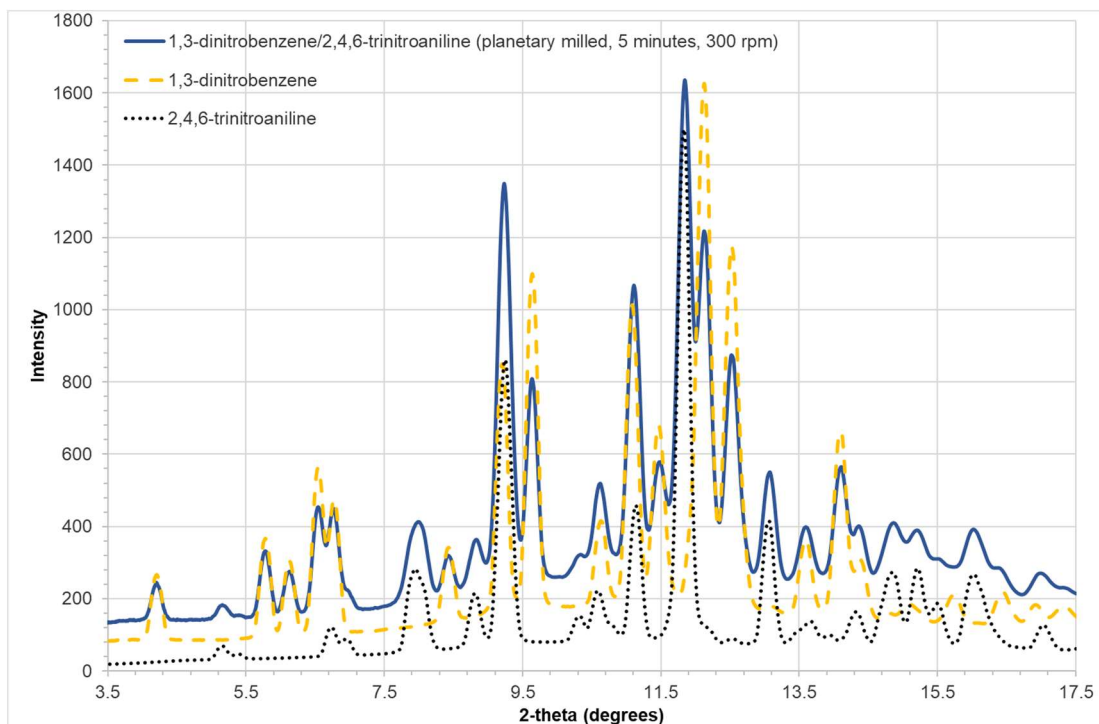


Figure B.31 - Powder x-ray pattern of 1,3-dinitrobenzene/2,4,6-trinitroaniline produced by planetary milling for 5 minutes for 300 rpm.

B.5 2,4-dinitrotoluene/2,4-dinitroaniline

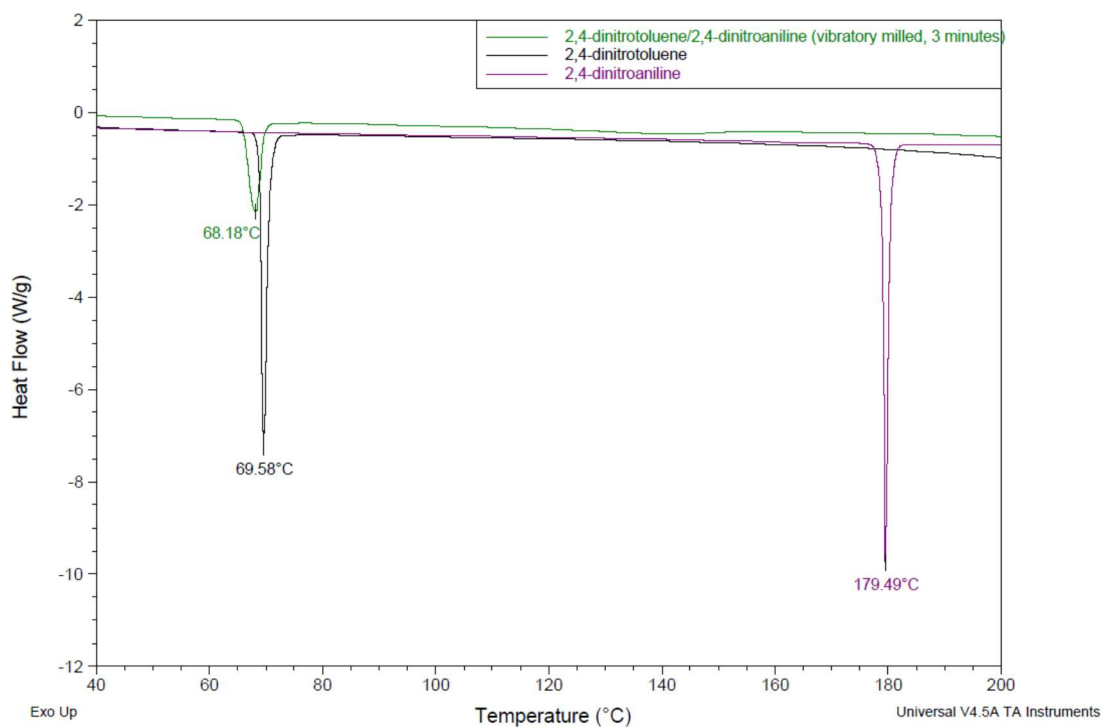


Figure B.32 - Thermal analysis of 2,4-dinitrotoluene/2,4-dinitroaniline produced by vibratory milling for 3 minutes.

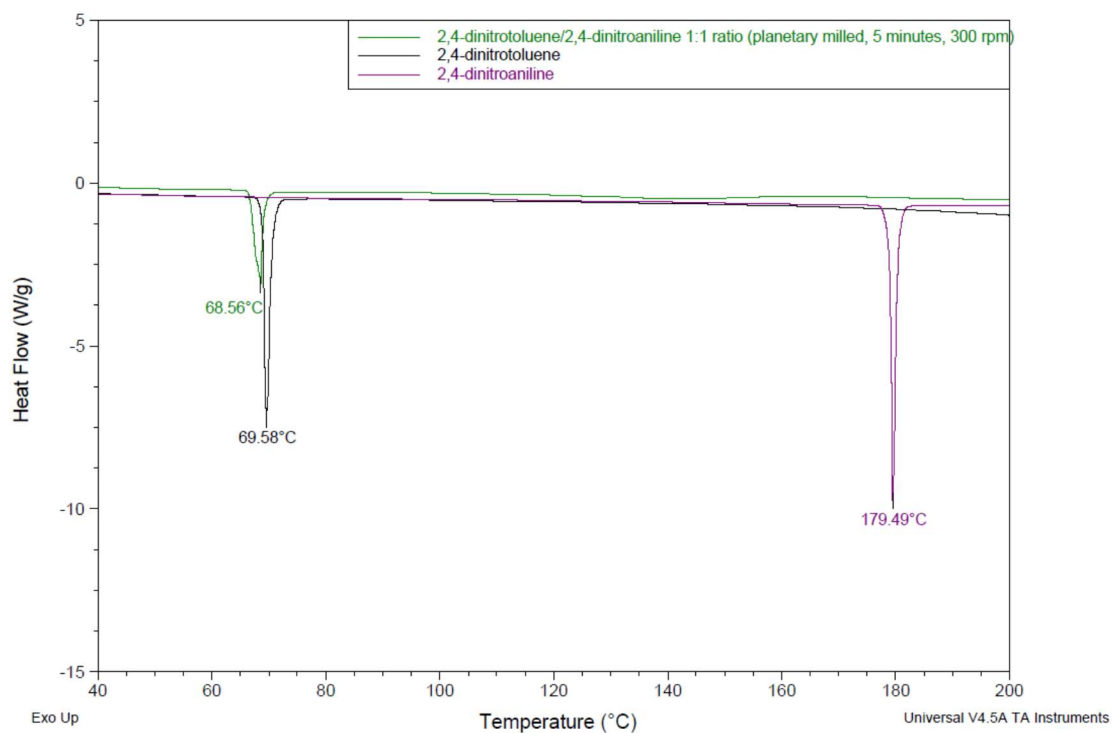


Figure B.33 - Thermal analysis of 2,4-dinitrotoluene/2,4-dinitroaniline produced by planetary milling for 5 minutes at 300 rpm.

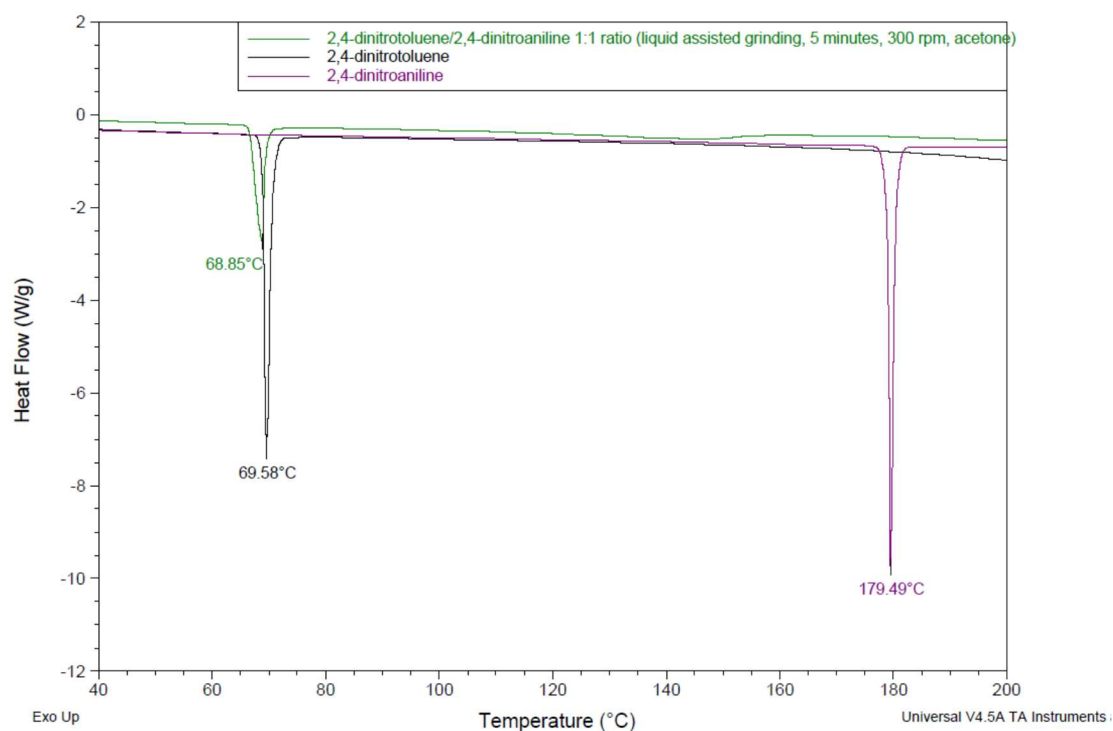


Figure B.34 - Thermal analysis of 2,4-dinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

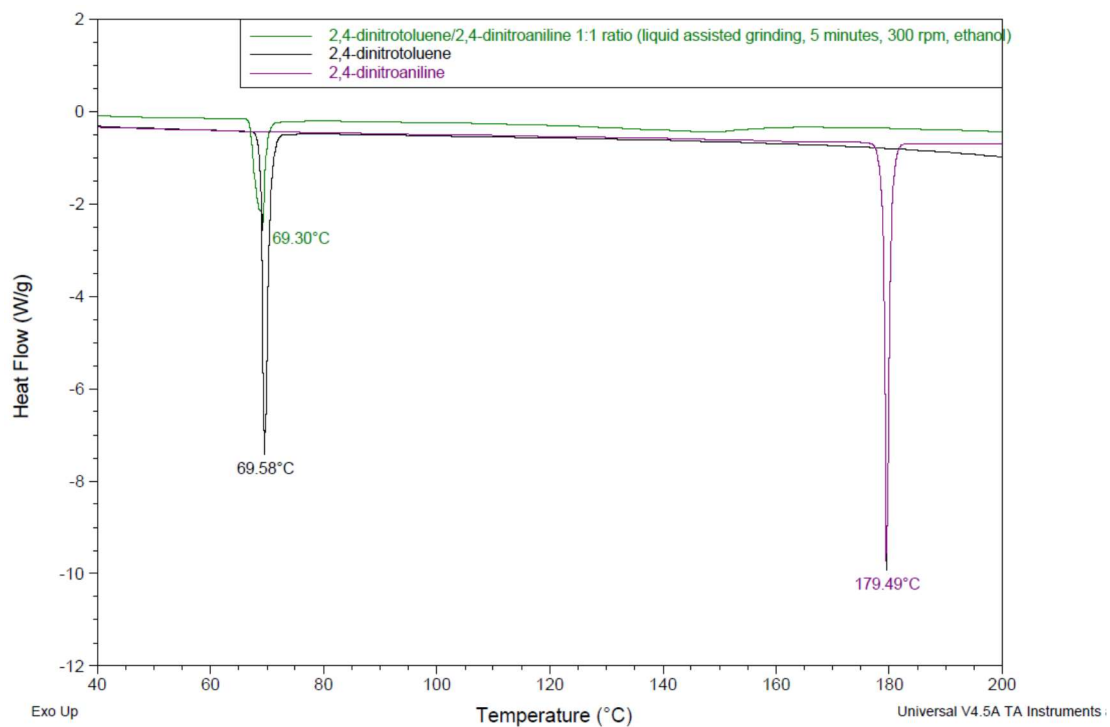


Figure B.35 - Thermal analysis of 2,4-dinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

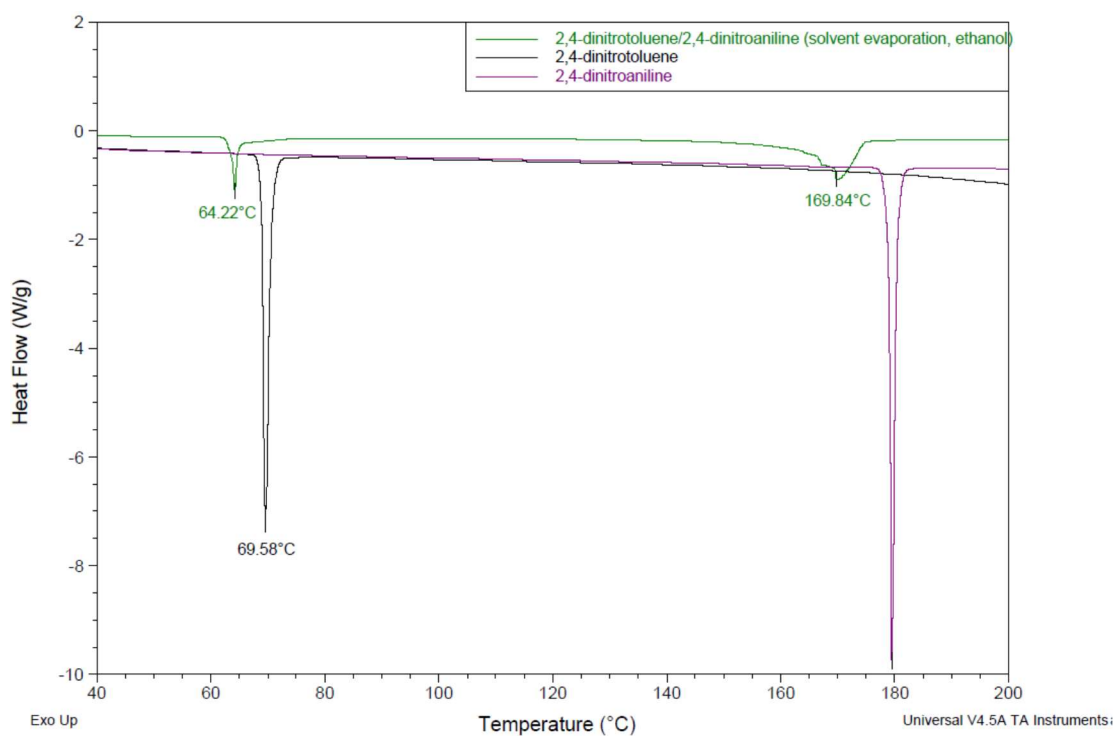


Figure B.36 - Thermal analysis of 2,4-dinitrotoluene/2,4-dinitroaniline produced by solvent evaporation with ethanol.

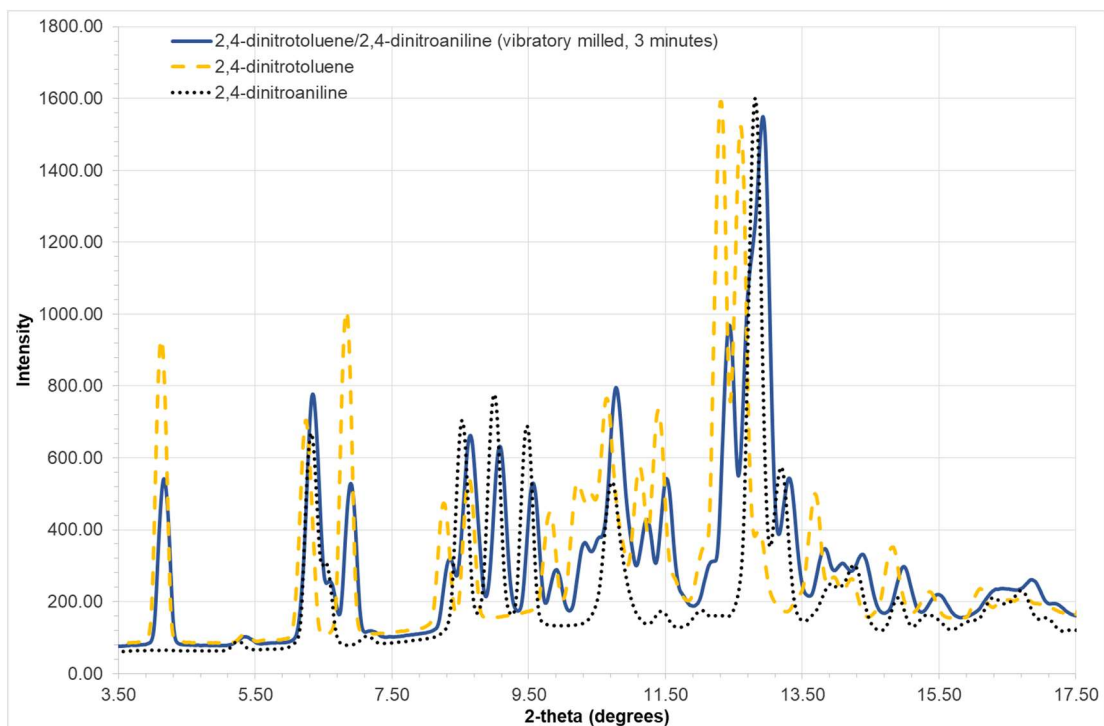


Figure B.37 – Powder x-ray pattern of 2,4-dinitrotoluene/2,4-dinitroaniline produced by vibratory milling for 3 minutes.

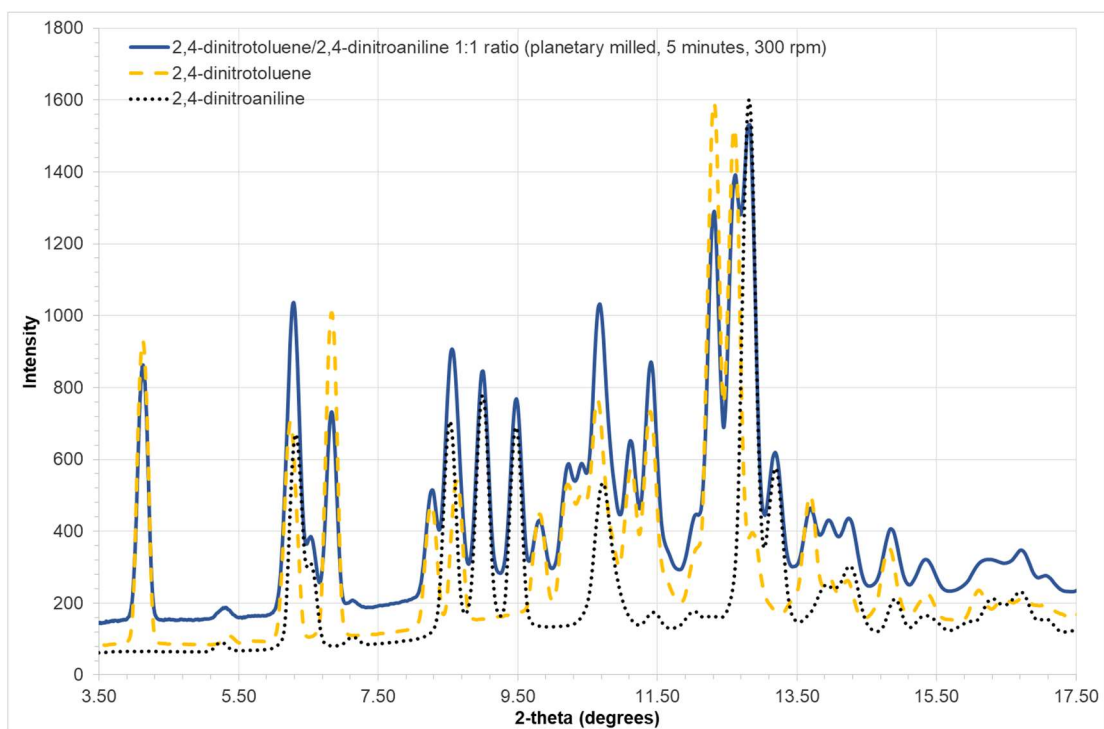


Figure B.38 - Powder x-ray pattern of 2,4-dinitrotoluene/2,4-dinitroaniline produced by planetary milling for 5 minutes, 300 rpm.

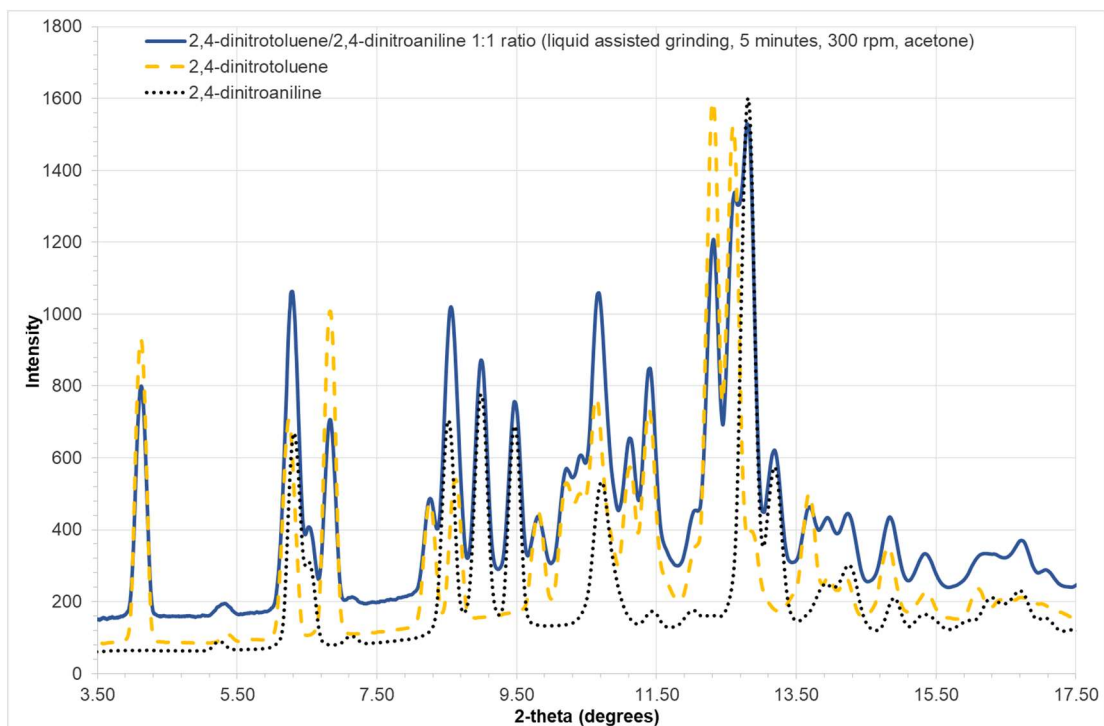


Figure B.39 - Powder x-ray pattern of 2,4-dinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes, 300 rpm with acetone.

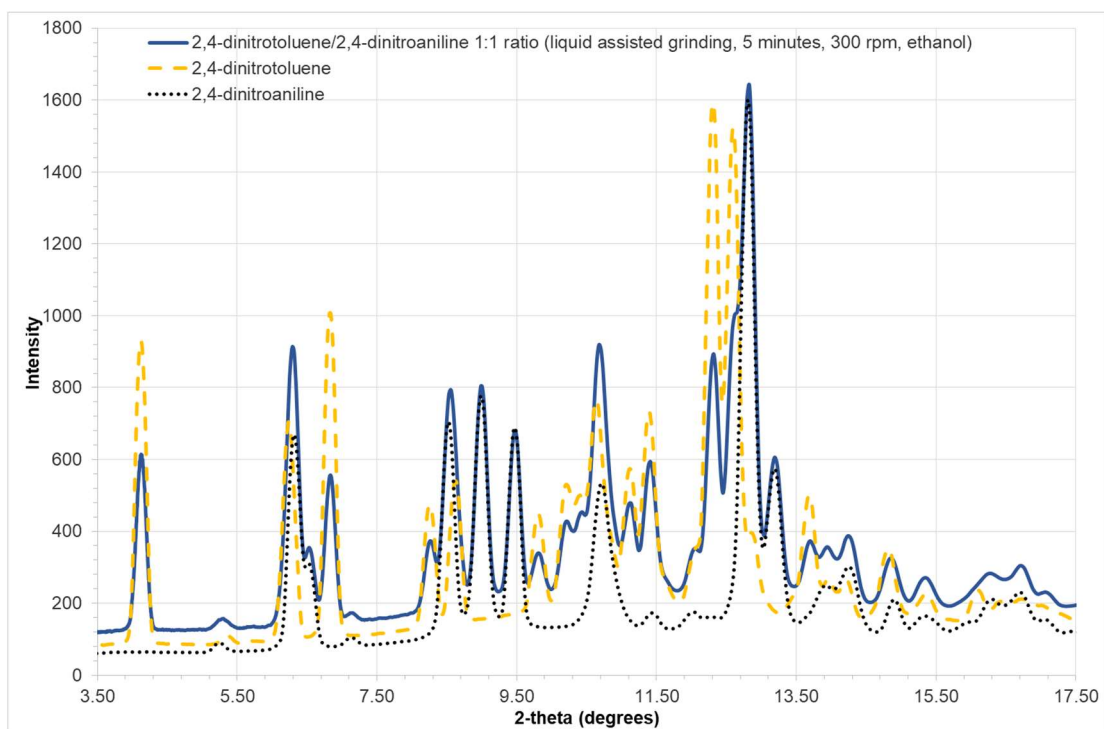


Figure B.40 - Powder x-ray pattern of 2,4-dinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes, 300 rpm with ethanol.

B.6 2,4-dinitrotoluene/2,4-dinitroanisole

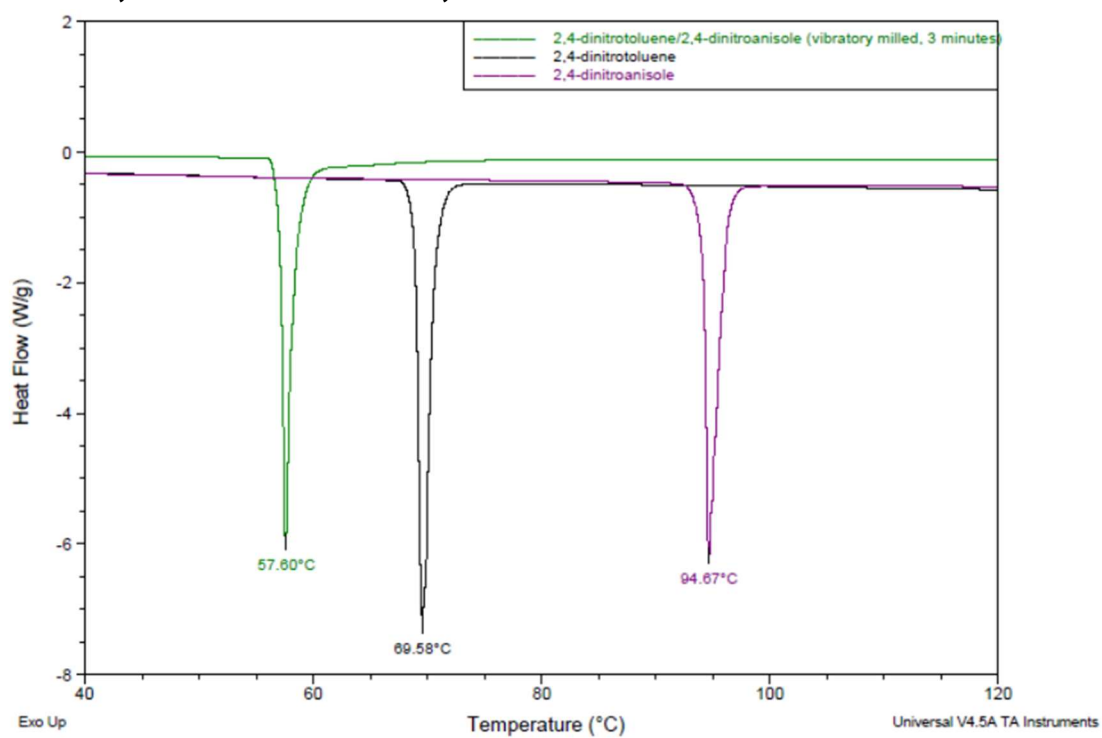


Figure B.41 – Thermal analysis of 2,4-dinitrotoluene/2,4-dinitroanisole produced by vibratory milling for 3 minutes.

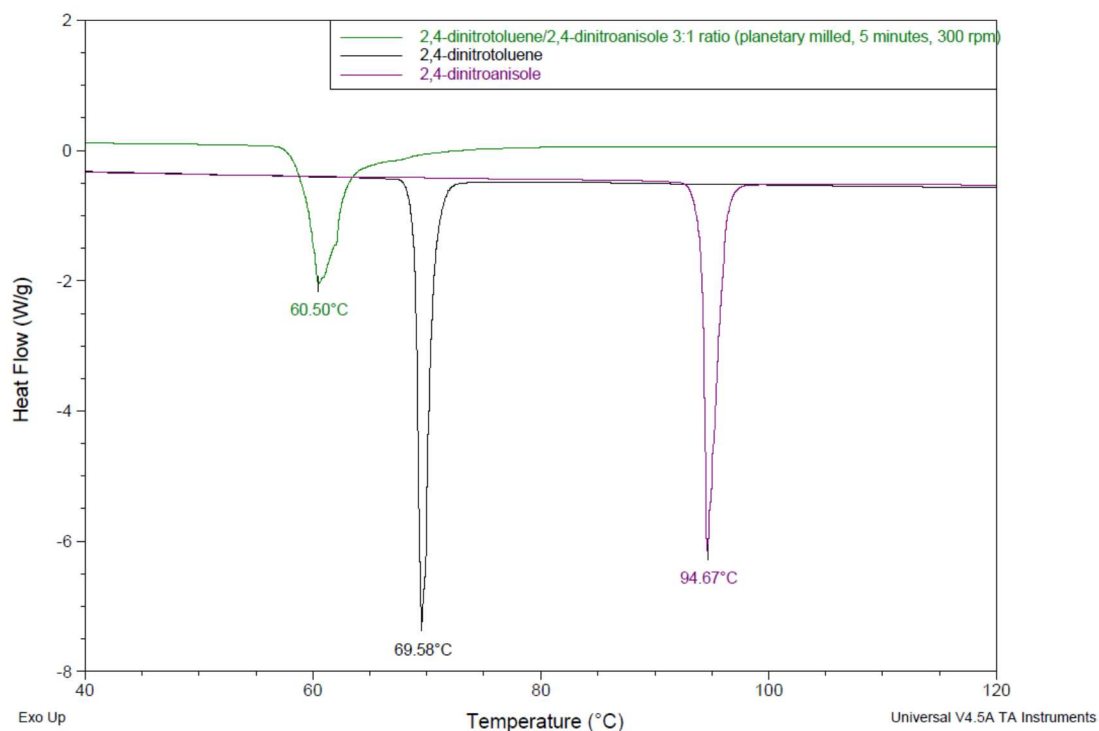


Figure B.42 - Thermal analysis of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

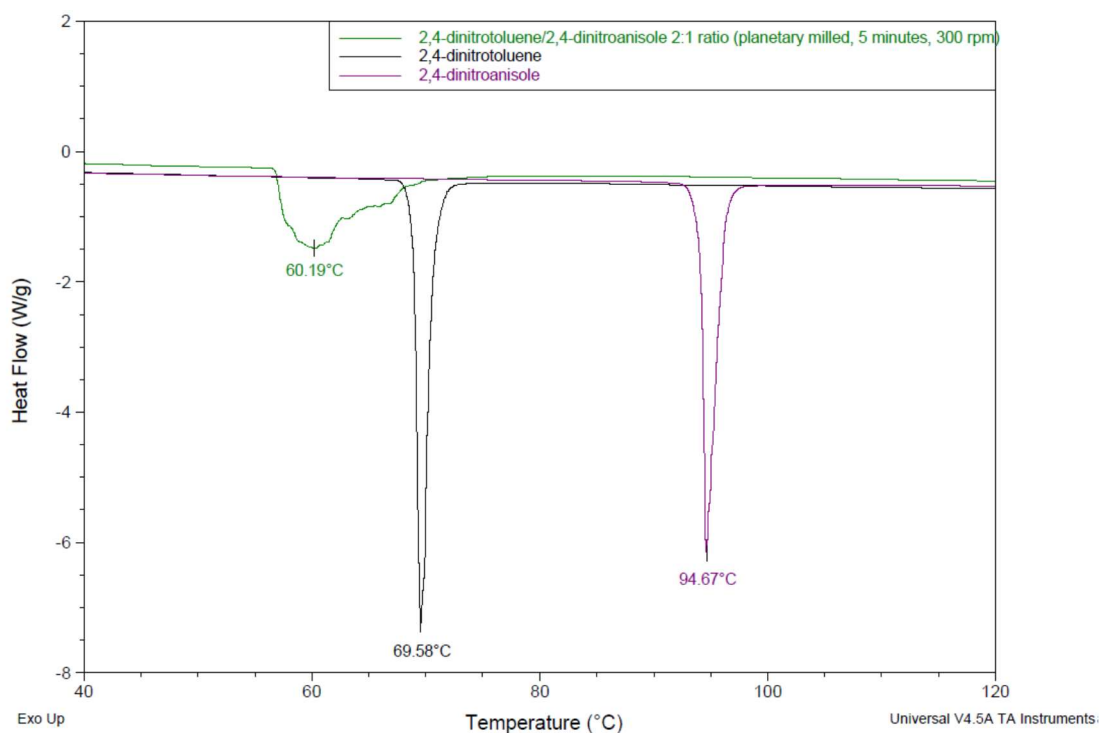


Figure B.43 - Thermal analysis of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

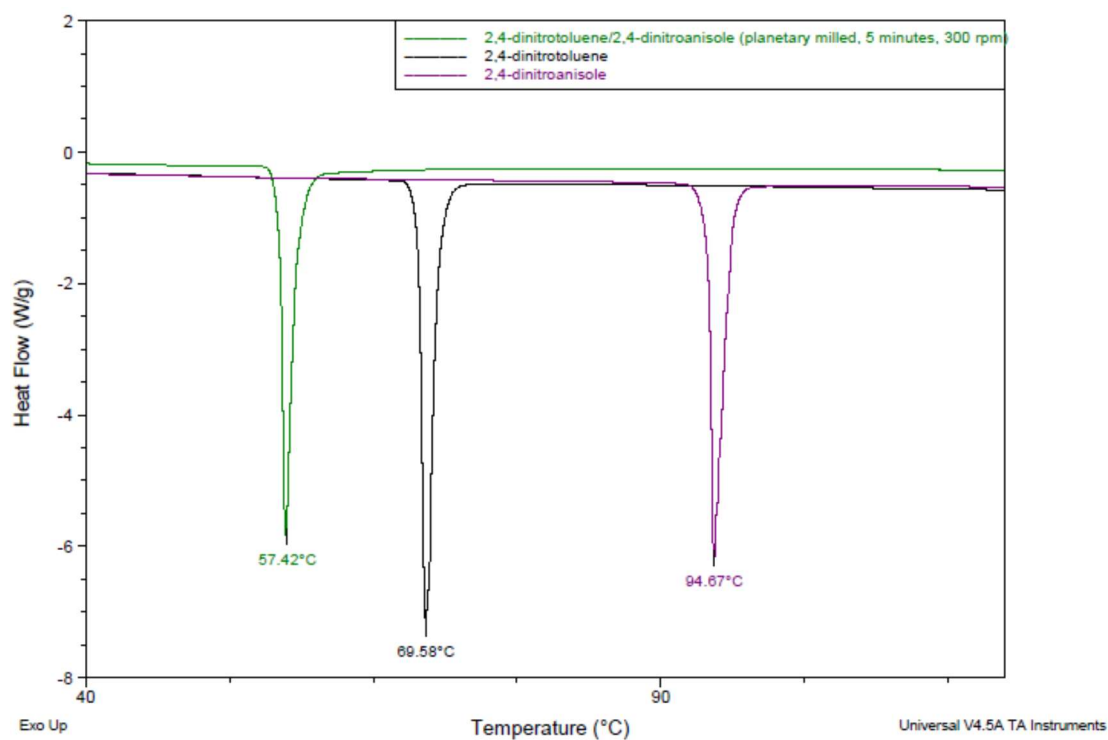


Figure B.44 - Thermal analysis of 2,4-dinitrotoluene/2,4-dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

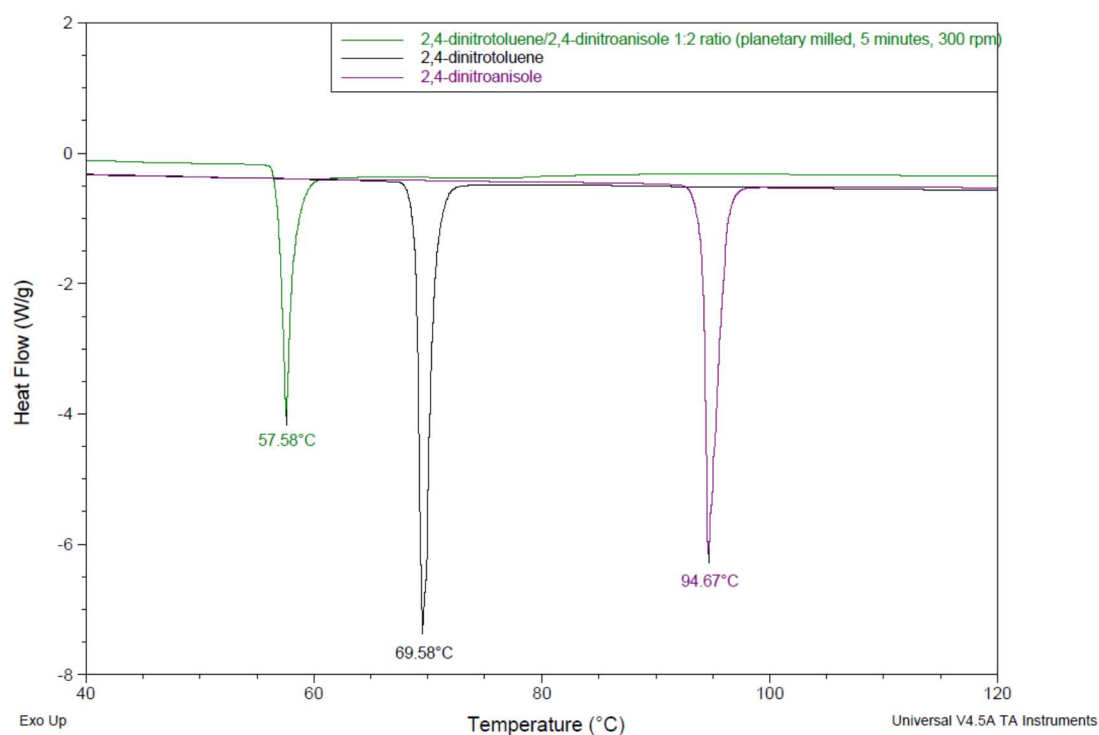


Figure B.45 - Thermal analysis of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

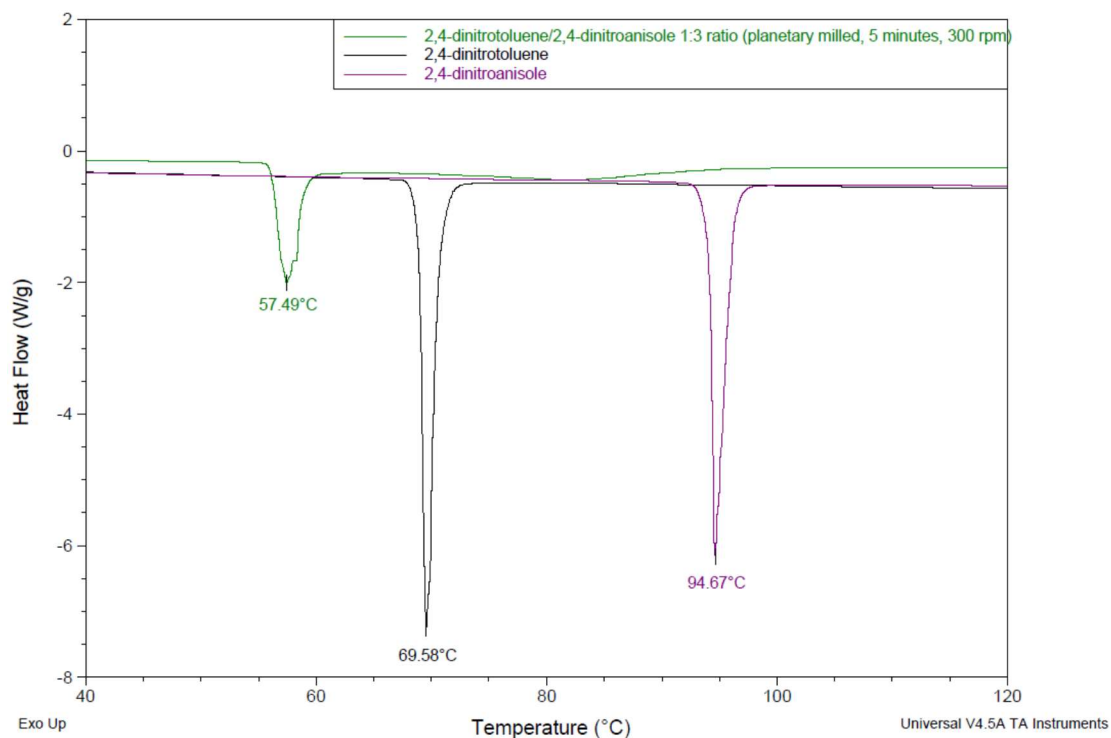


Figure B.46 - Thermal analysis of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

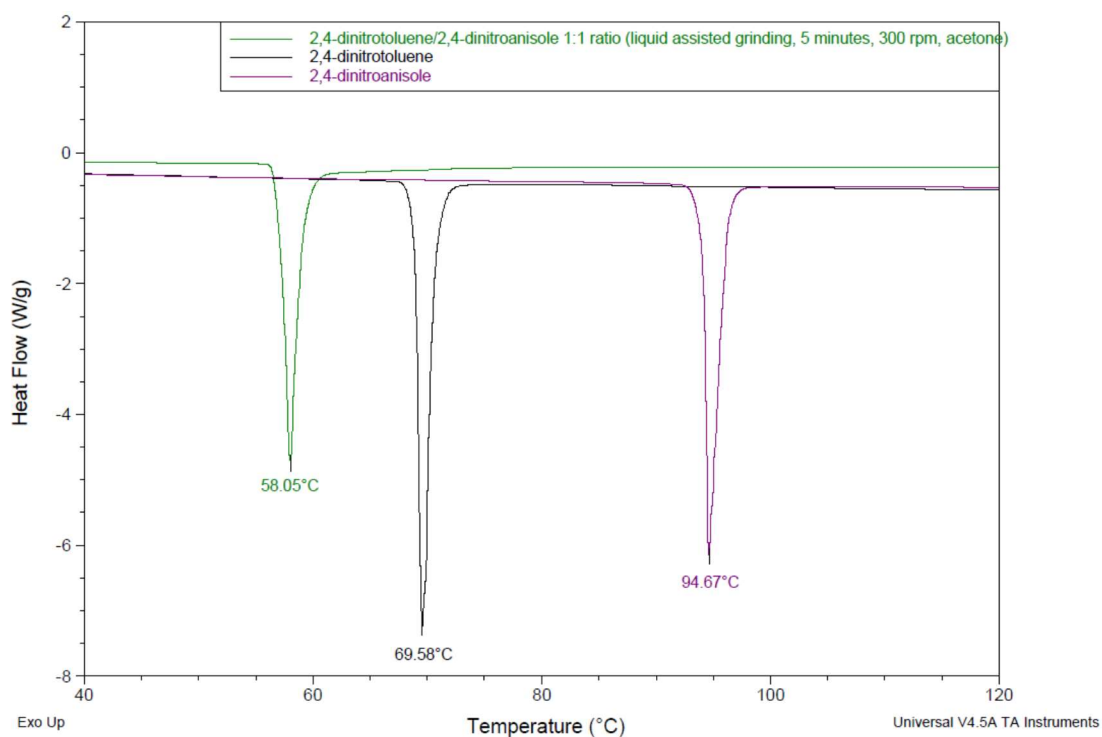


Figure B.47 - Thermal analysis of 2,4 dinitrotoluene/2,4 dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

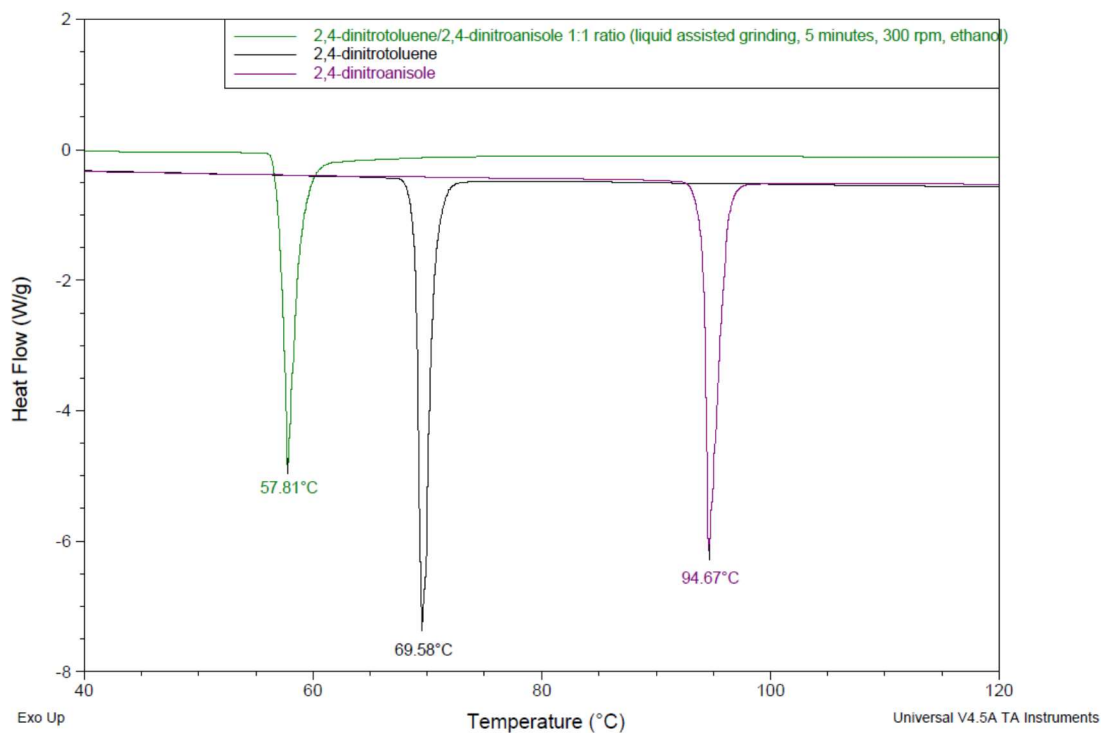


Figure B.48 - Thermal analysis of 2,4 dinitrotoluene/2,4 dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

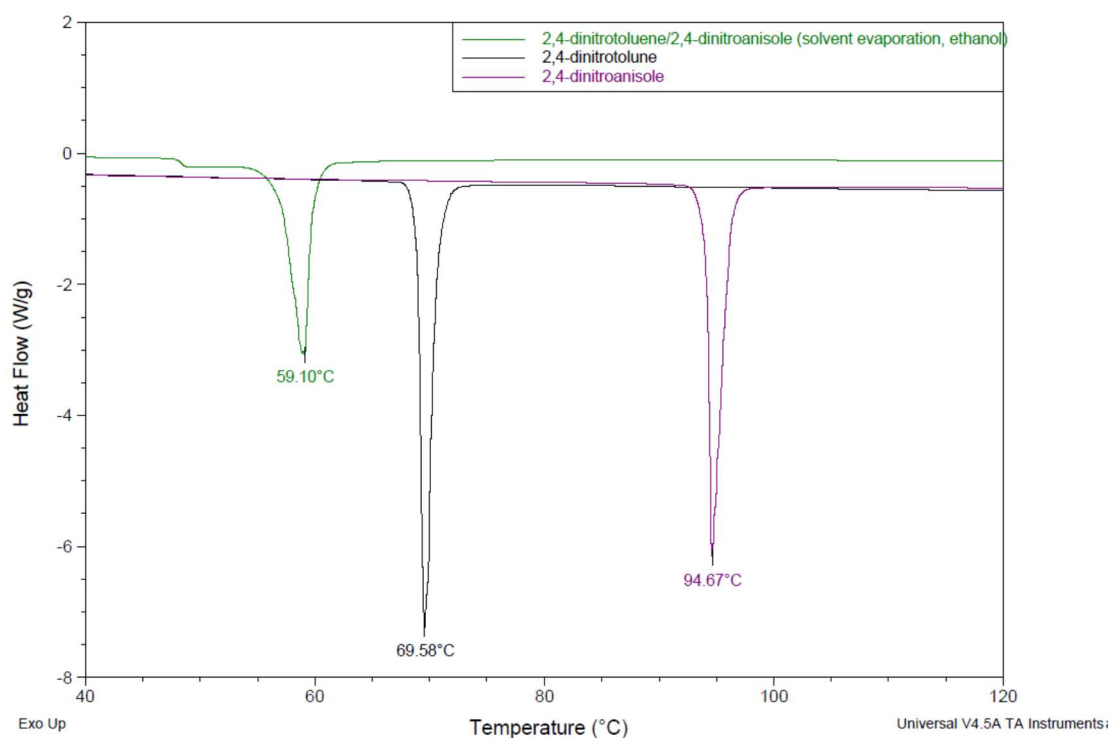


Figure B.49 - Thermal analysis of 2,4 dinitrotoluene/2,4 dinitroanisole produced by solvent evaporation with ethanol.

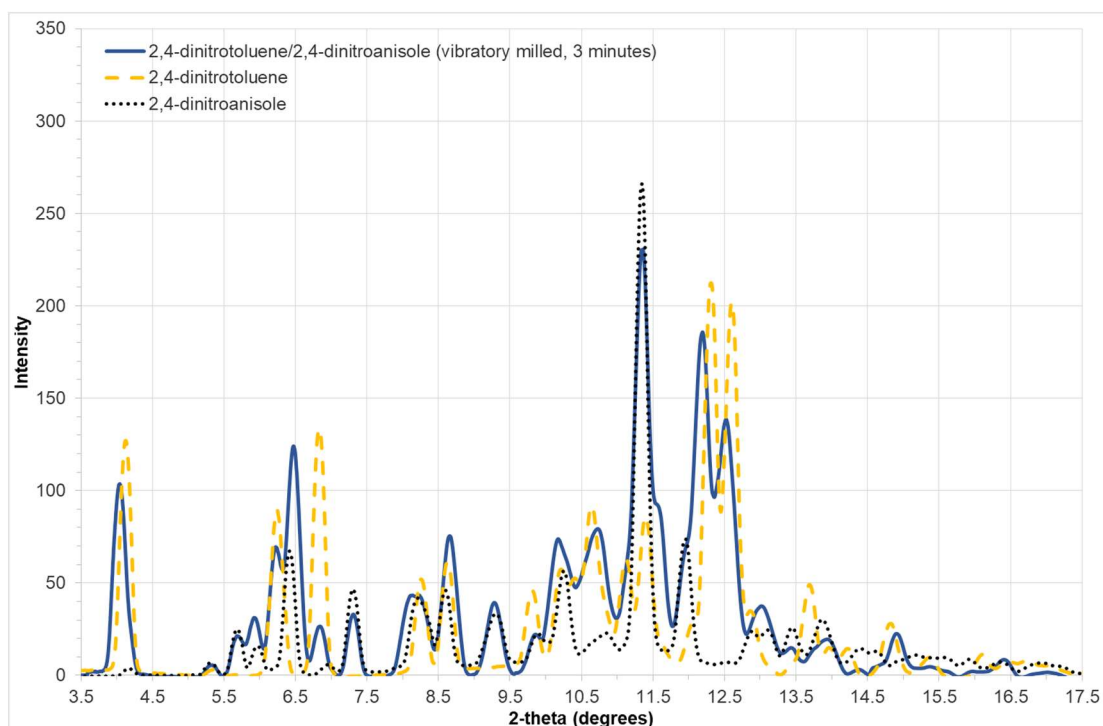


Figure B.50 – Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by vibratory milling for 3 minutes.

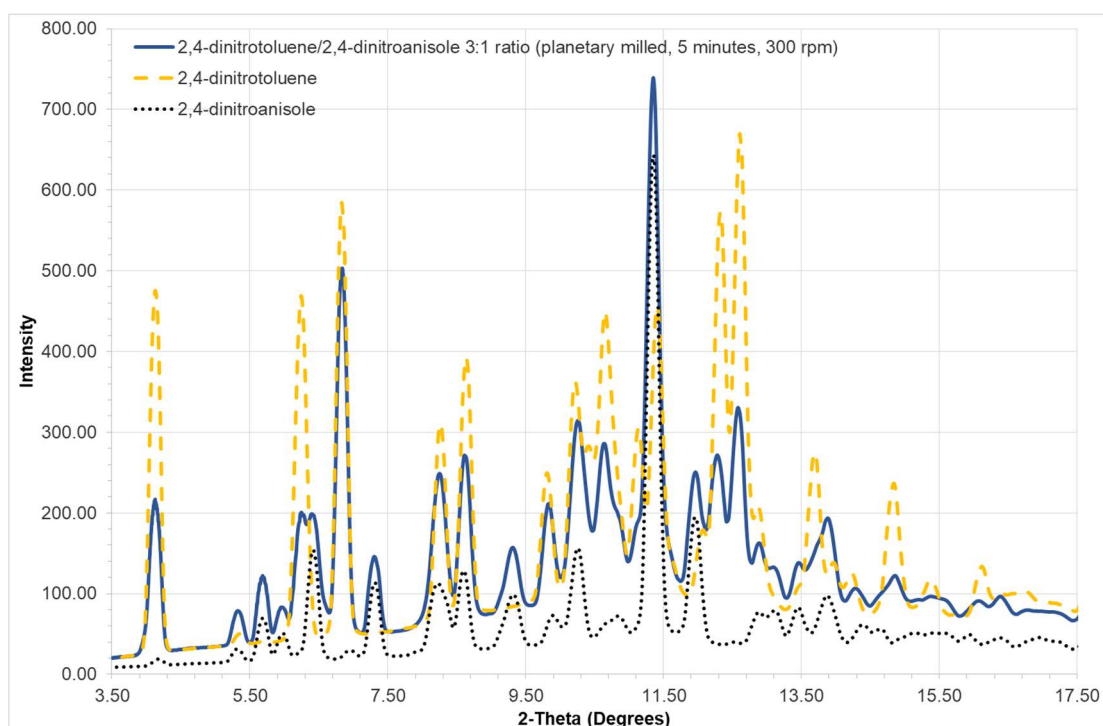


Figure B.51 - Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

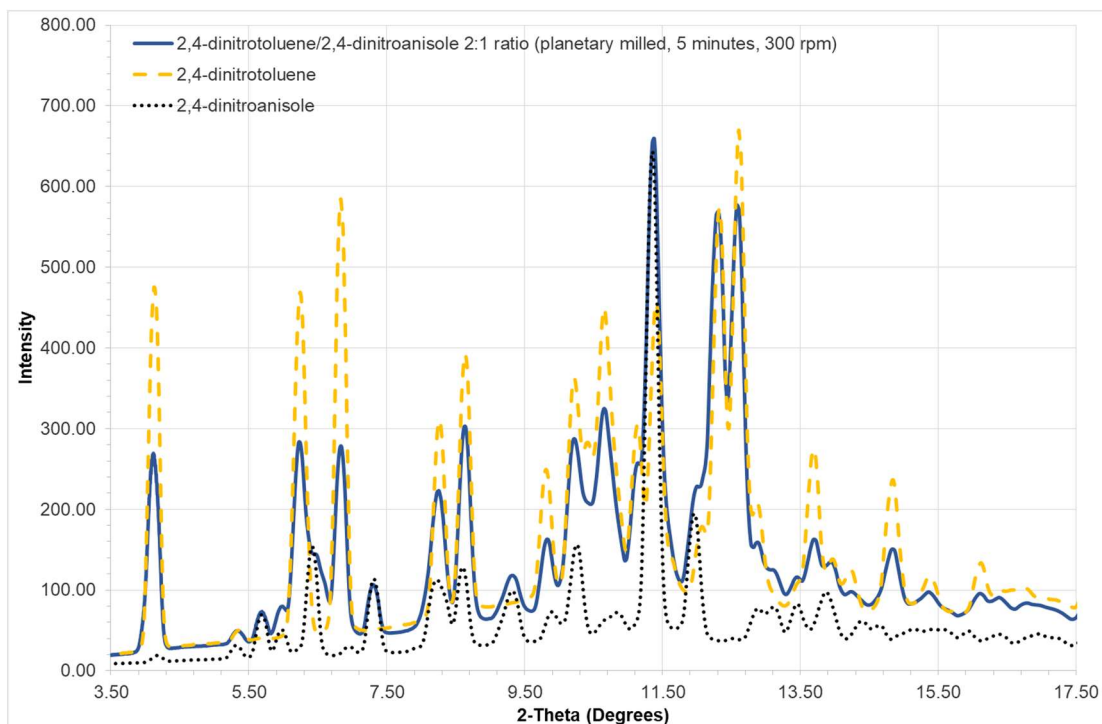


Figure B.52 - Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

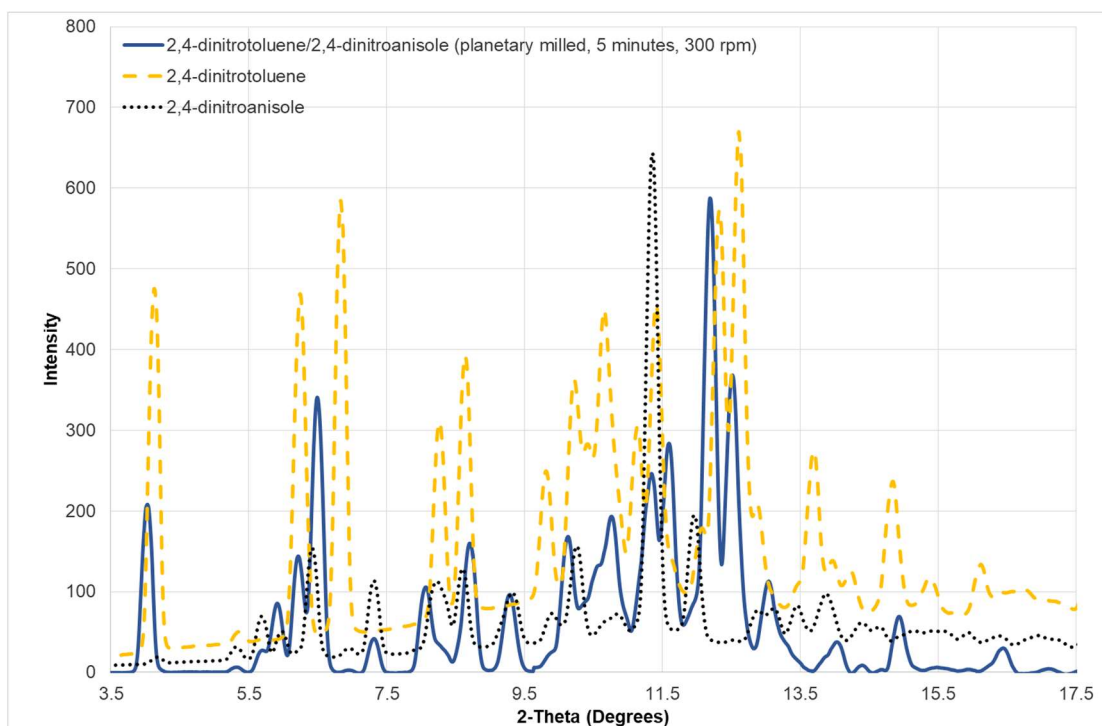


Figure B.53 - Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

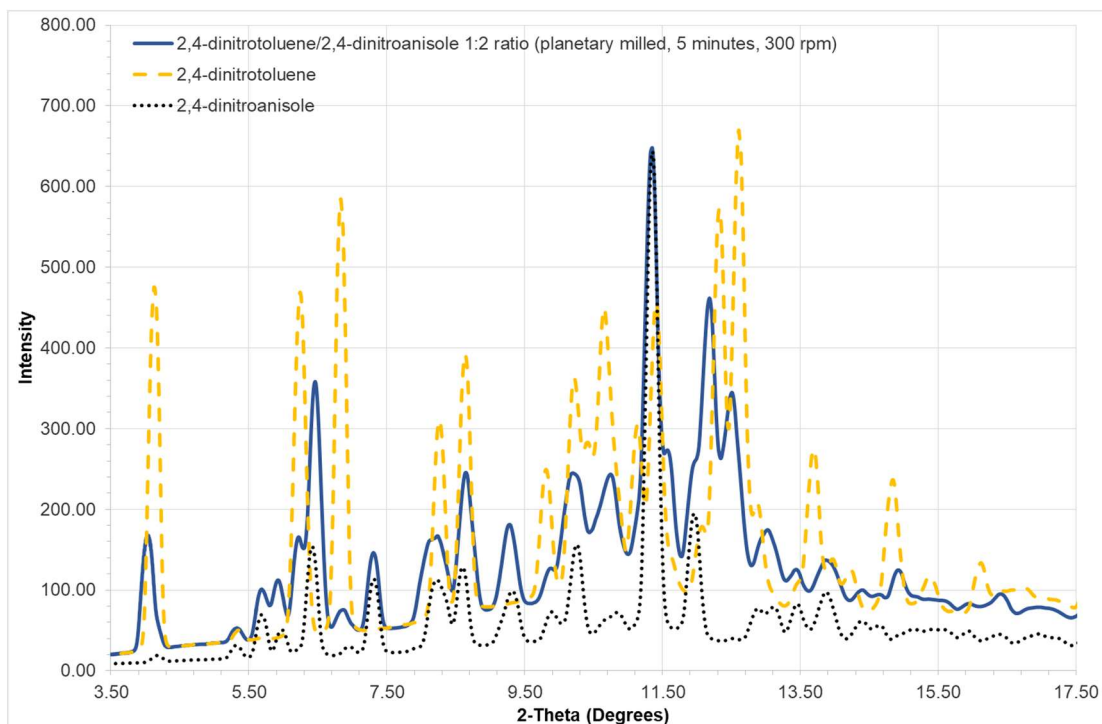


Figure B.54 - Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

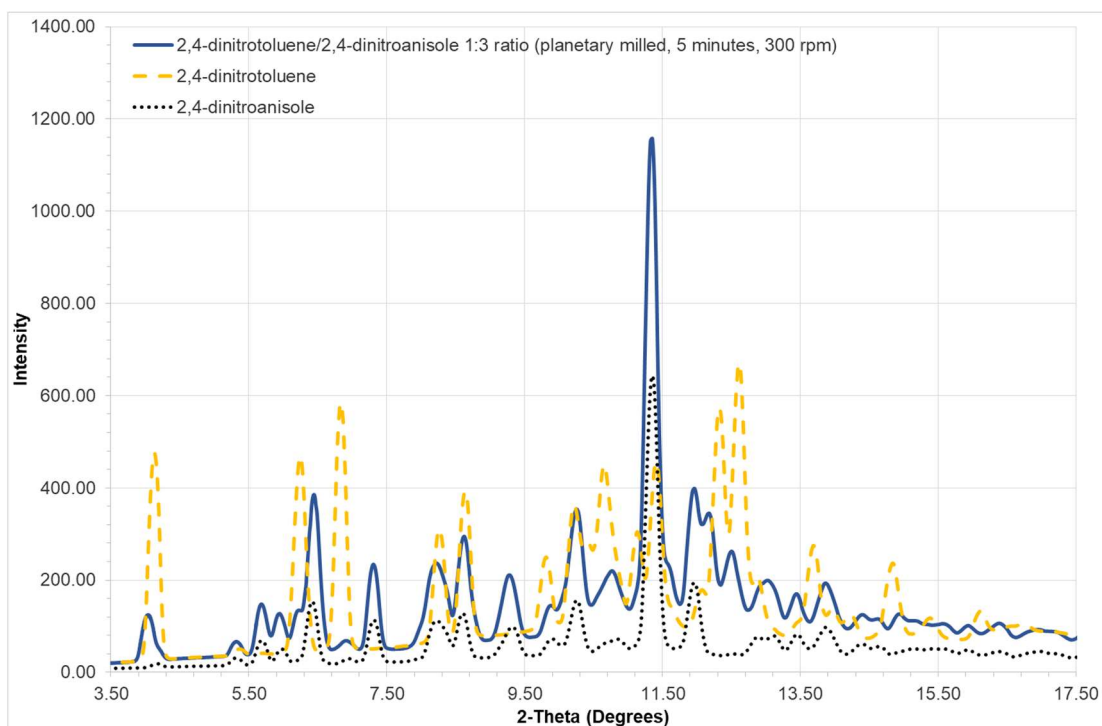


Figure B.55 - Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

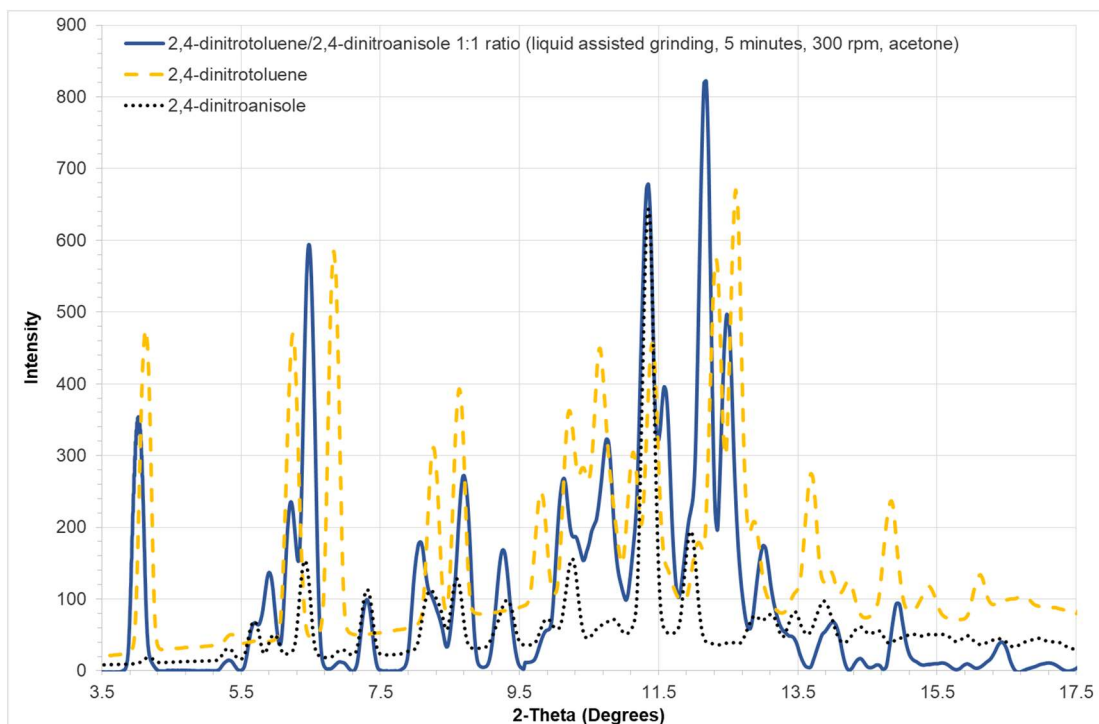


Figure B.56 - Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

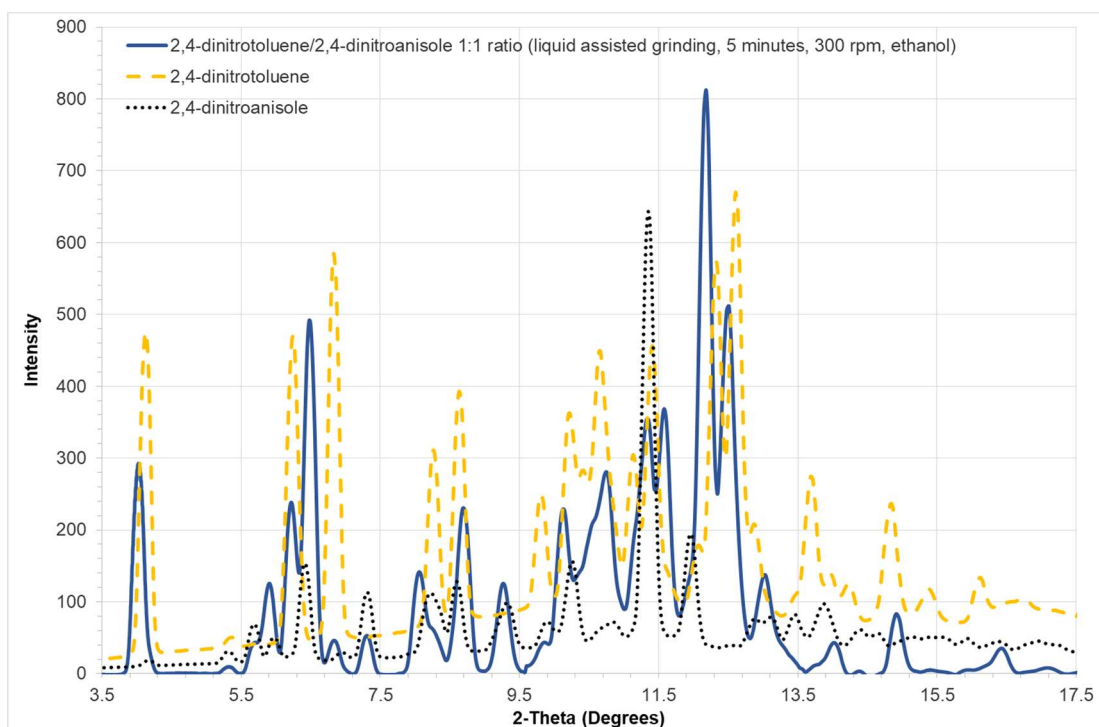


Figure B.57 - Powder x-ray pattern of 2,4 dinitrotoluene/2,4 dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.7 2,4-dinitrotoluene/1,3-dinitrobenzene

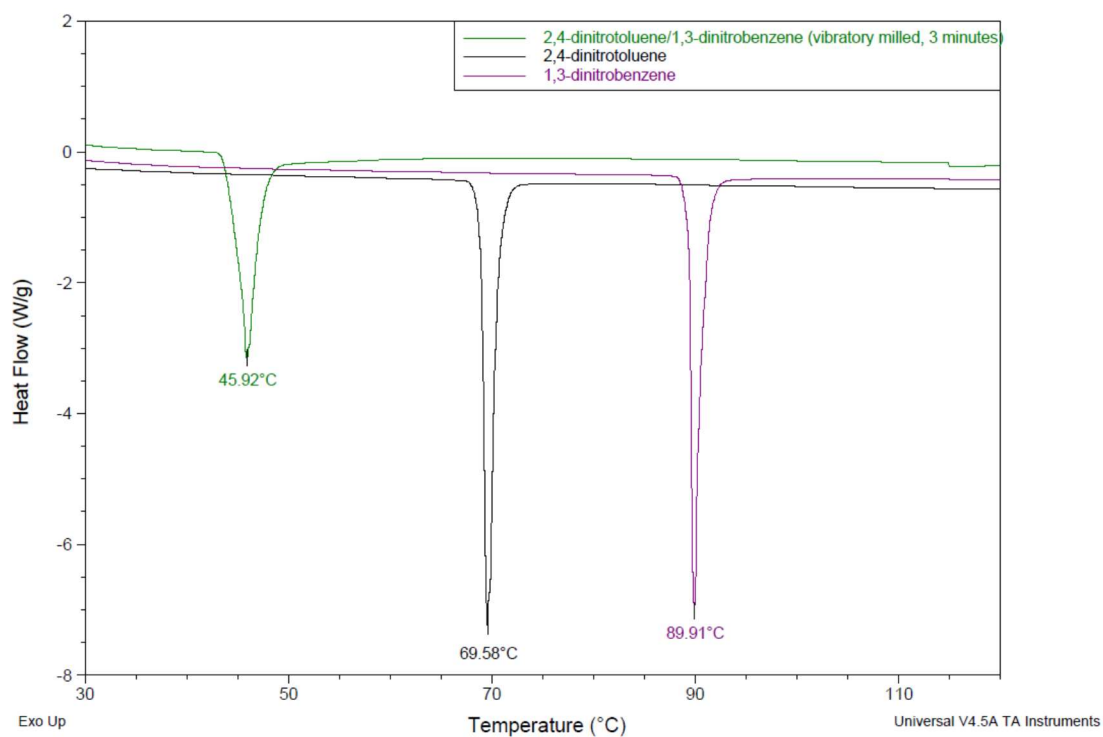


Figure B.58 - Thermal analysis of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by vibratory milling for 3 minutes.

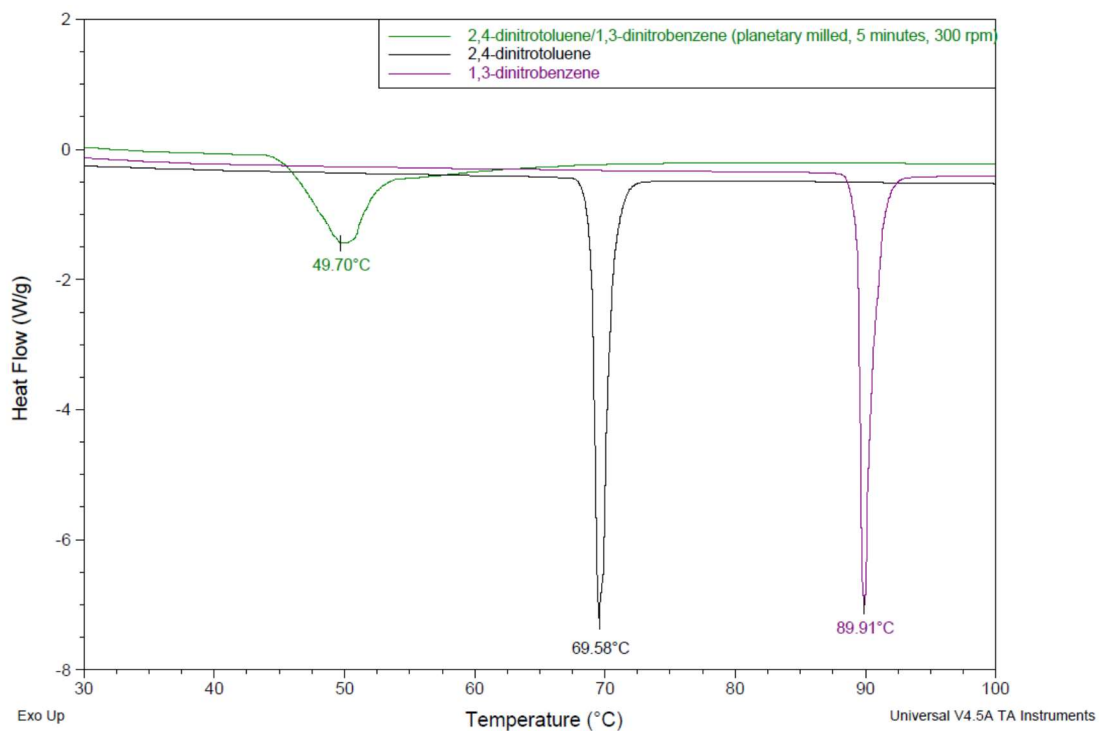


Figure B.59 - Thermal analysis of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

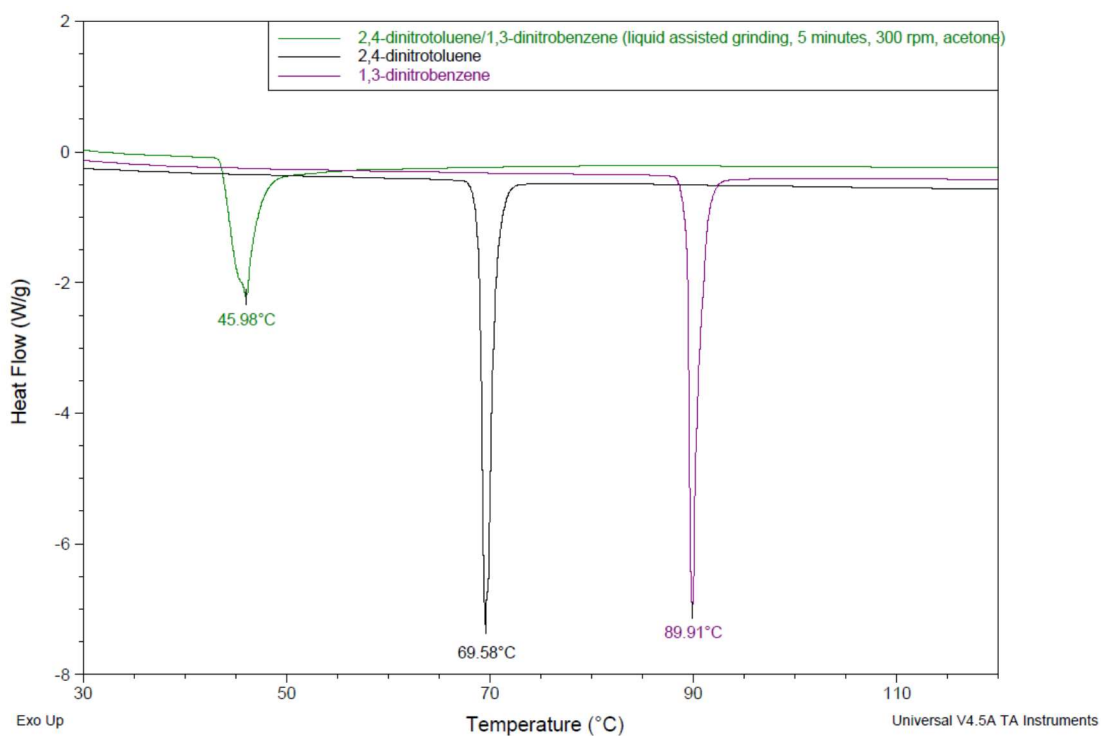


Figure B.60 - Thermal analysis of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

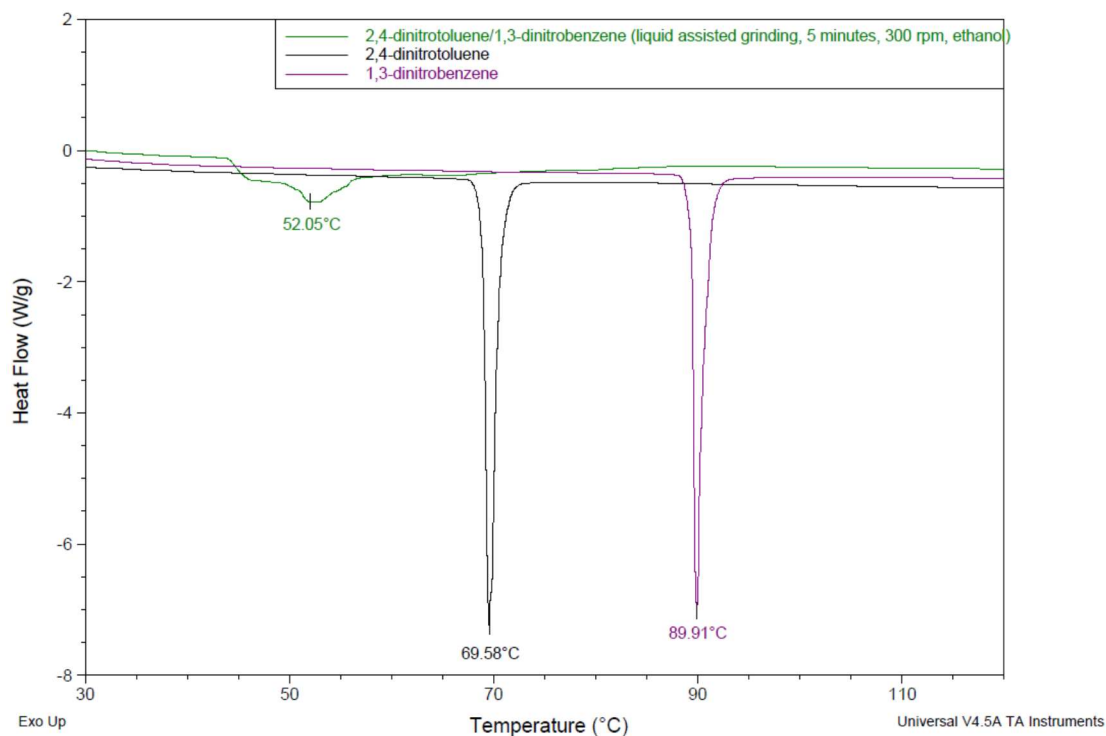


Figure B.61 - Thermal analysis of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

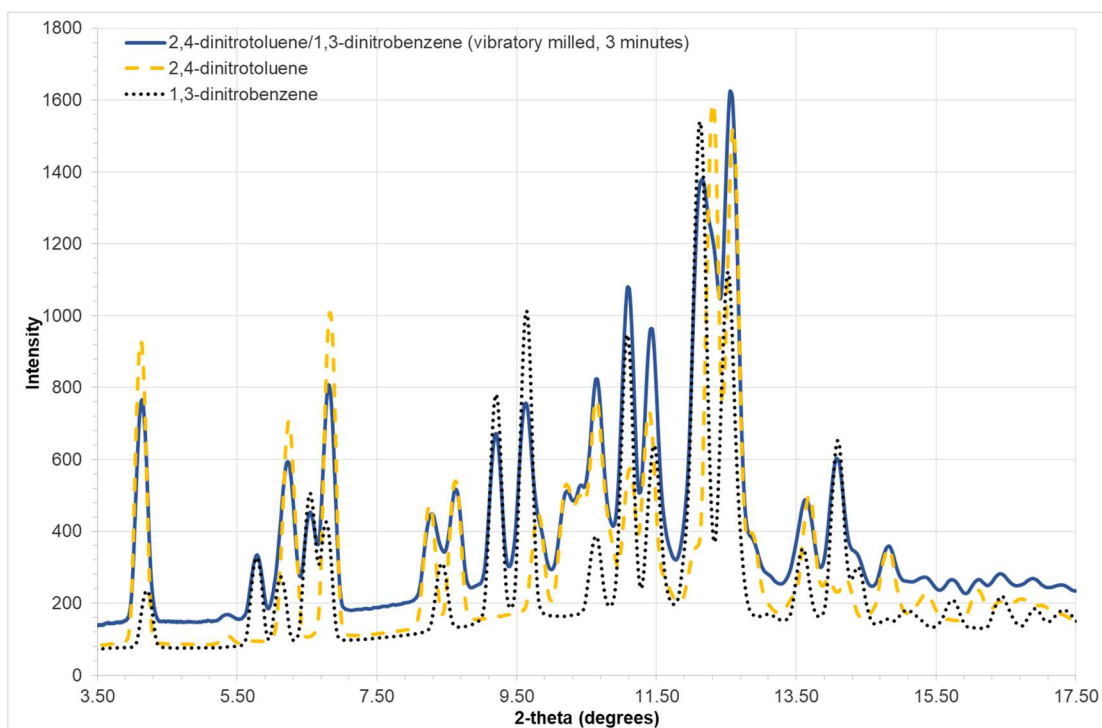


Figure B.62 – Powder x-ray pattern of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by vibratory milling for 3 minutes.

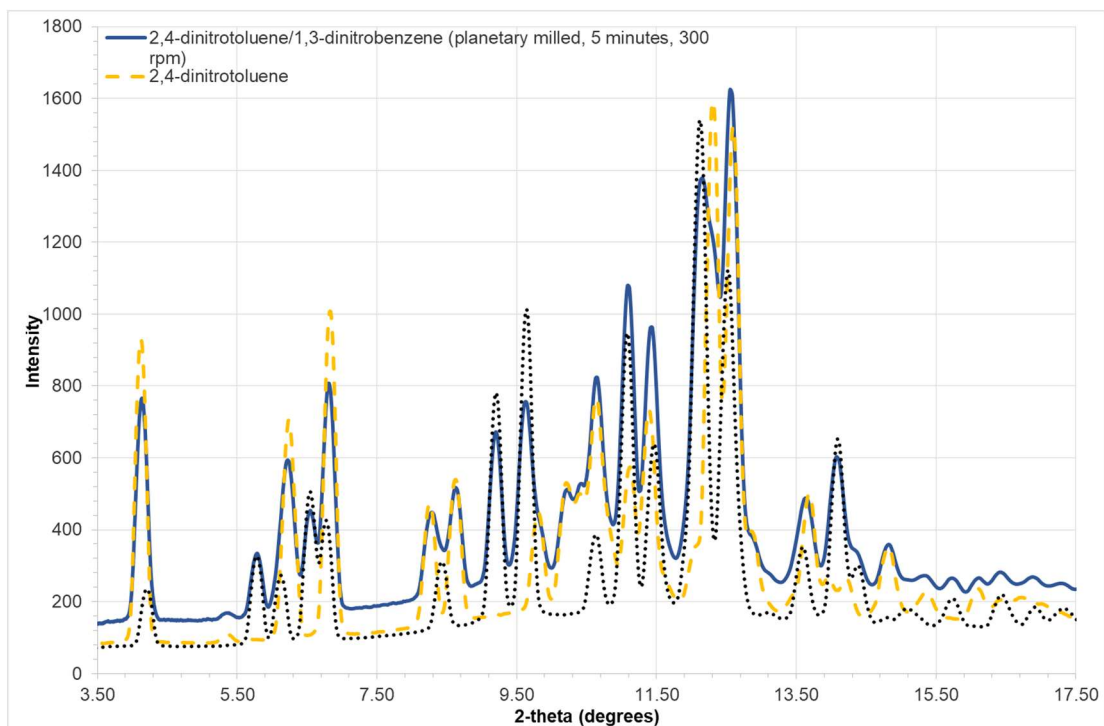


Figure B.63 - Powder x-ray pattern of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

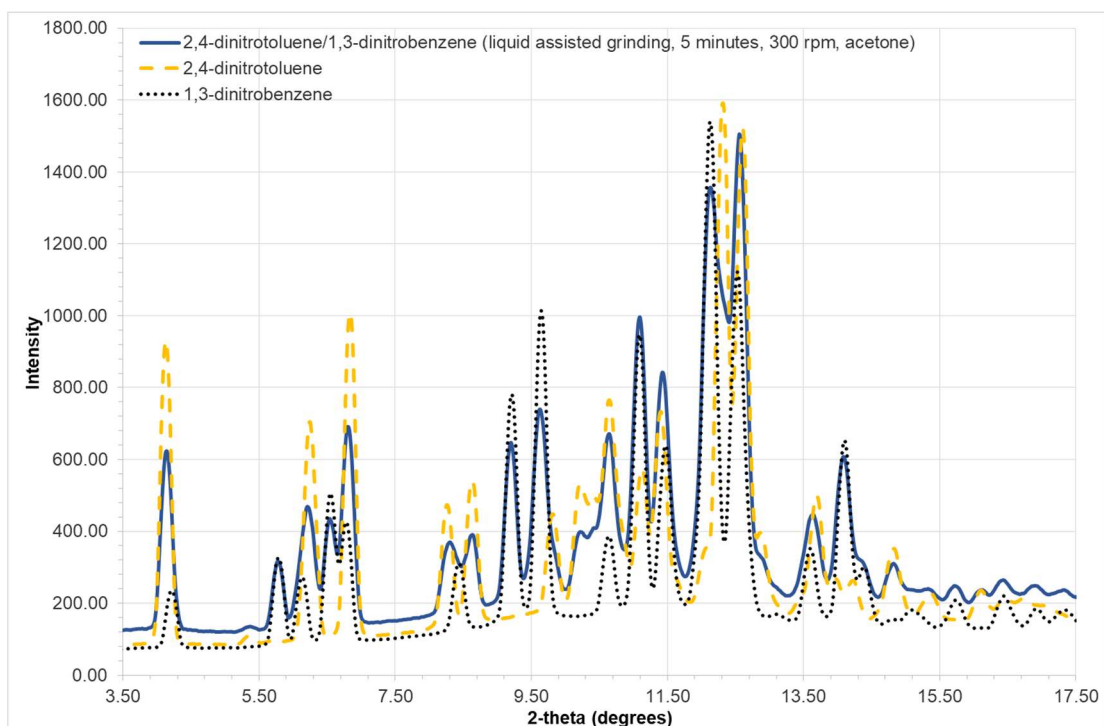


Figure B.64 - Powder x-ray pattern of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

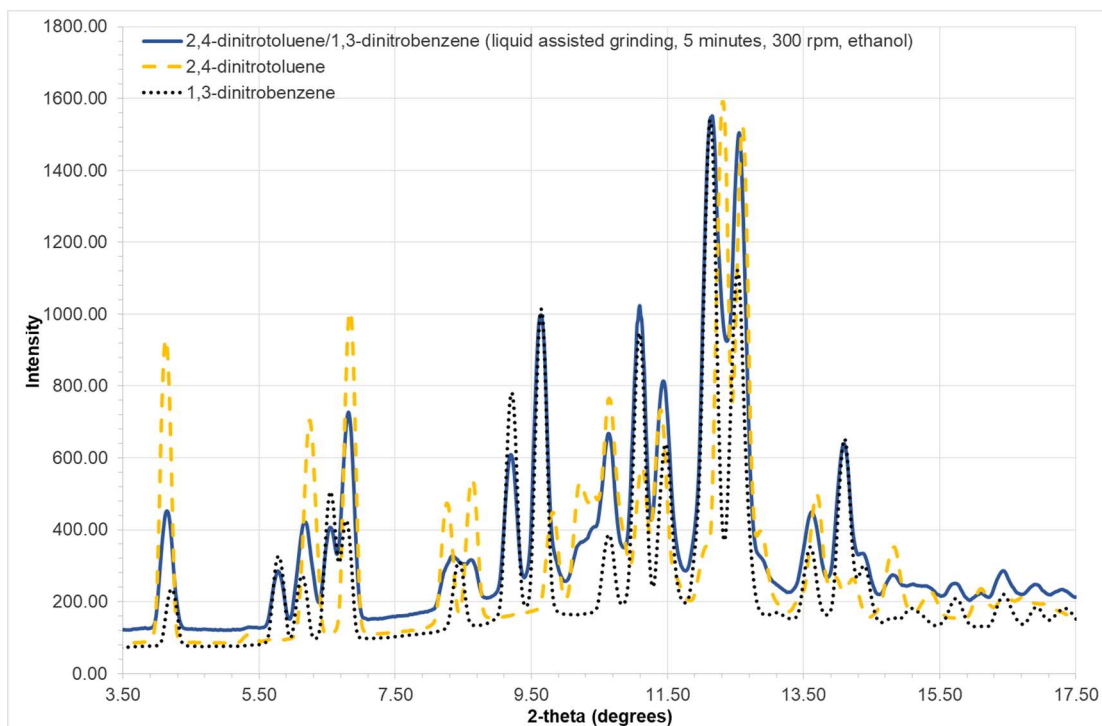


Figure B.65 - Powder x-ray pattern of 2,4-dinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.8 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene

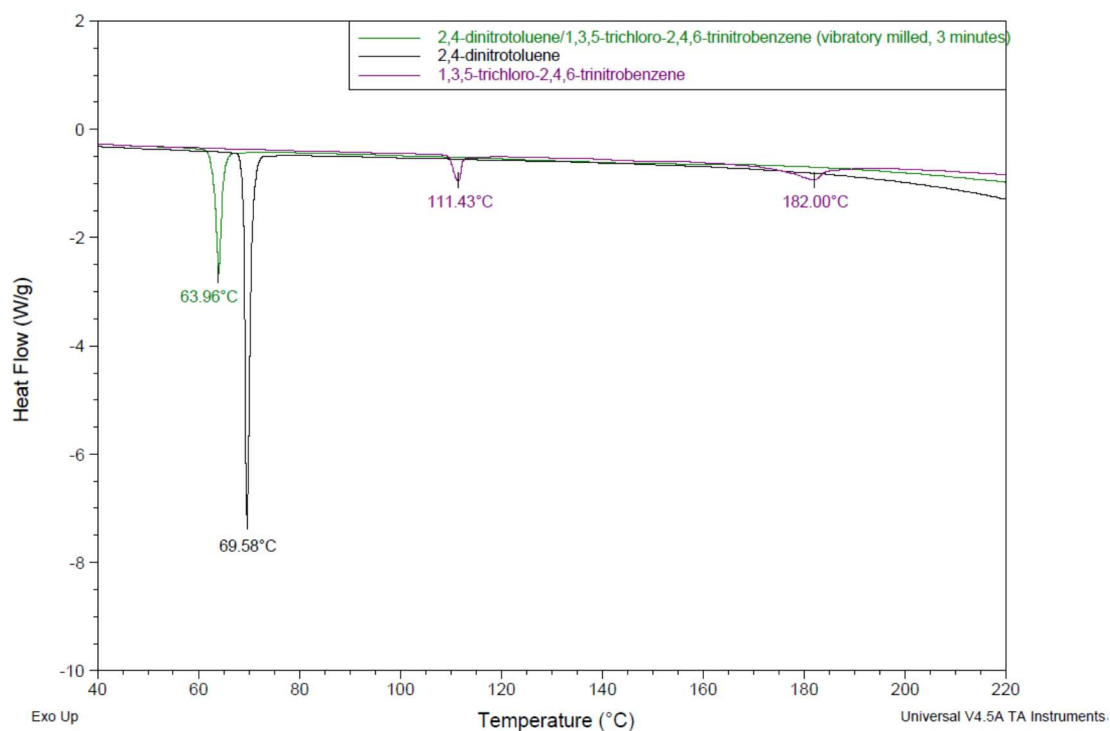


Figure B.66 - Thermal analysis of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by vibratory milling for 3 minutes.

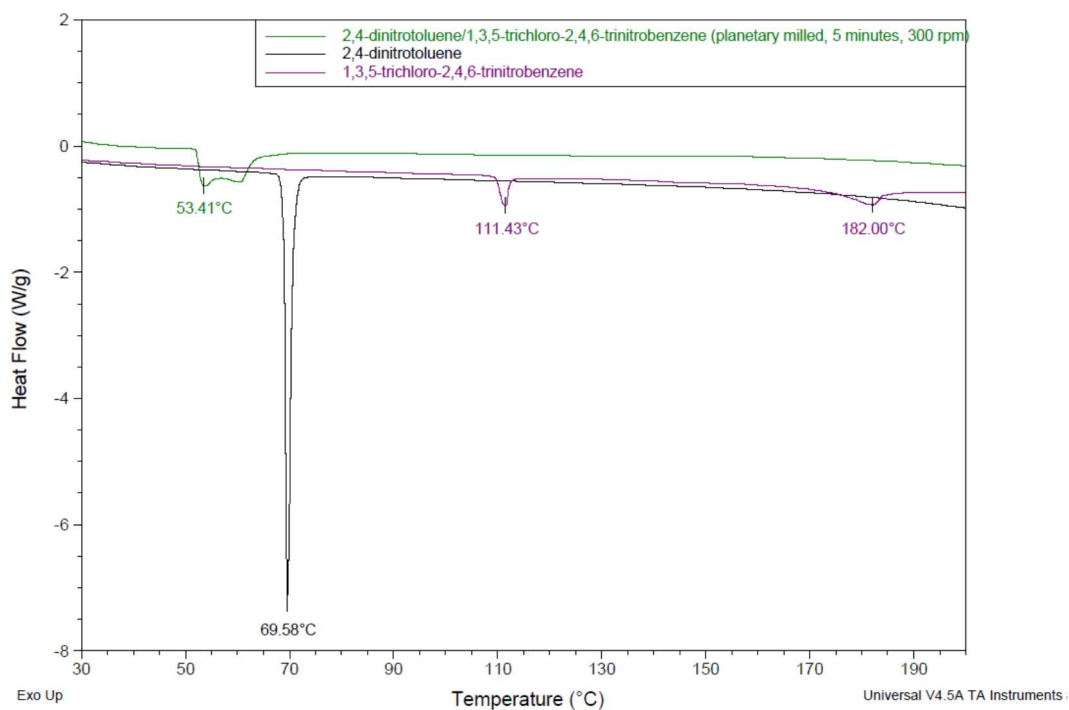


Figure B.67 - Thermal analysis of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

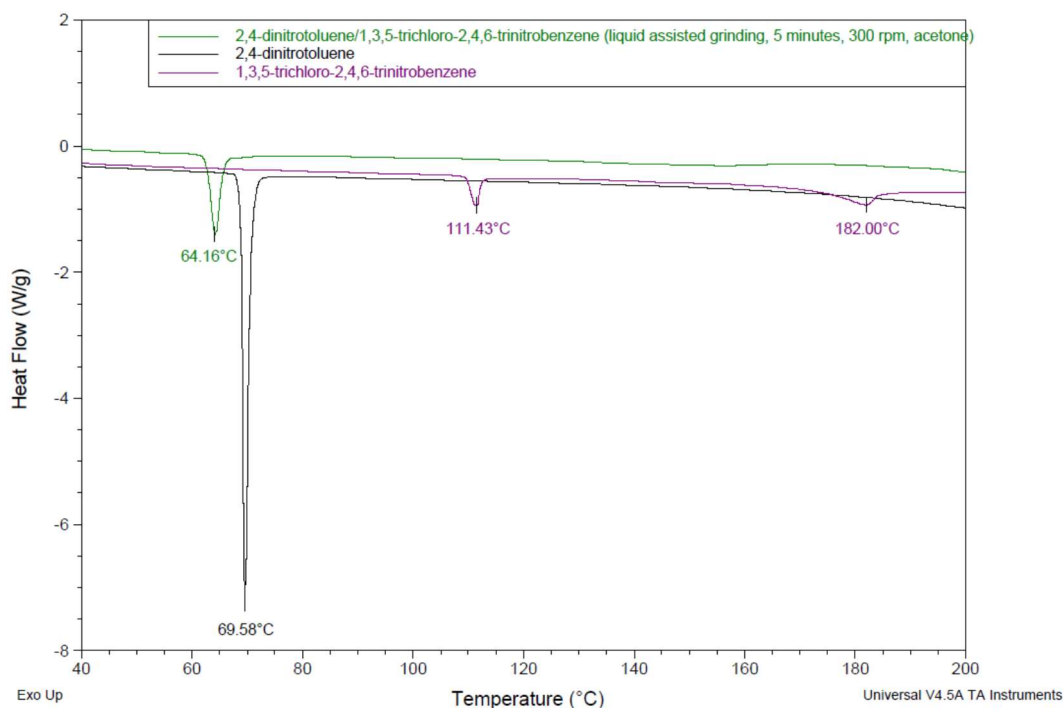


Figure B.68 - Thermal analysis of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

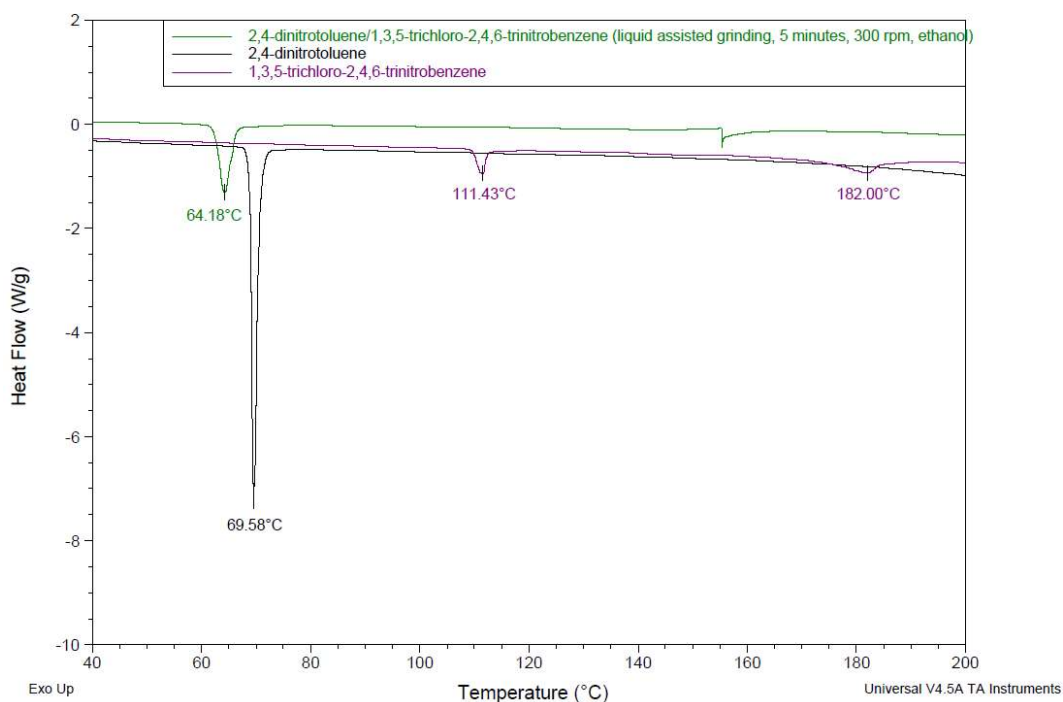


Figure B.69 - Thermal analysis of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

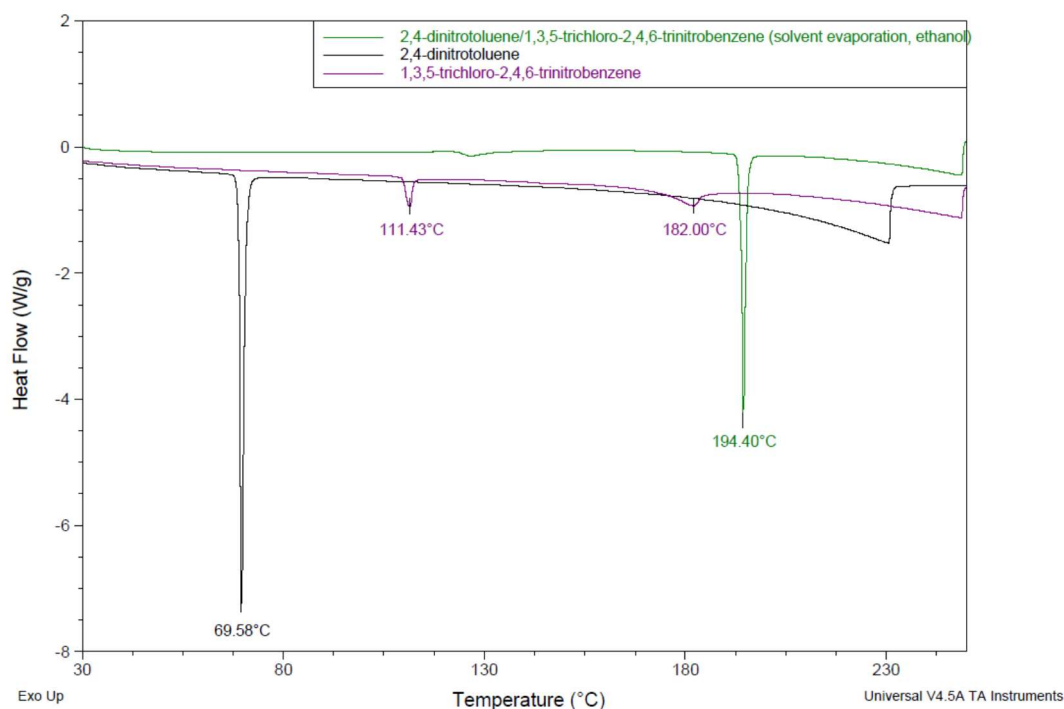


Figure B.70 - Thermal analysis of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by solvent evaporation with ethanol.

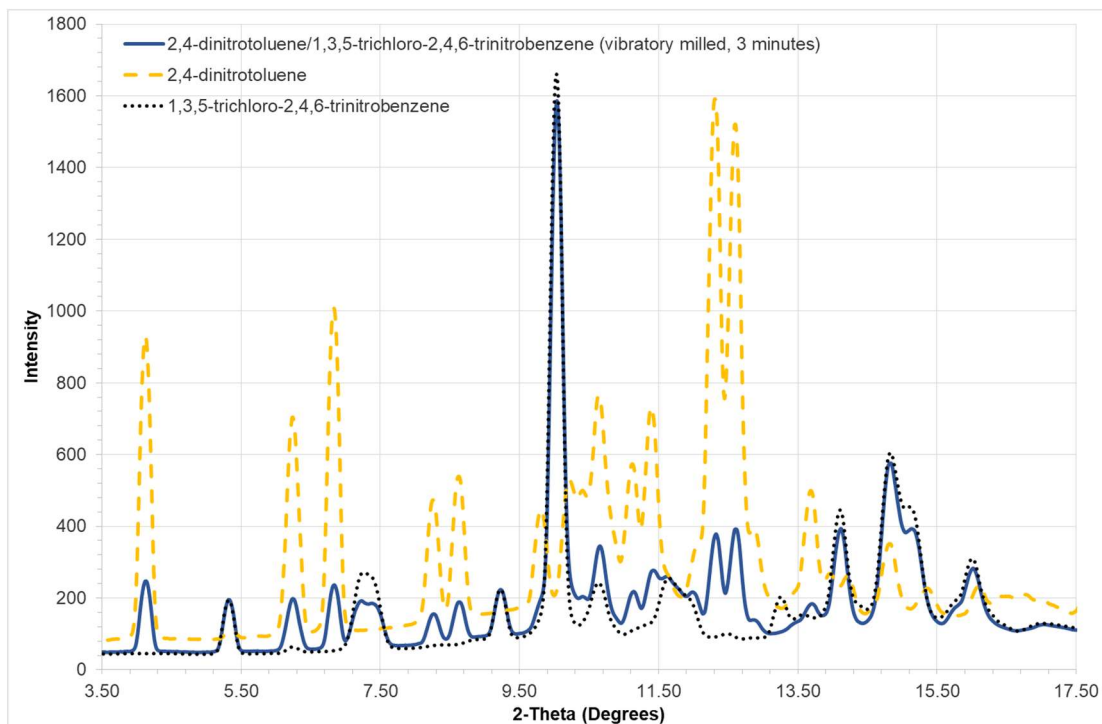


Figure B.71 – Powder x-ray pattern of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by vibratory milling for 3 minutes.

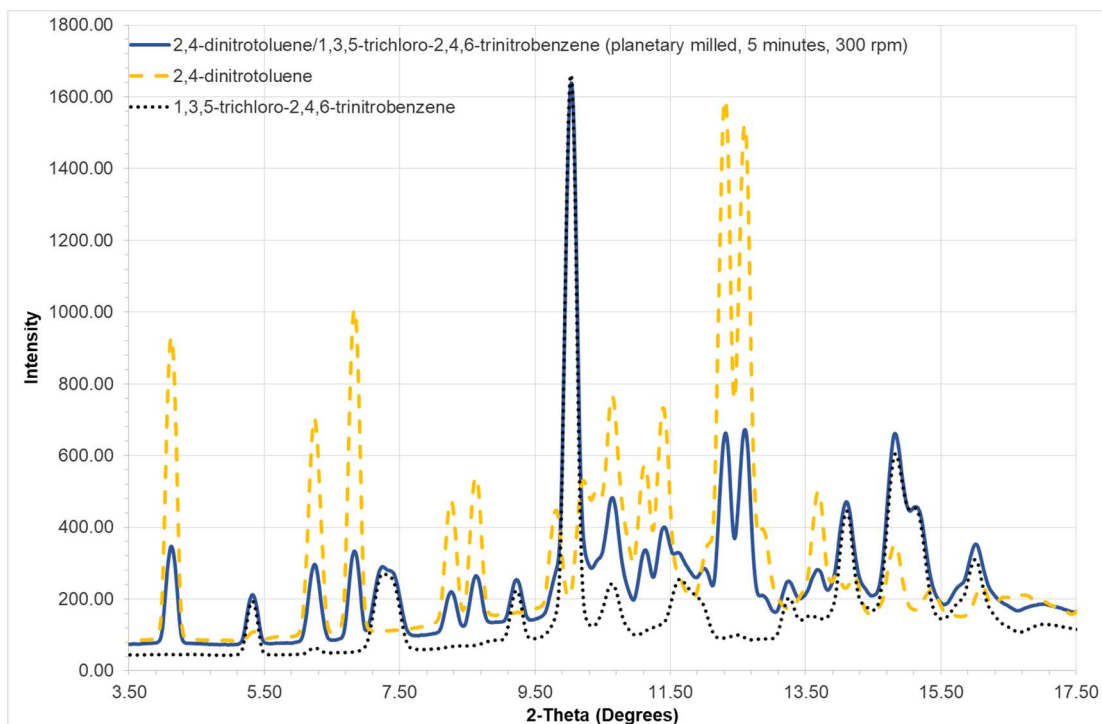


Figure B.72 - Powder x-ray pattern of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

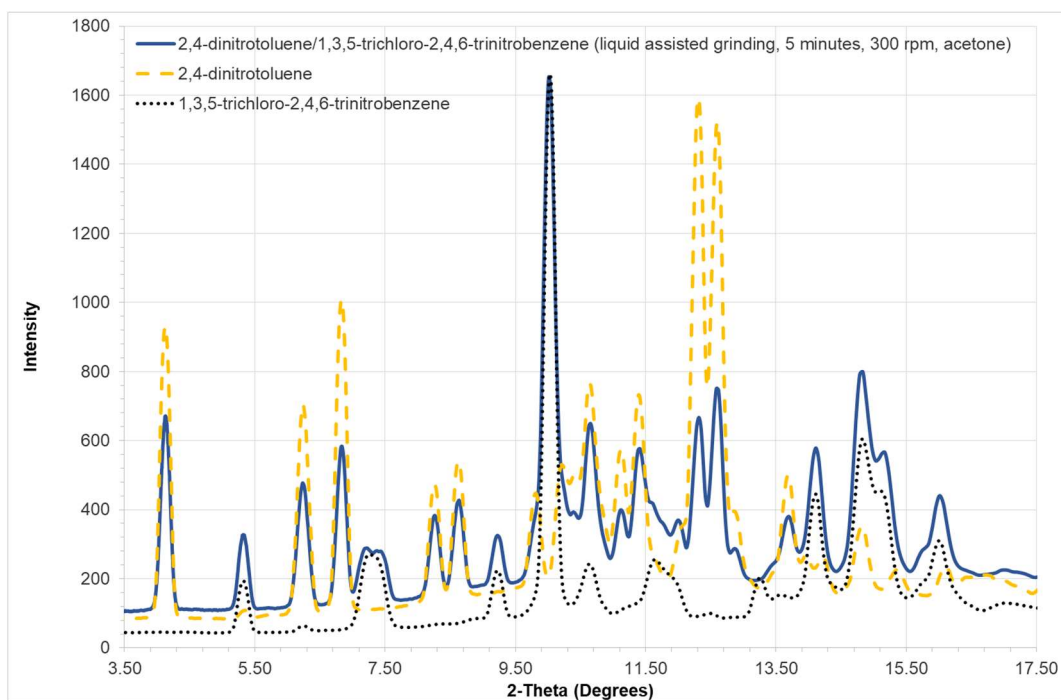


Figure B.73 - Powder x-ray pattern of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

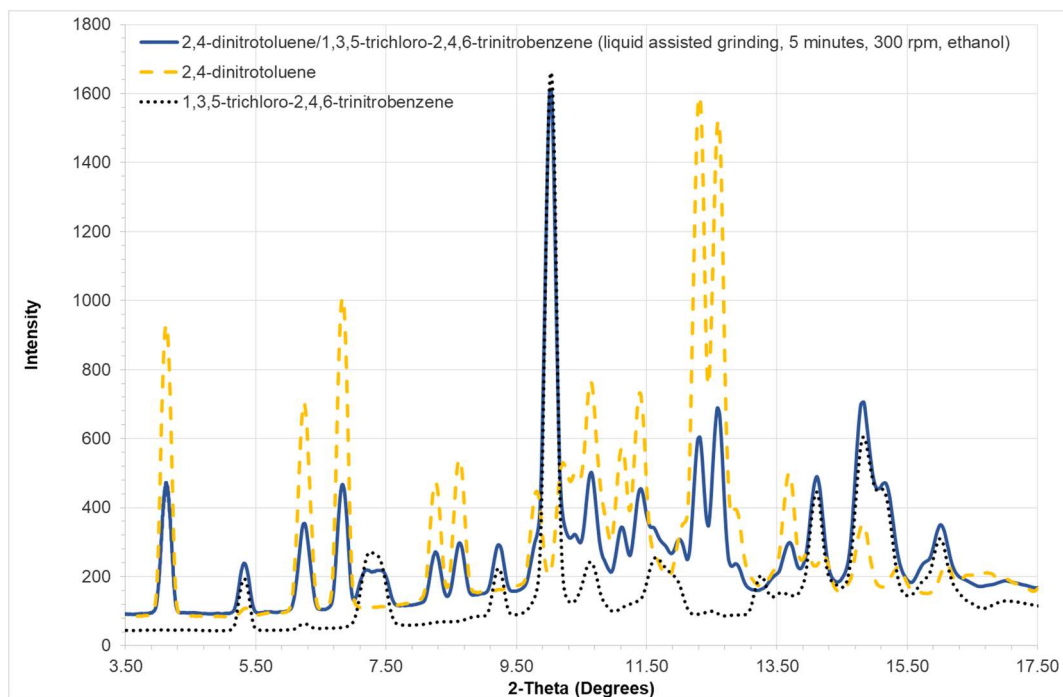


Figure B.74 - Powder x-ray pattern of 2,4-dinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.9 2,4-dinitrotoluene/2,4,6-trinitroaniline

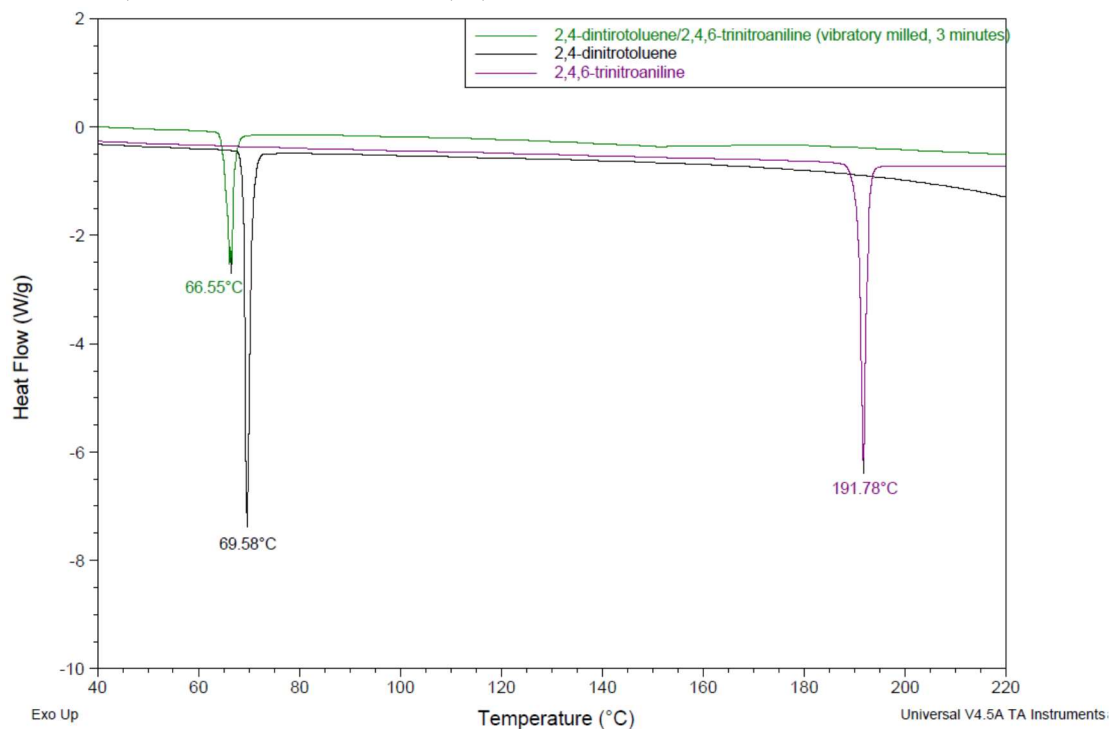


Figure B.75 – Thermal analysis of 2,4-dinitrotoluene/2,4,6-trinitroaniline produced by vibratory milling for 3 minutes.

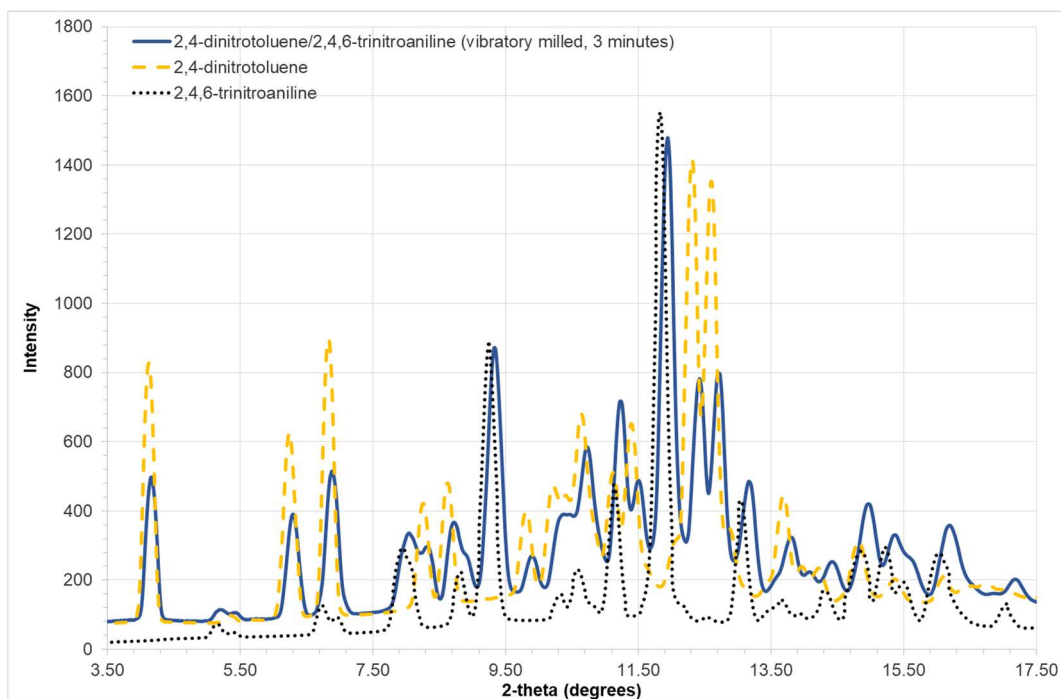


Figure B.76 – Powder x-ray pattern of 2,4-dinitrotoluene/2,4,6-trinitroaniline produced by vibratory milling for 3 minutes.

B.10 2,4-dinitrotoluene/2,4,6-trinitrotoluene

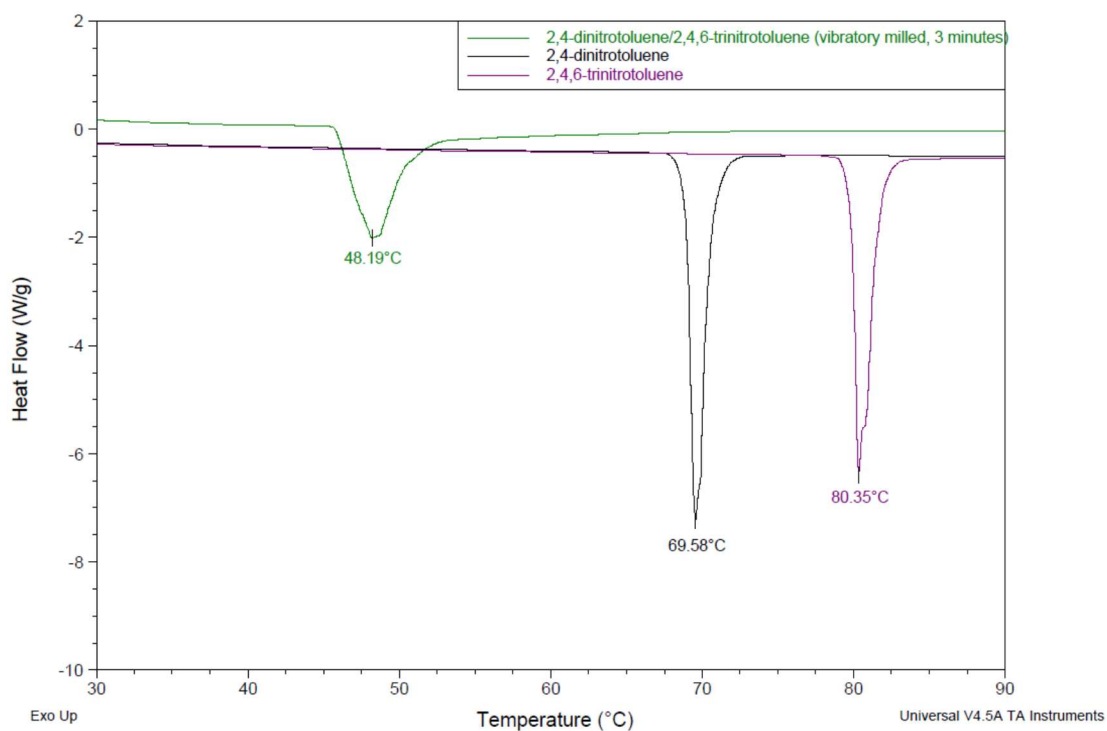


Figure B.77 - Thermal analysis of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by vibratory milling for 3 minutes.

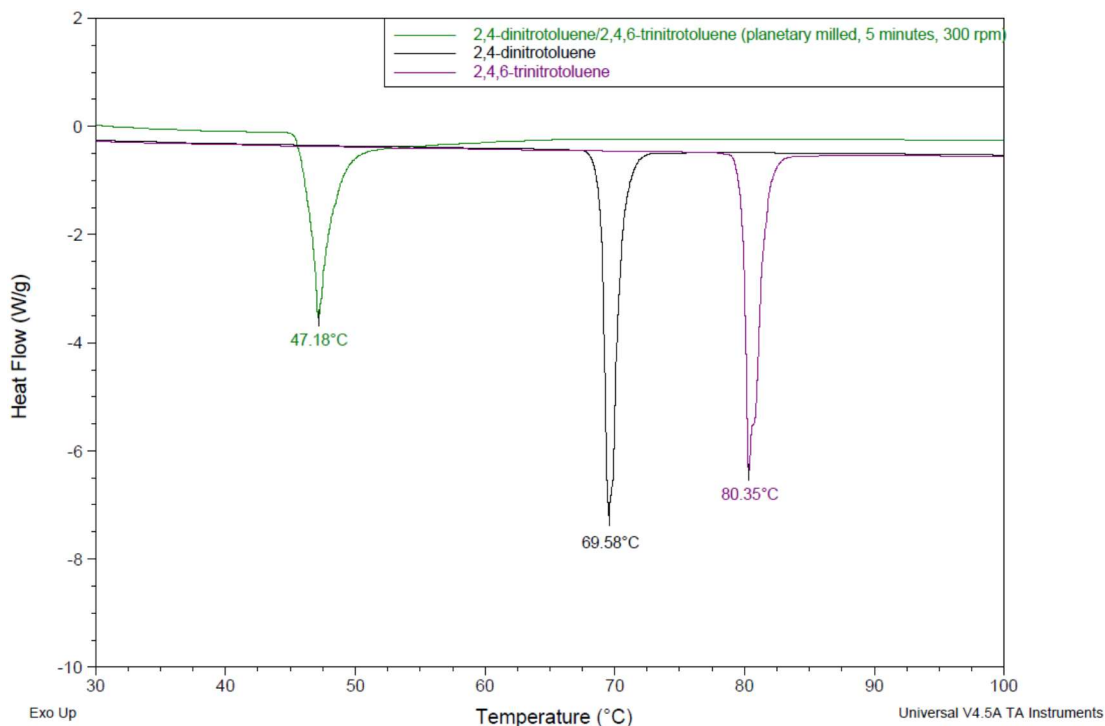


Figure B.78 - Thermal analysis of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by planetary milling for 5 minutes at 300 rpm.

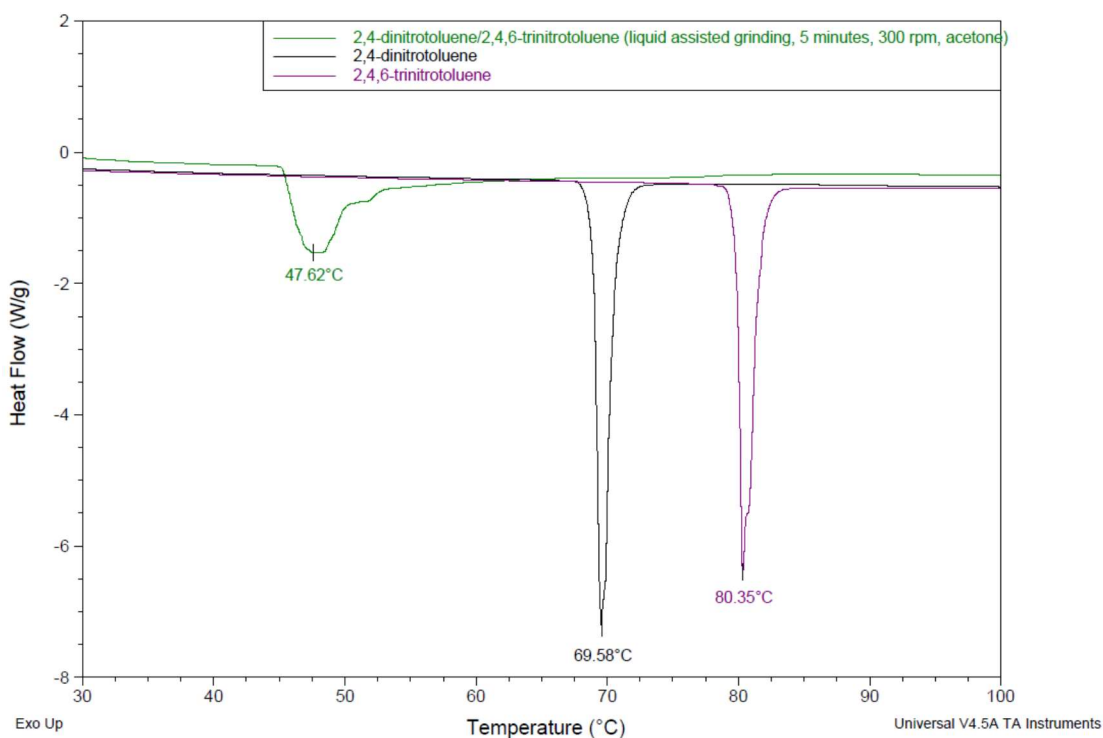


Figure B.79 - Thermal analysis of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

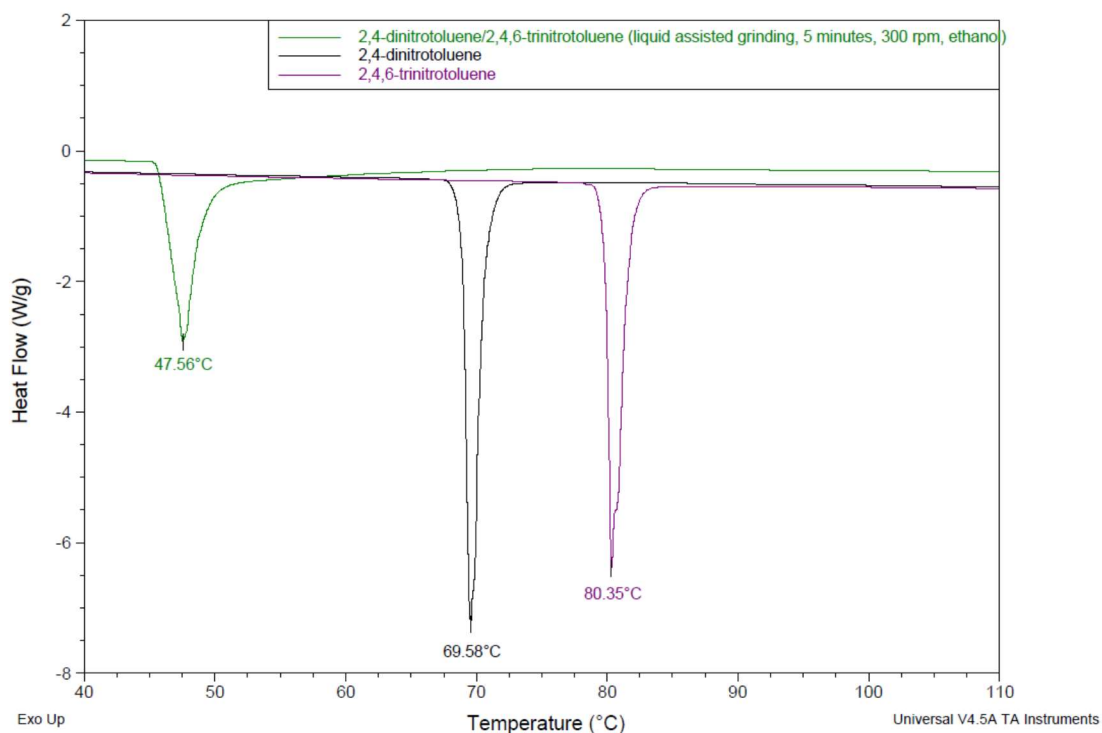


Figure B.80 - Thermal analysis of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

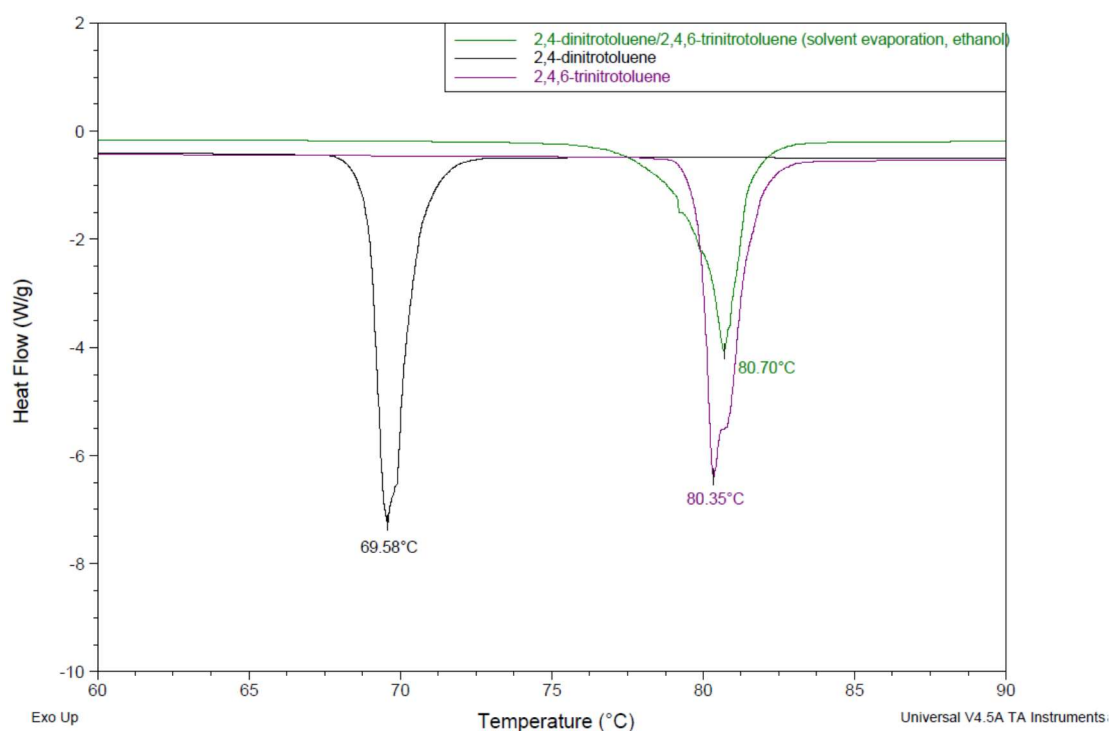


Figure B.81 - Thermal analysis of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by solvent evaporation with ethanol.

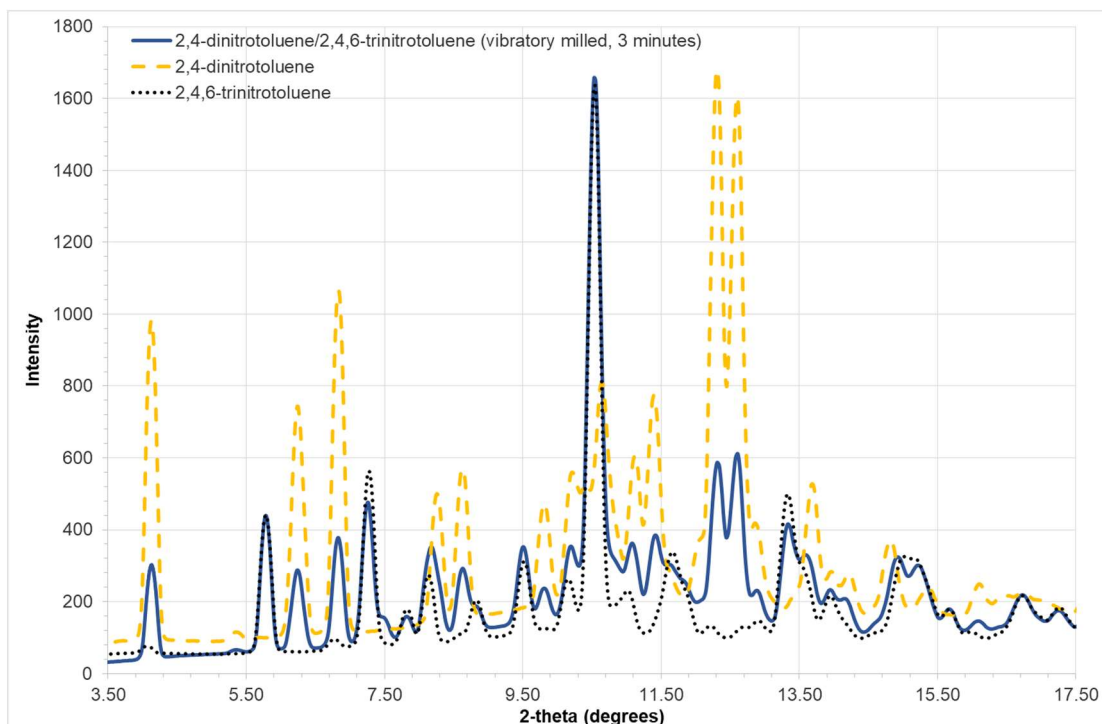


Figure B.82 – Powder x-ray pattern of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by vibratory milling for 3 minutes.

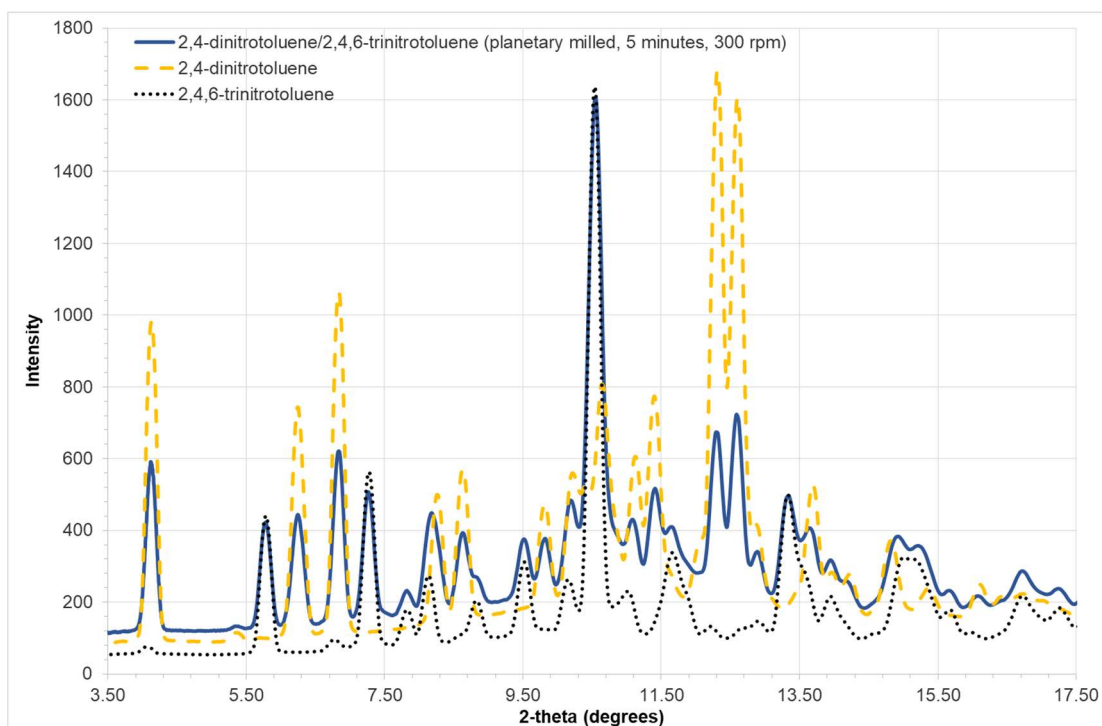


Figure B.83 - Powder x-ray pattern of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by planetary milling for 5 minutes at 300 rpm.

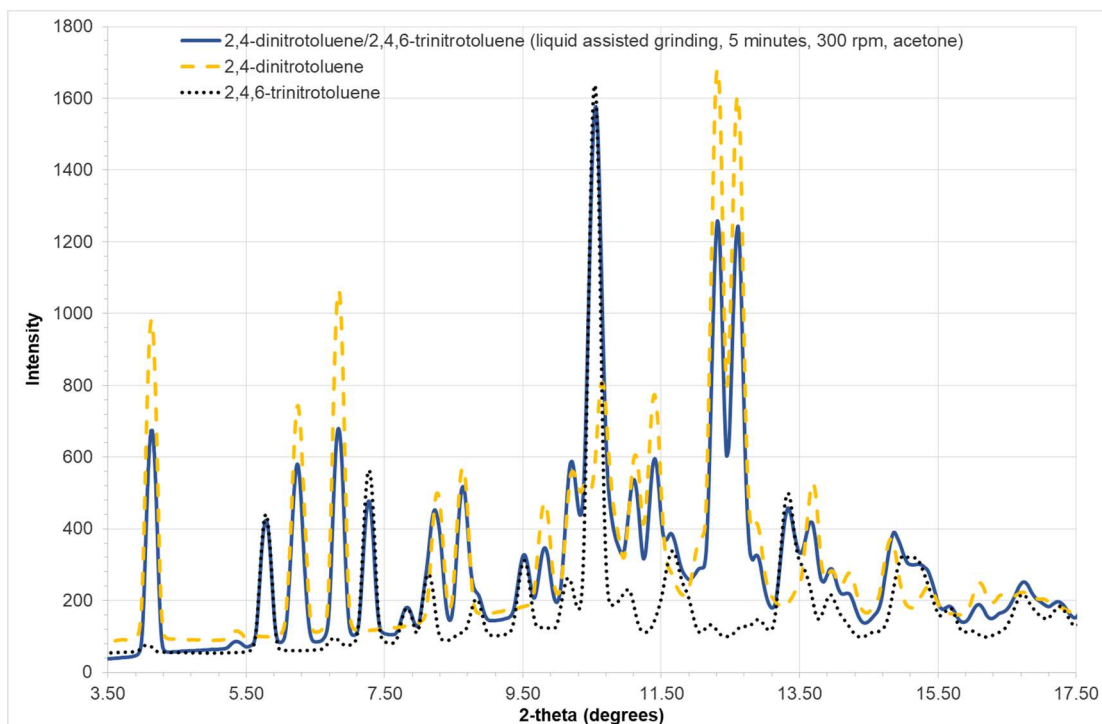


Figure B.84 - Powder x-ray pattern of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

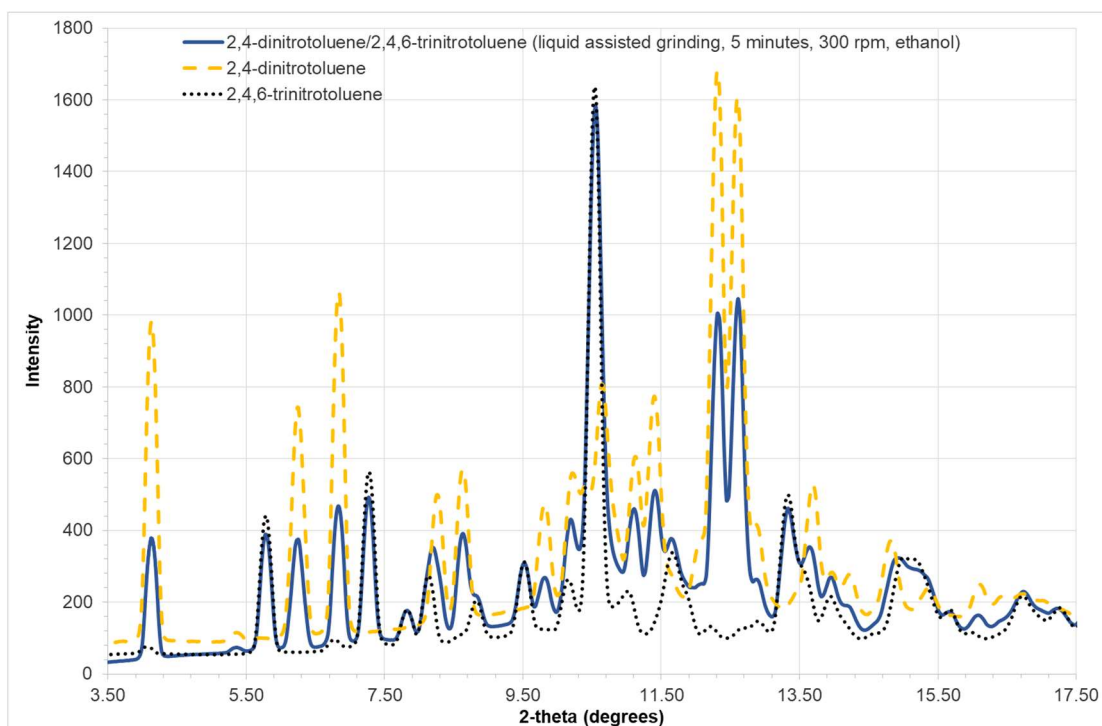


Figure B.85 - Powder x-ray pattern of 2,4-dinitrotoluene/2,4,6-trinitrotoluene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.11 2,4,6-trinitrotoluene/2,4-dinitroaniline

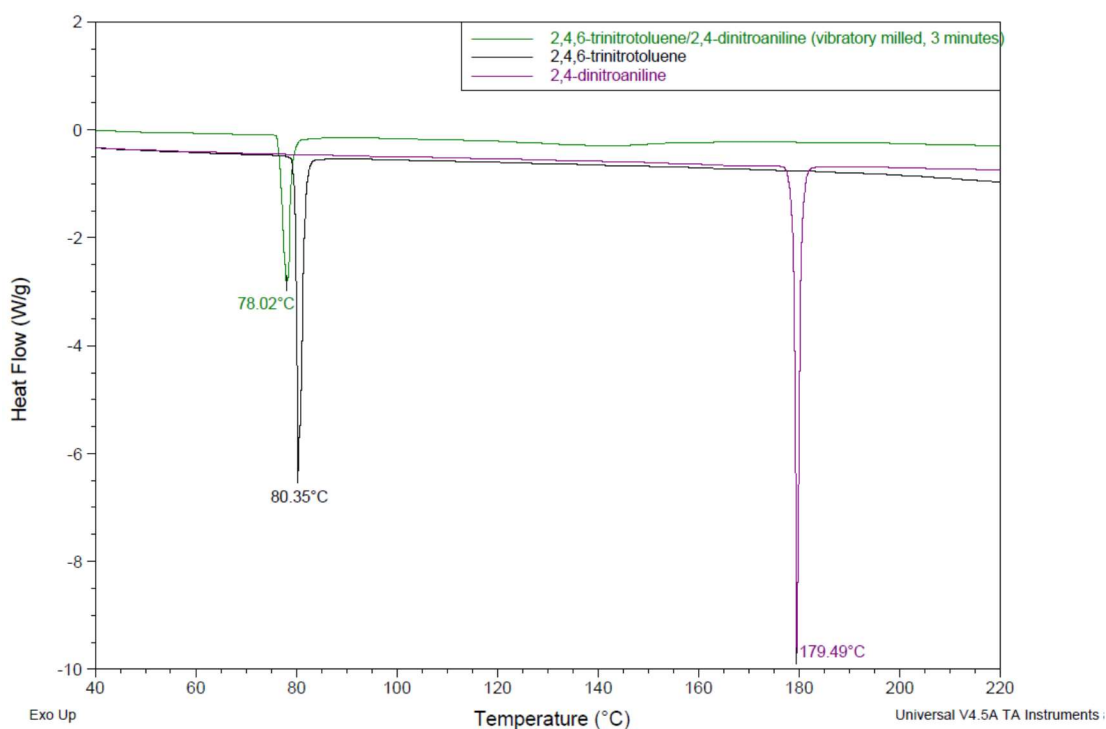


Figure B.86 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by vibratory milling for 3 minutes.

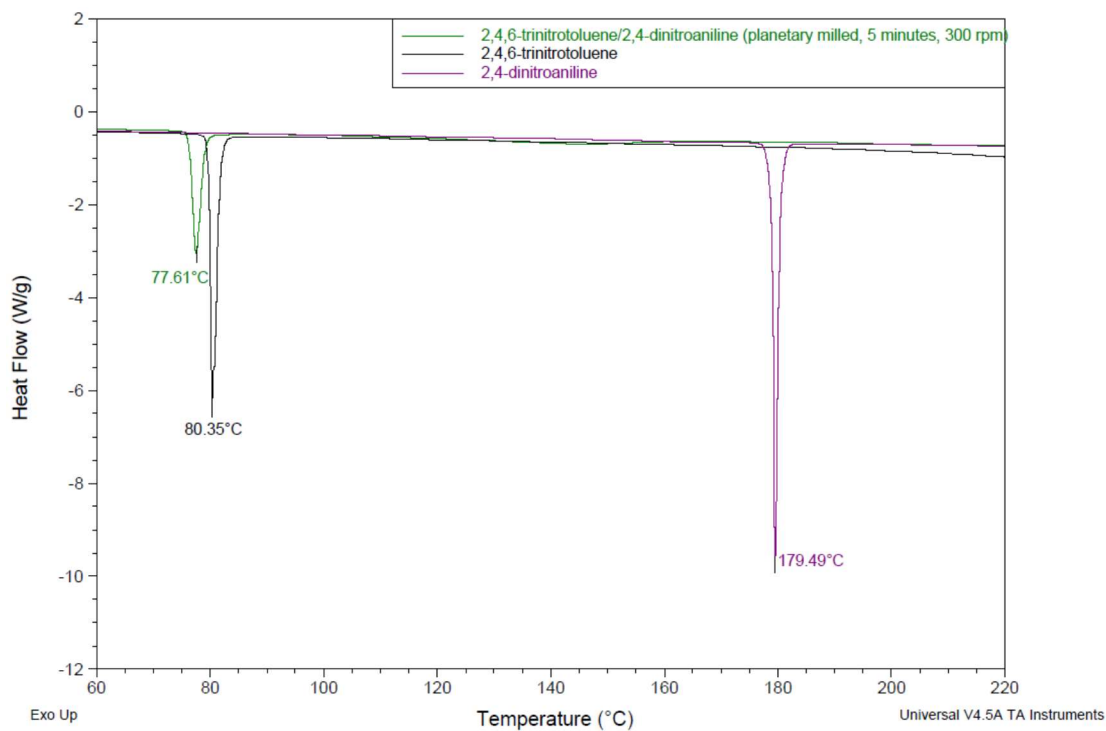


Figure B.87 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by planetary milling for 5 minutes at 300 rpm.

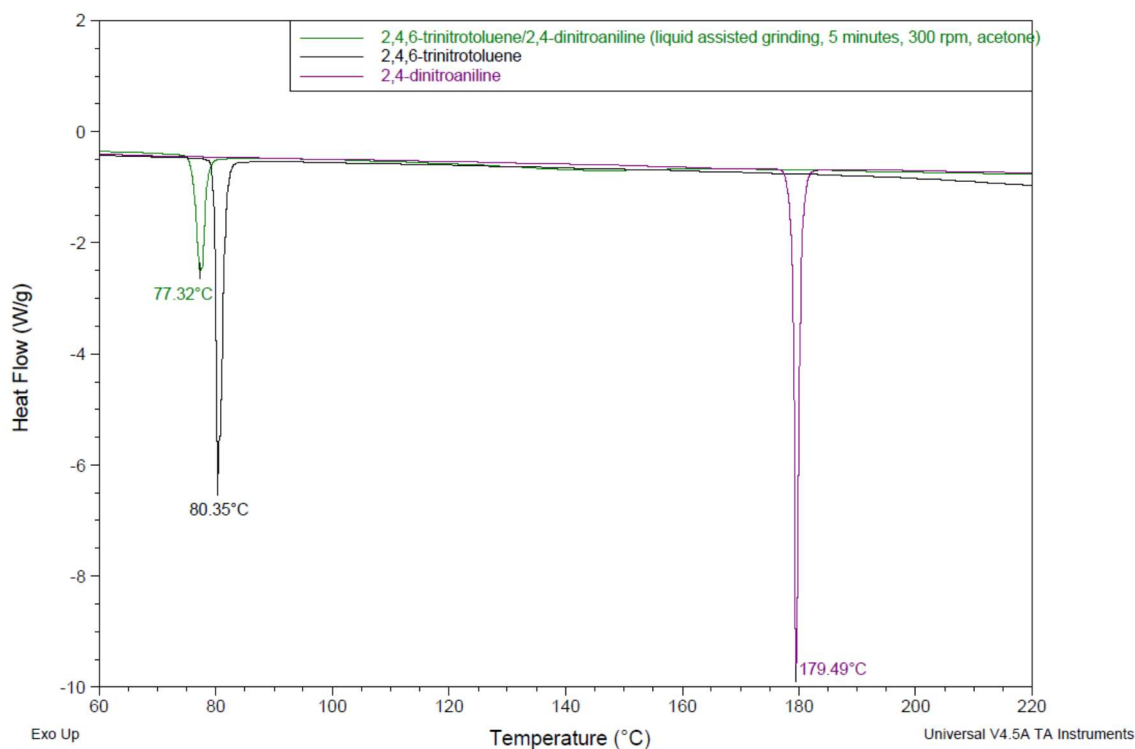


Figure B.88 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

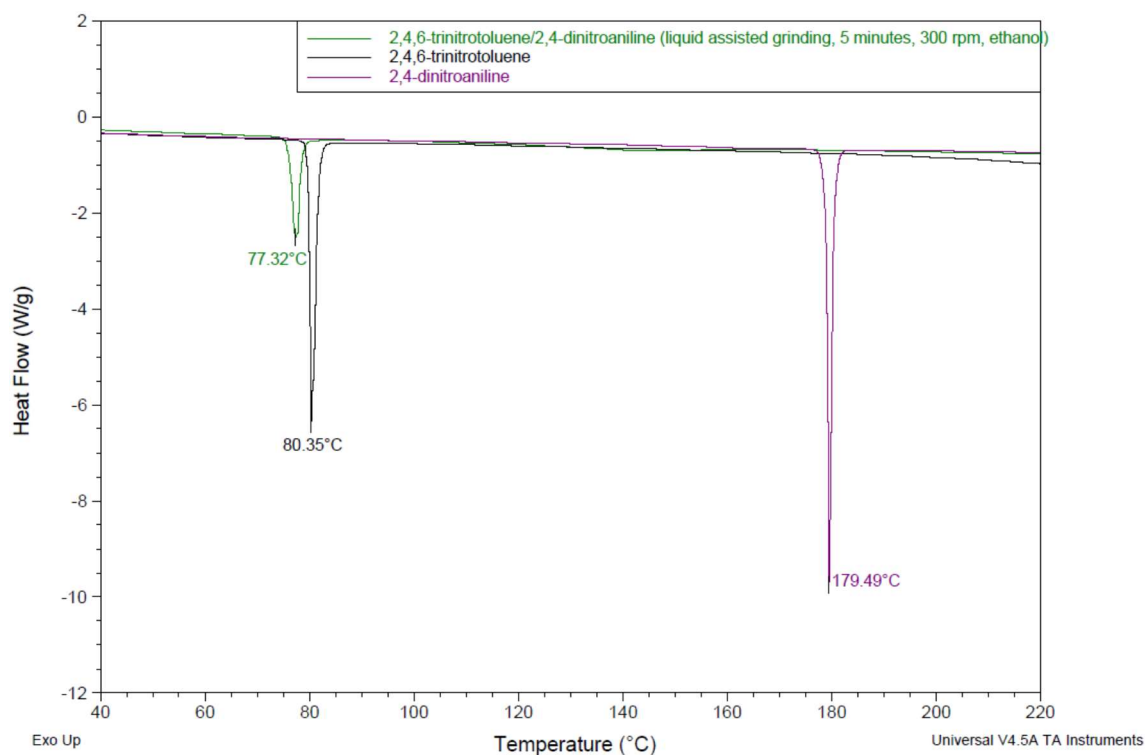


Figure B.89 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

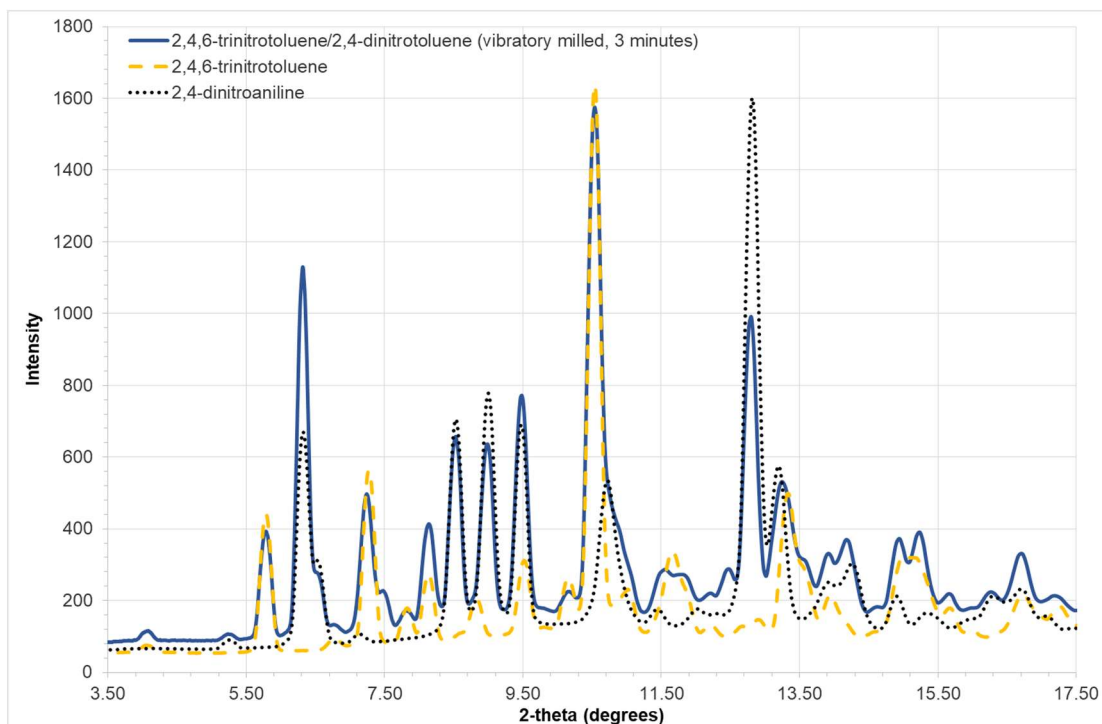


Figure B.90 – Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by vibratory milling for 3 minutes.

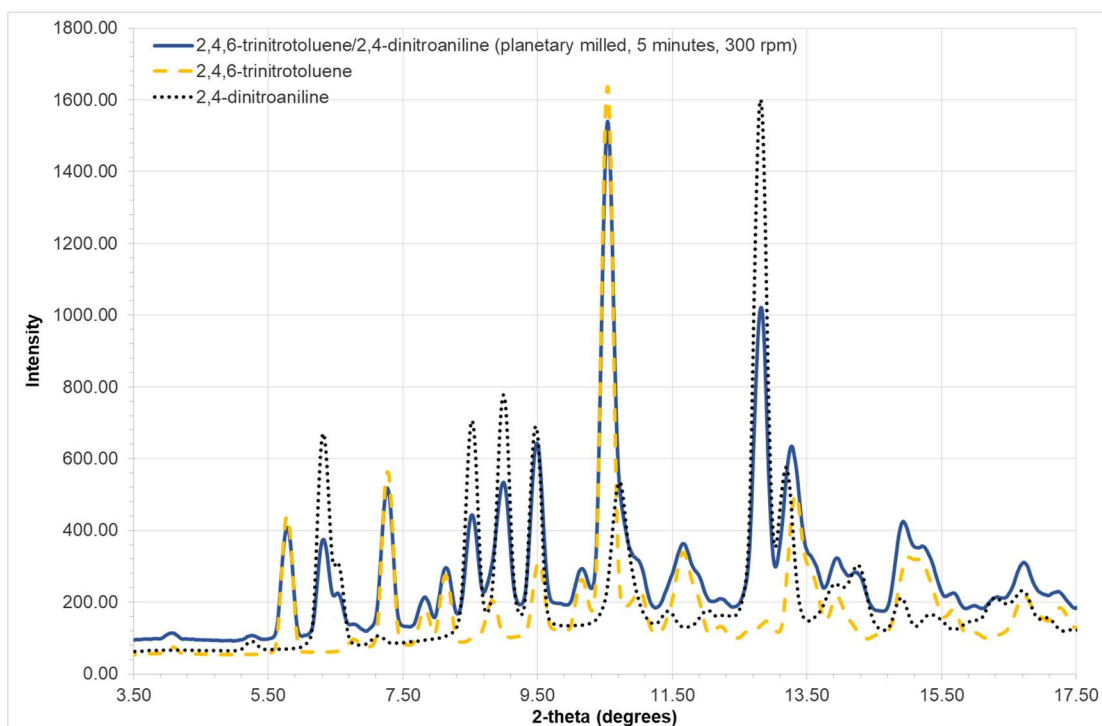


Figure B.91 – Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by planetary milling for 5 minutes at 300 rpm.

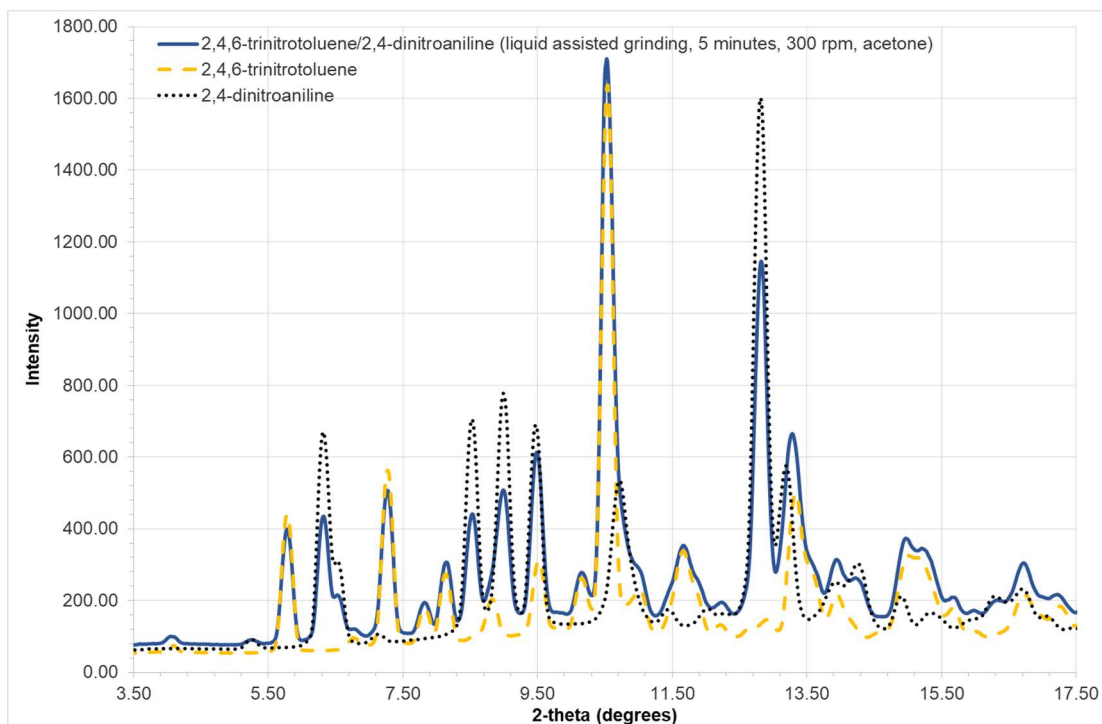


Figure B.92 - Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

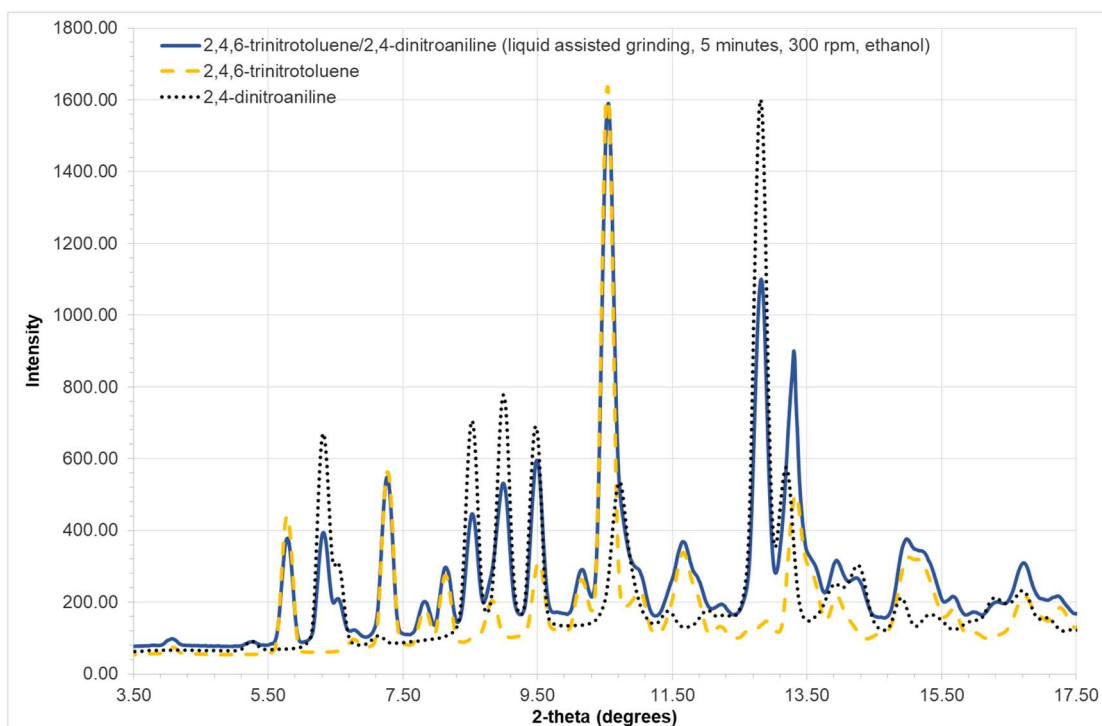


Figure B.93 - Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroaniline produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.12 2,4,6-trinitrotoluene/2,4-dinitroanisole

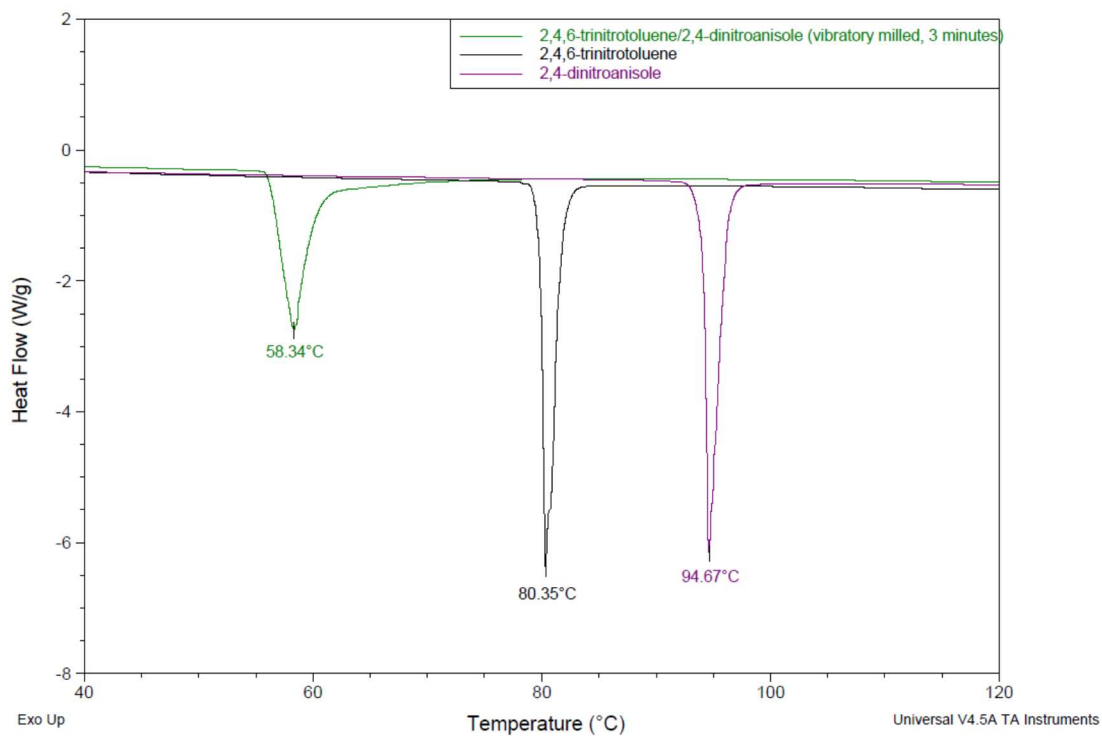


Figure B.94 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by vibratory milling for 3 minutes.

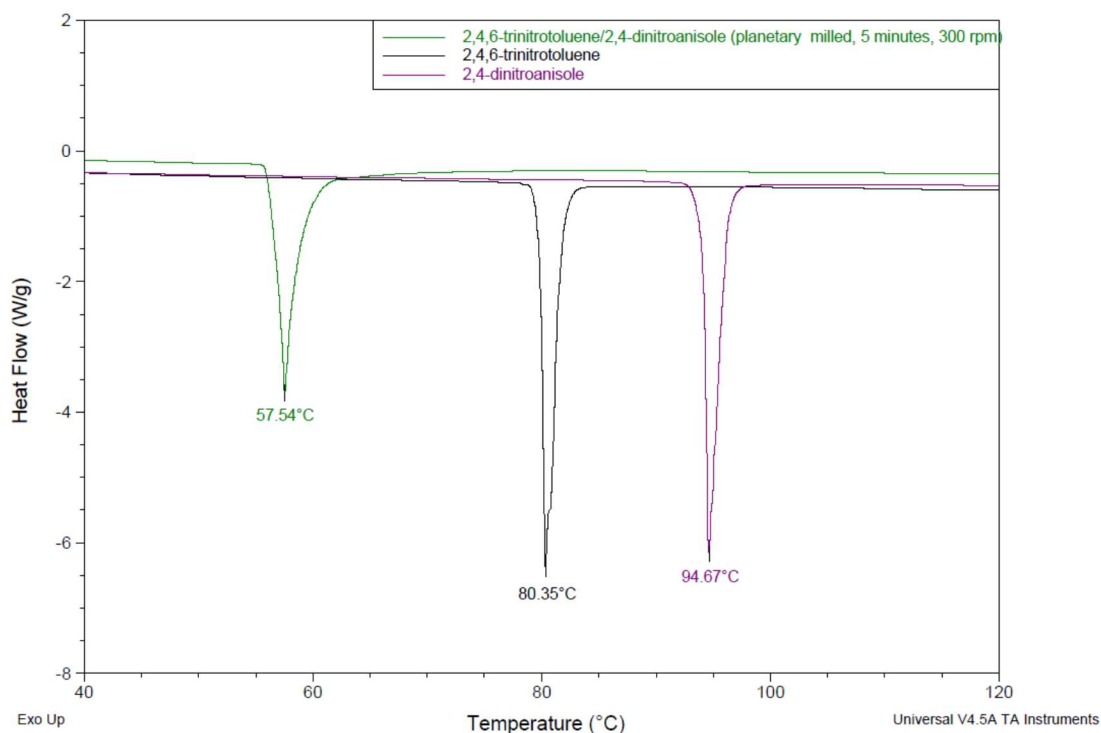


Figure B.95 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by planetary milling for 5 minutes at 300 rpm.

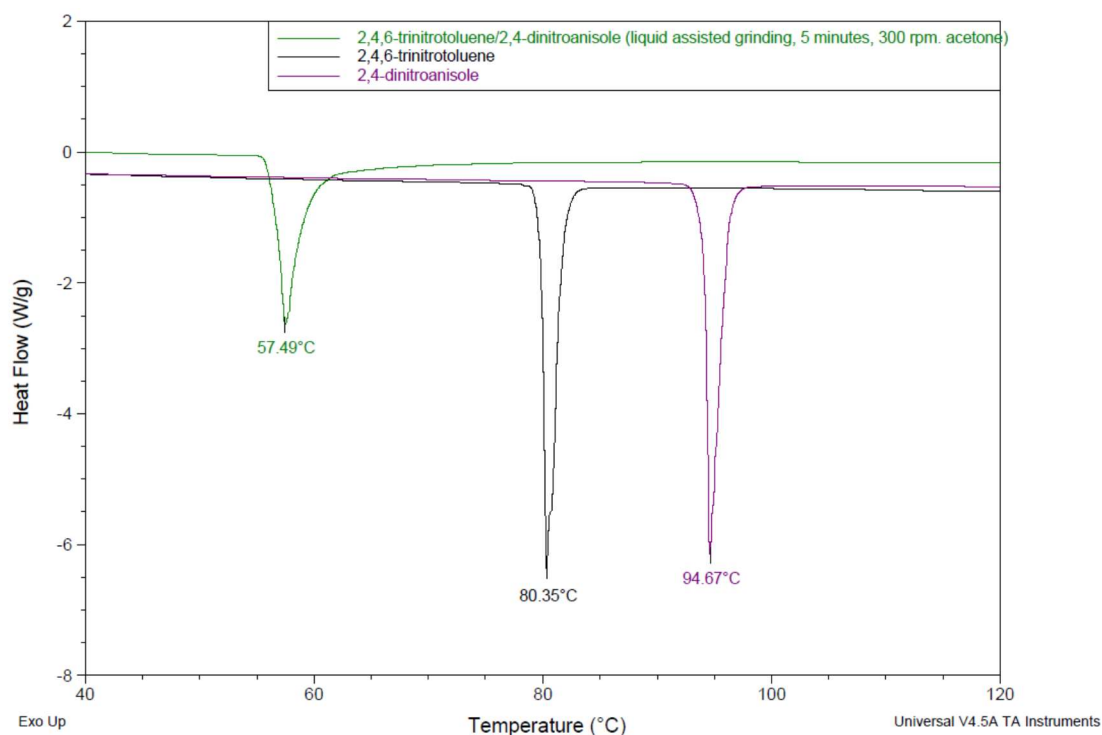


Figure B.96 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

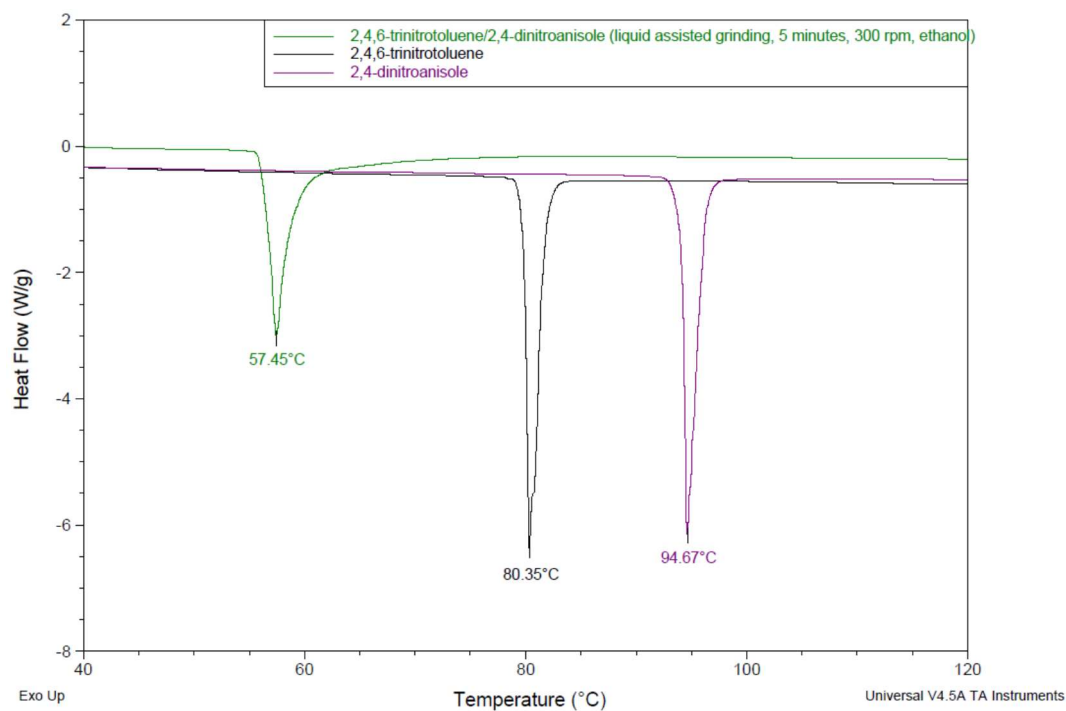


Figure B.97 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

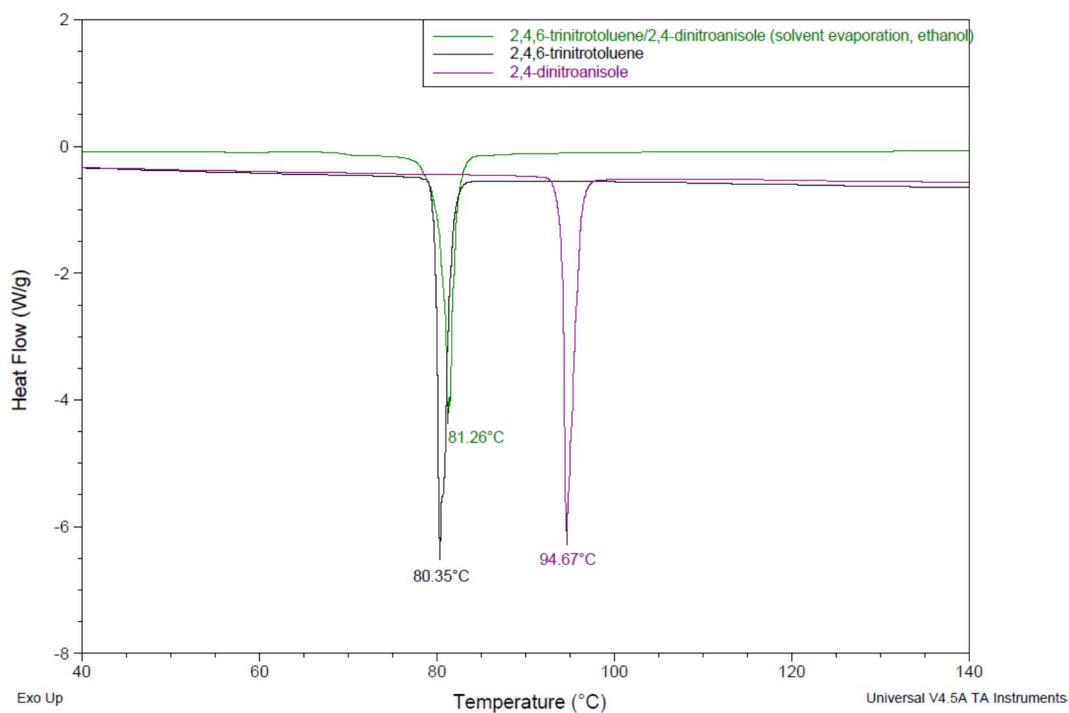


Figure B.98 - Thermal analysis of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by solvent evaporation with ethanol.

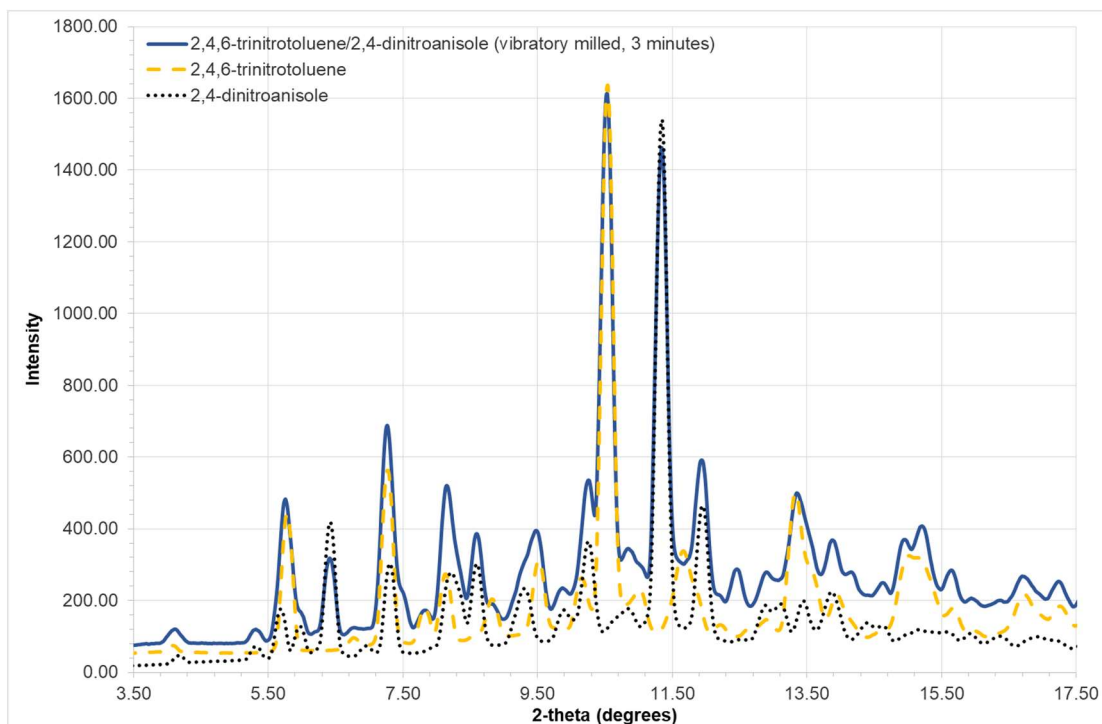


Figure B.99 – Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by vibratory milling for 3 minutes.

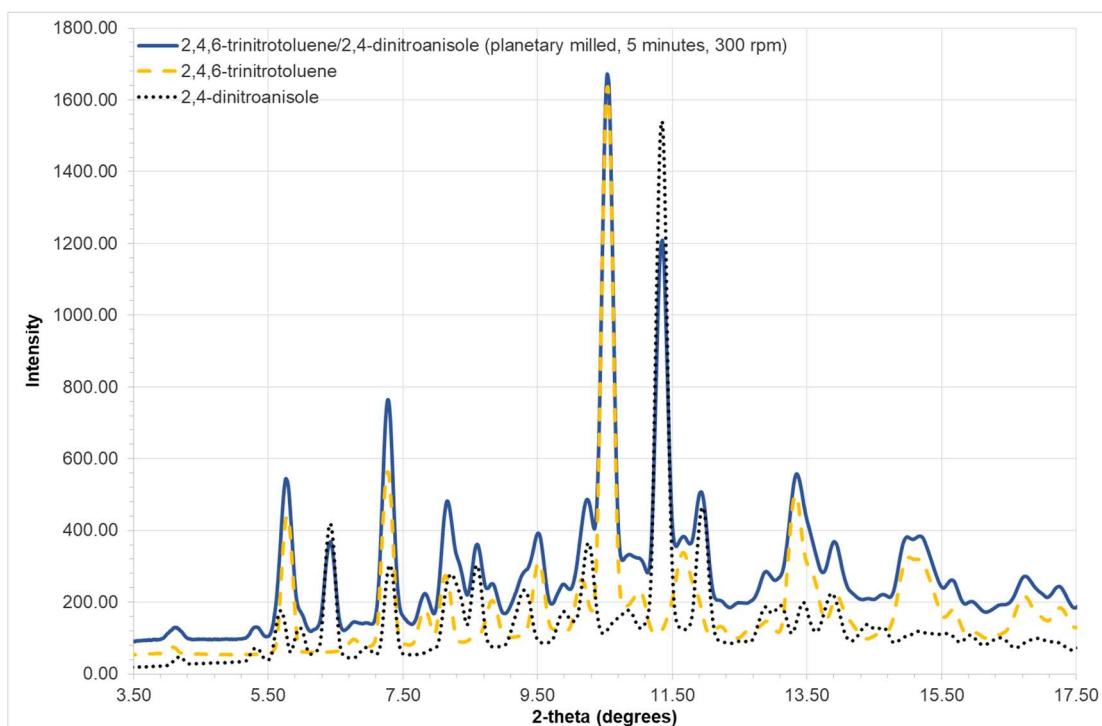


Figure B.100 - Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by planetary milling for 5 minutes at 300 rpm.

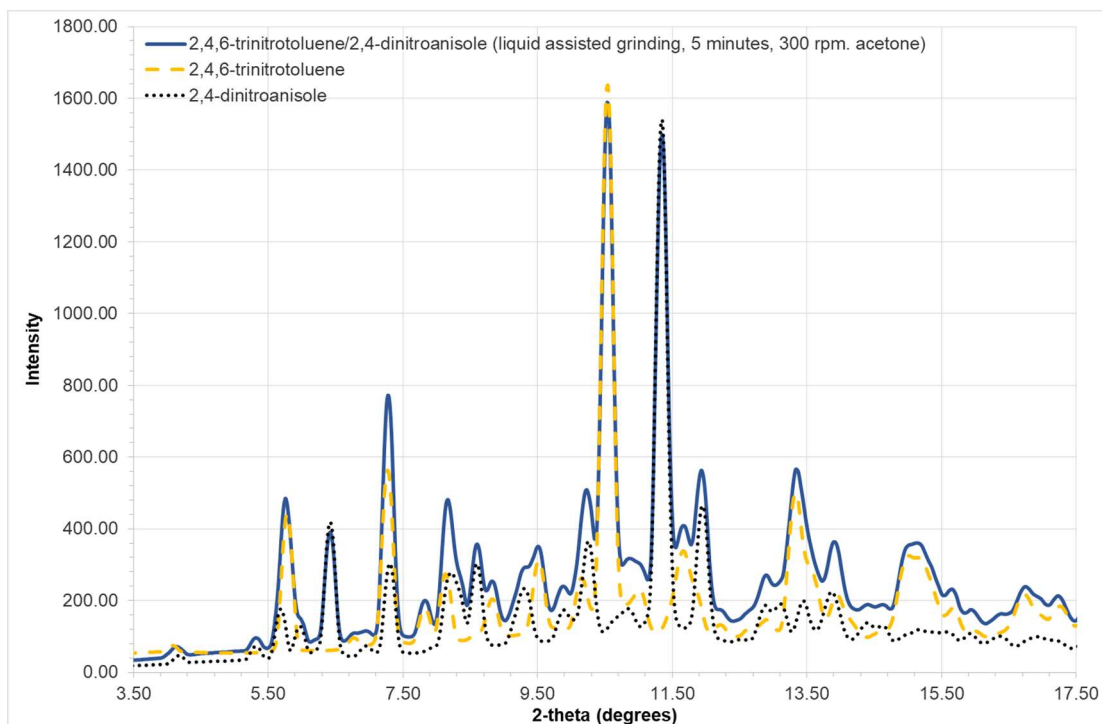


Figure B.101 - Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

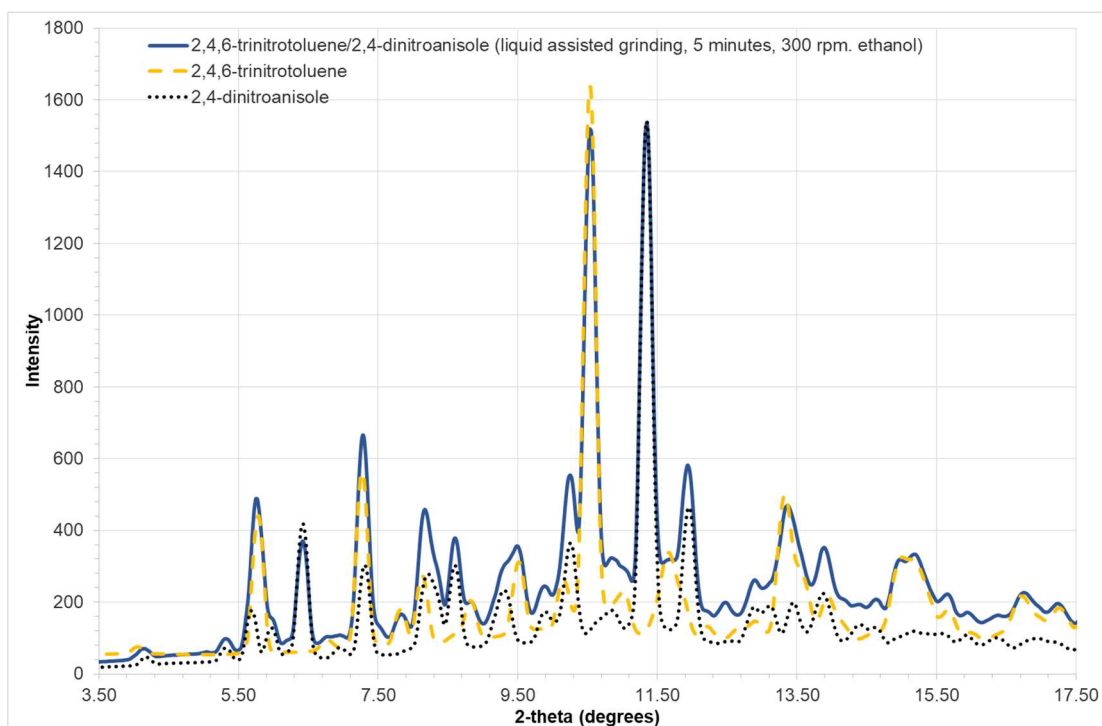


Figure B.102 - Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4-dinitroanisole produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.13 2,4,6-trinitrotoluene/1,3-dinitrobenzene

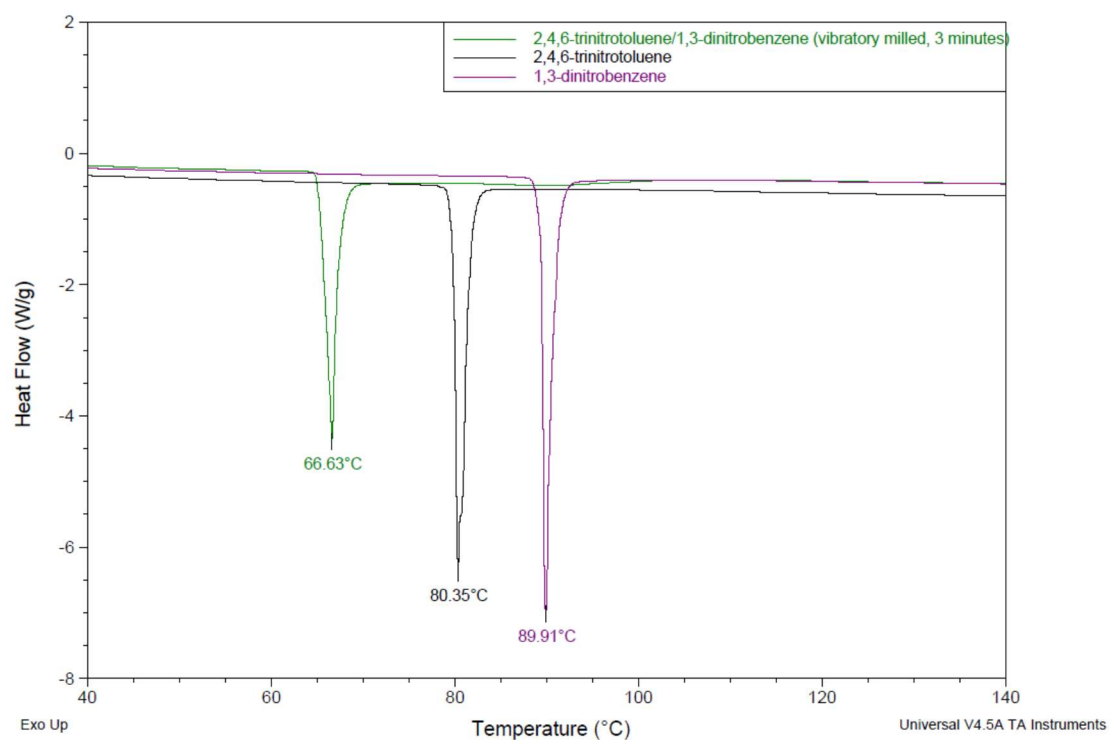


Figure B.103 – Thermal analysis of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by vibratory milling for 3 minutes.

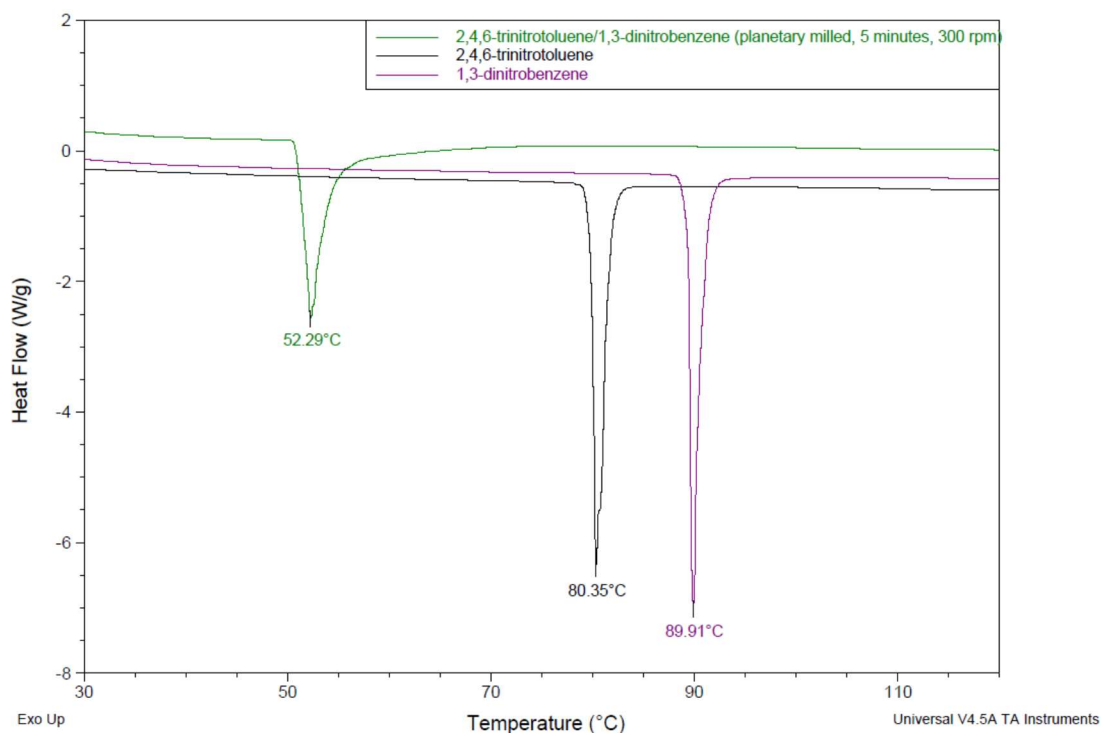


Figure B.104 - Thermal analysis of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

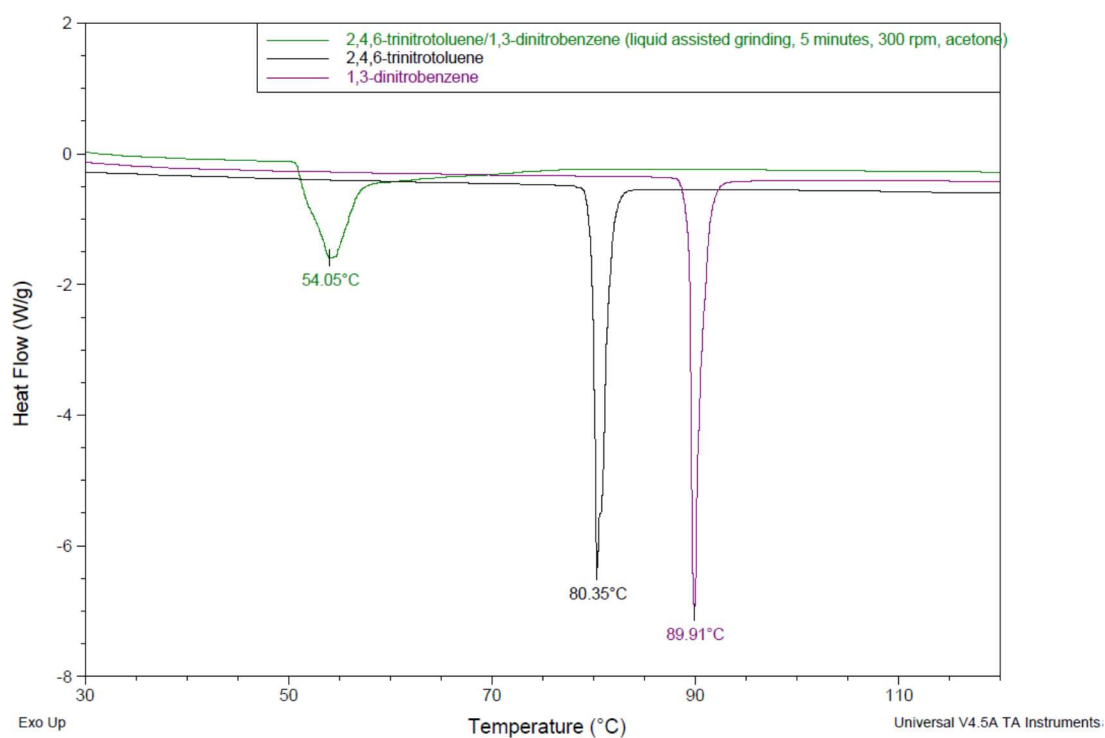


Figure B.105 - Thermal analysis of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

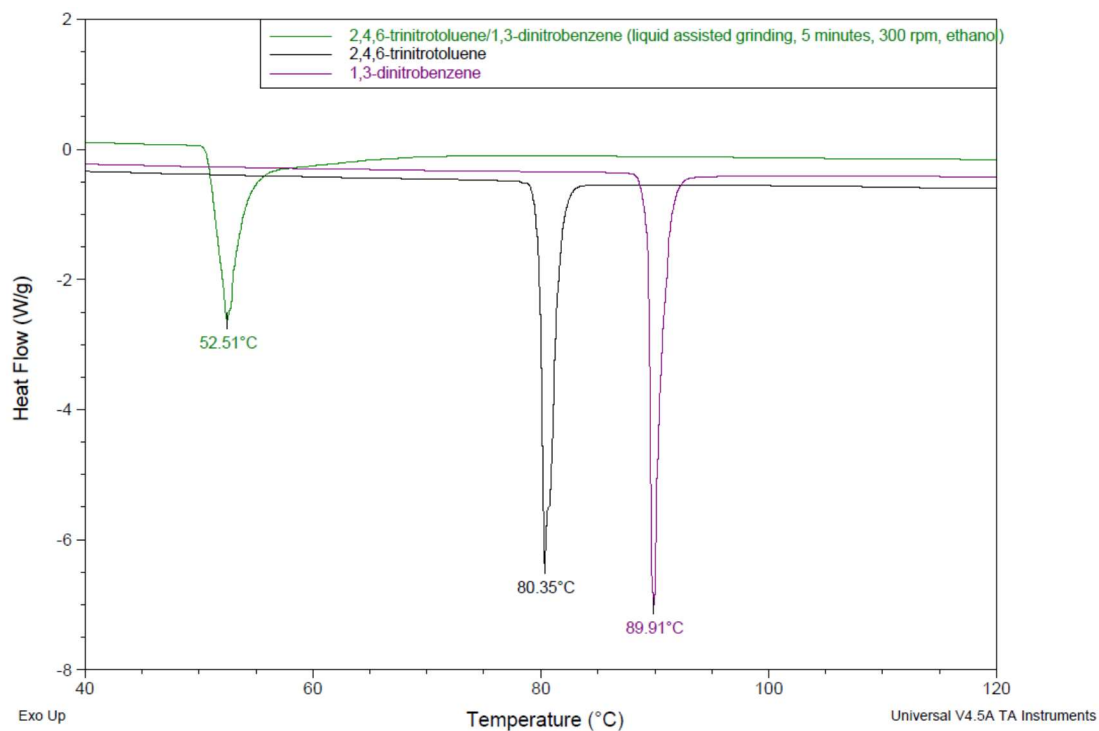


Figure B.106 - Thermal analysis of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

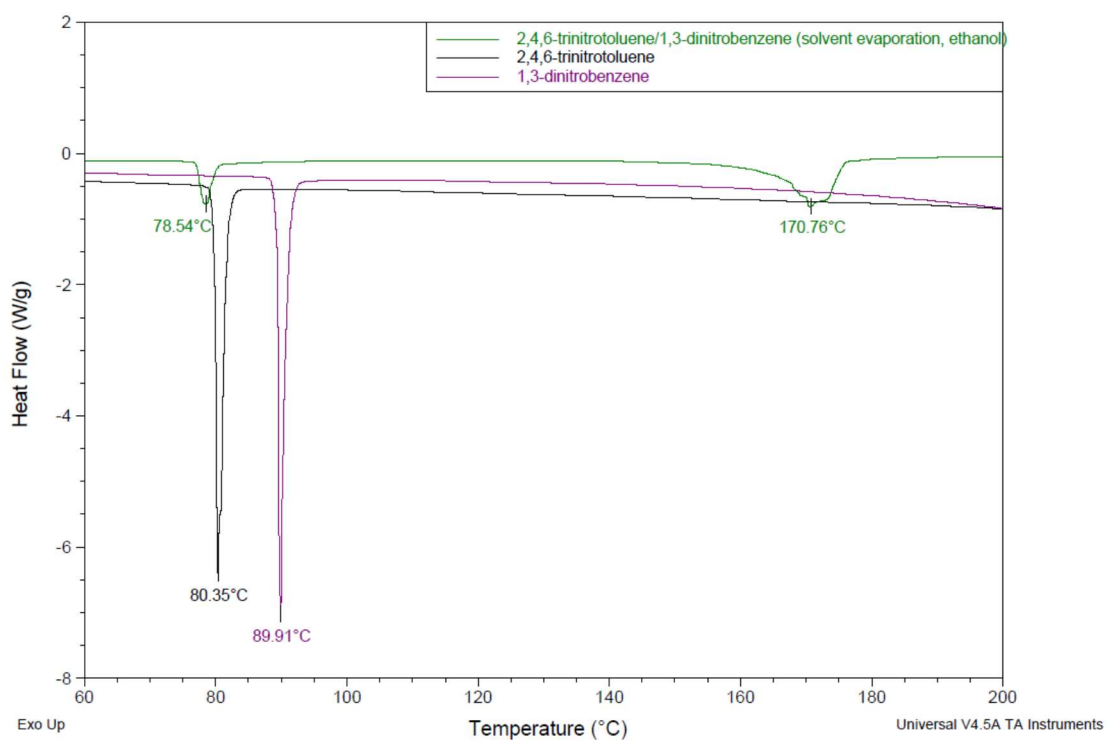


Figure B.107 - Thermal analysis of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by solvent evaporation with ethanol.

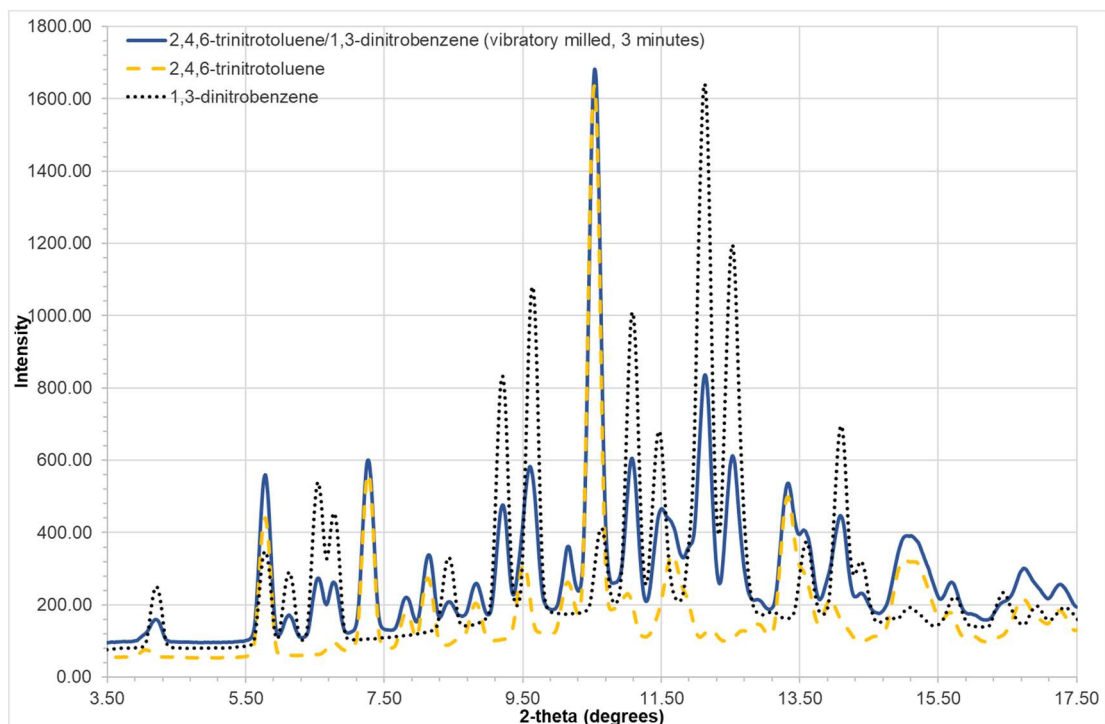


Figure B.108 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by vibratory milling for 3 minutes.

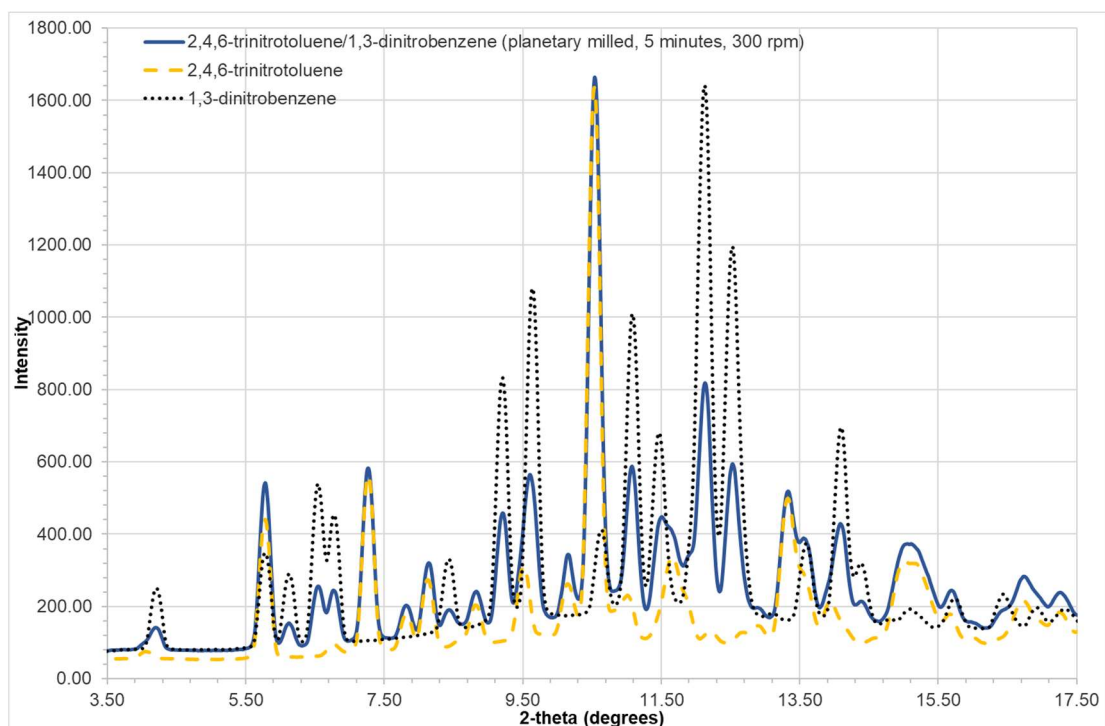


Figure B.109 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

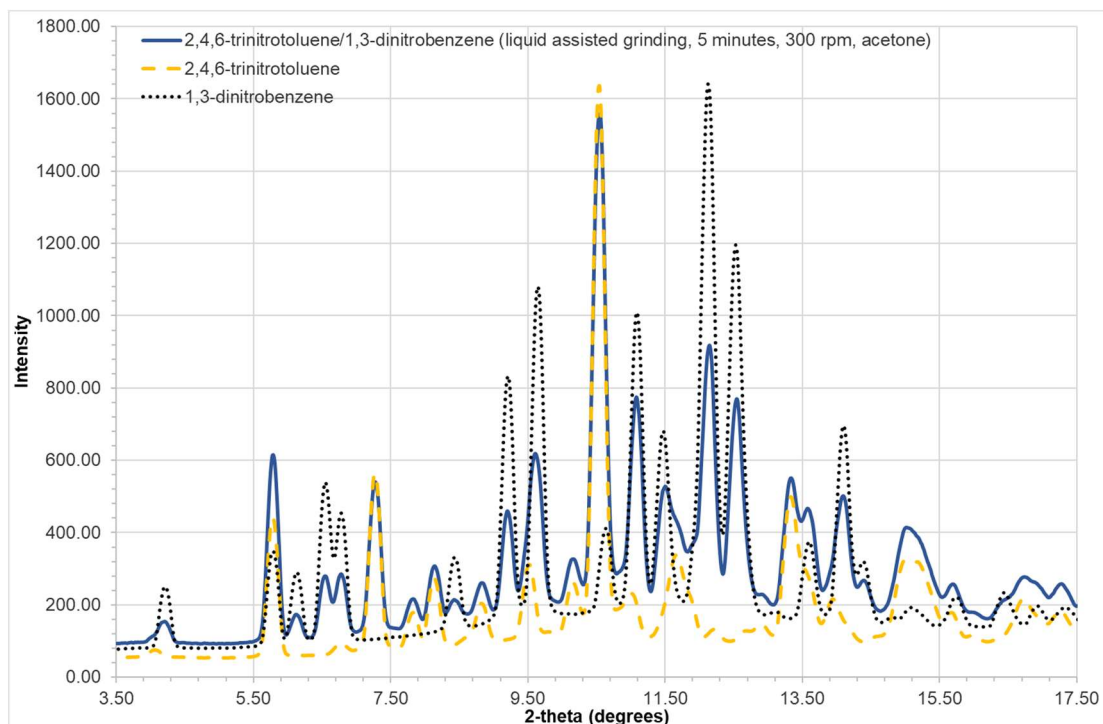


Figure B.110 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

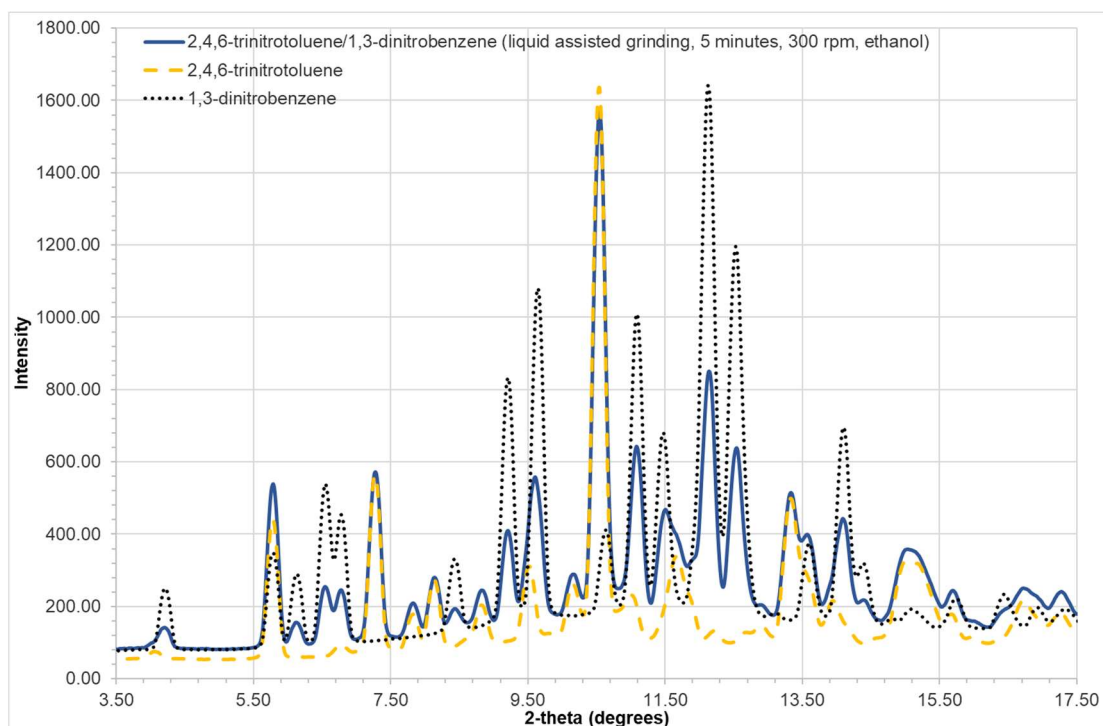


Figure B.111 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3-dinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.14 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene

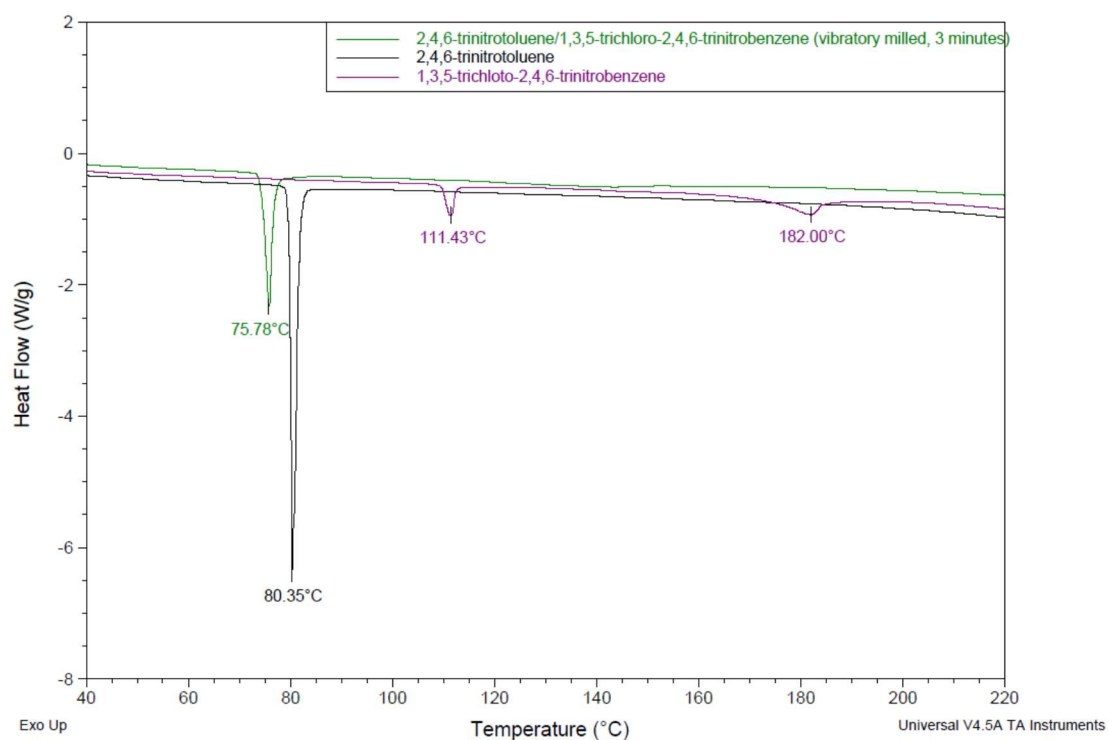


Figure B.112 – Thermal analysis of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by vibratory milling for 3 minutes.

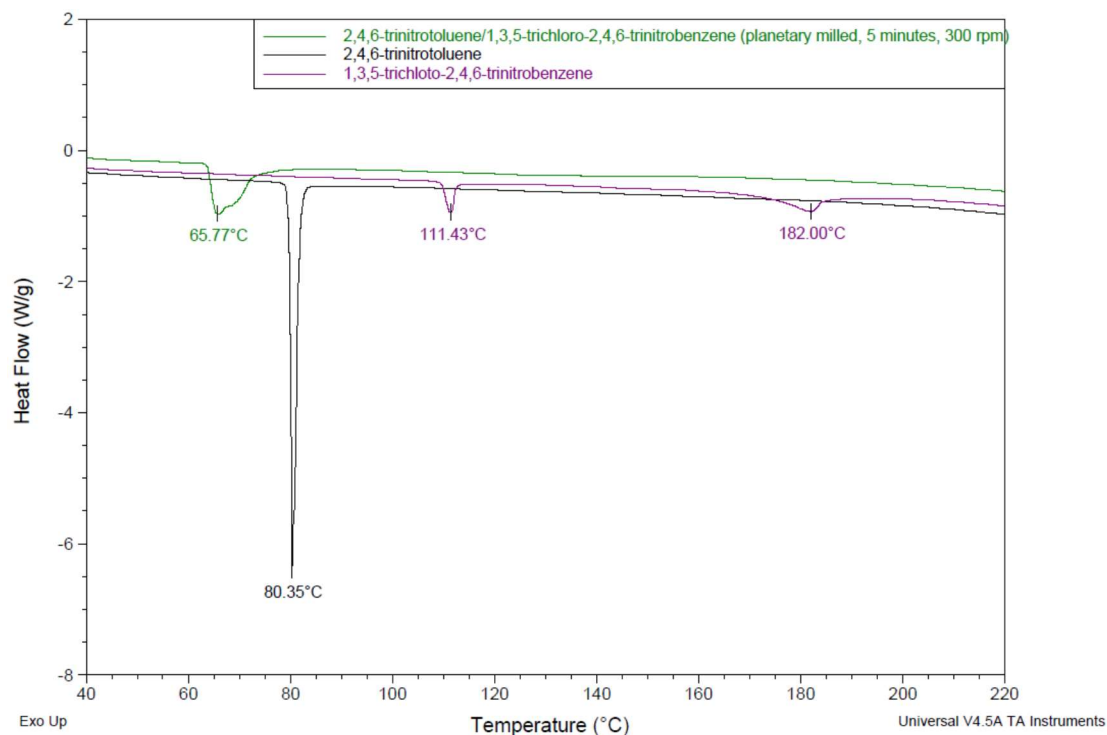


Figure B.113 - Thermal analysis of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

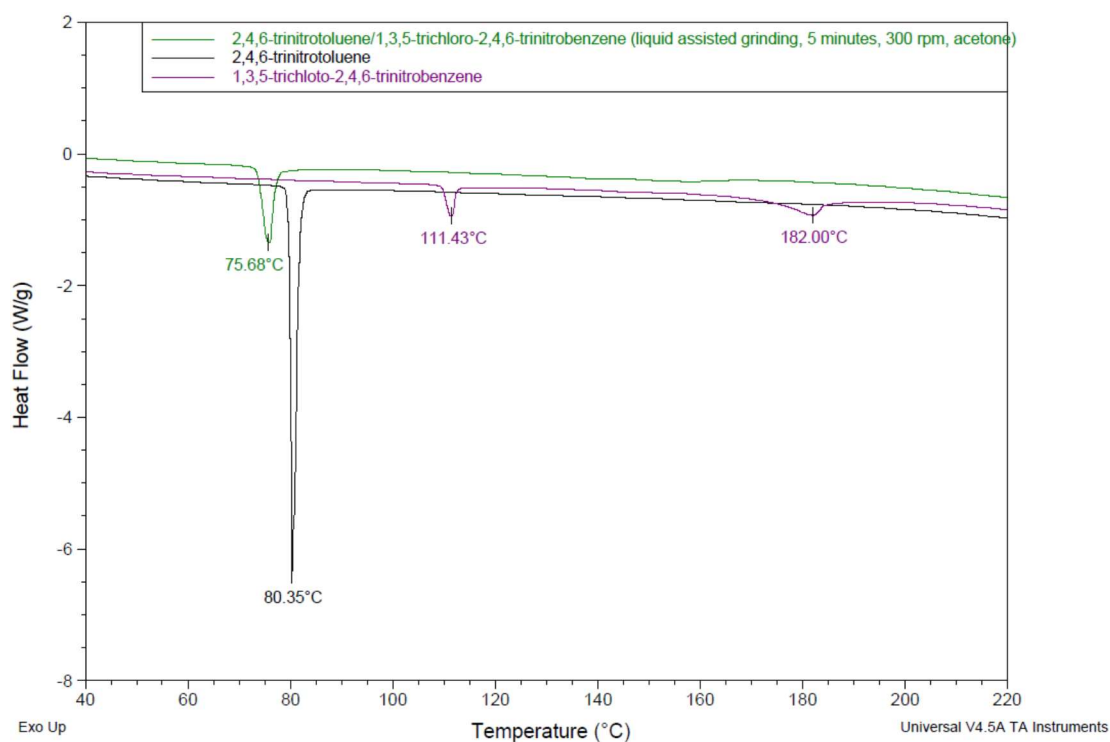


Figure B.114 - Thermal analysis of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

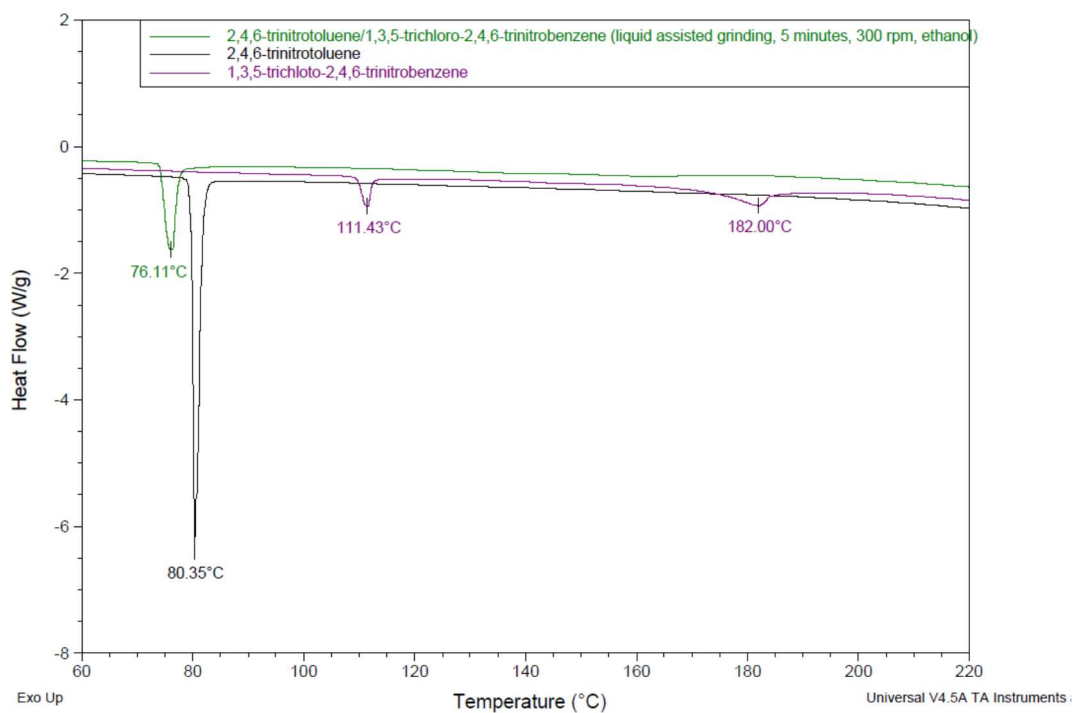


Figure B.115 - Thermal analysis of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

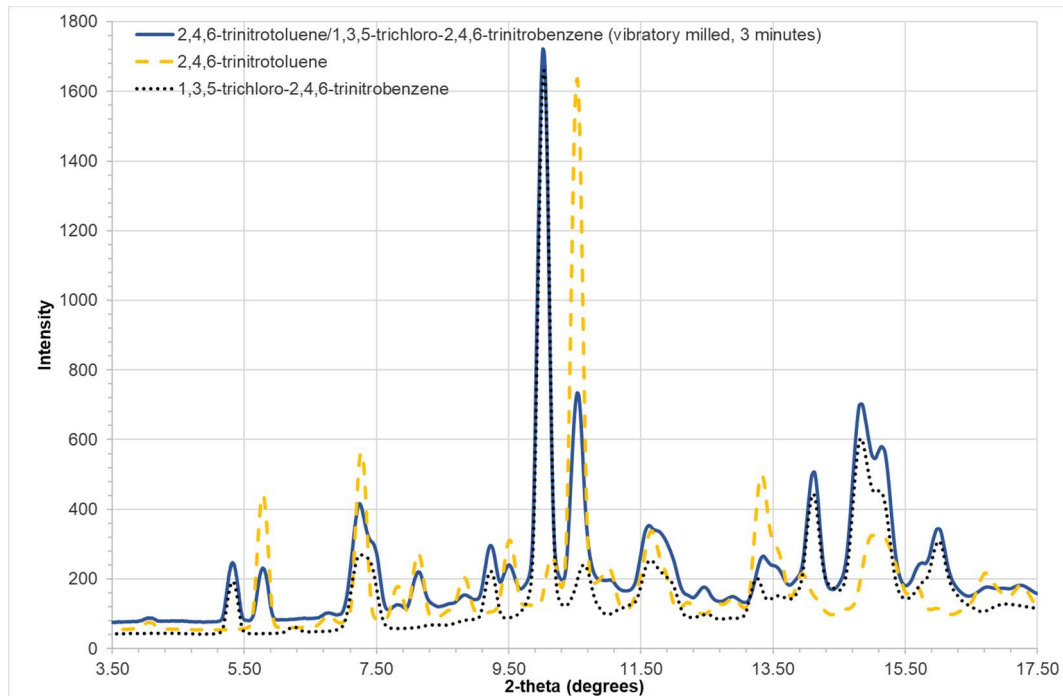


Figure B.116 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by vibratory milling for 3 minutes.

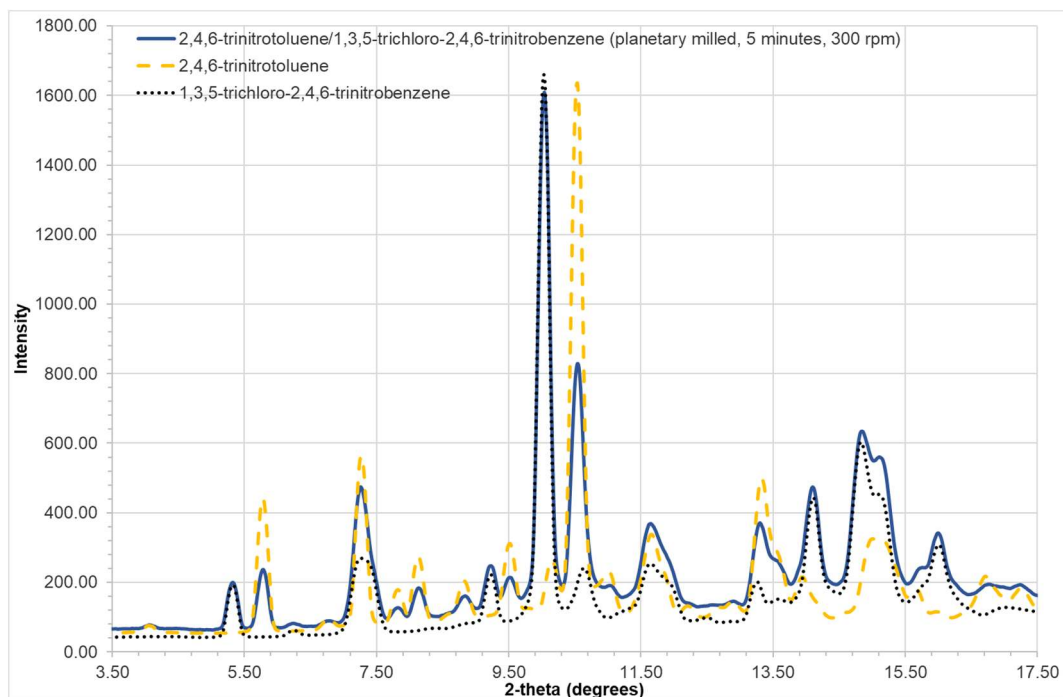


Figure B.117 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by planetary milling for 5 minutes at 300 rpm.

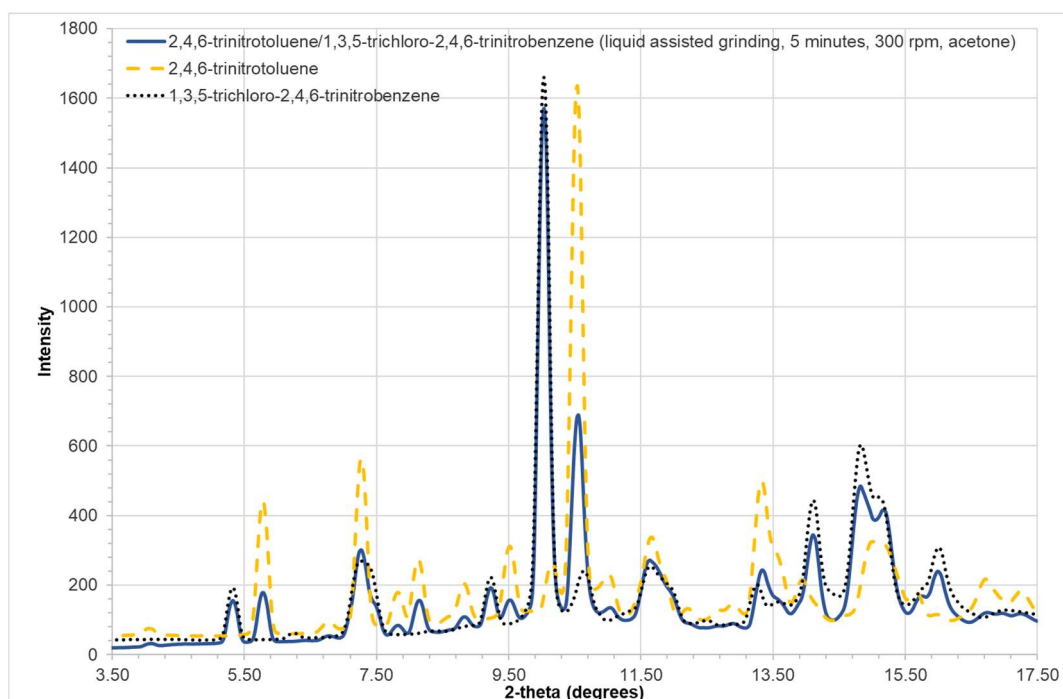


Figure B.118 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with acetone.

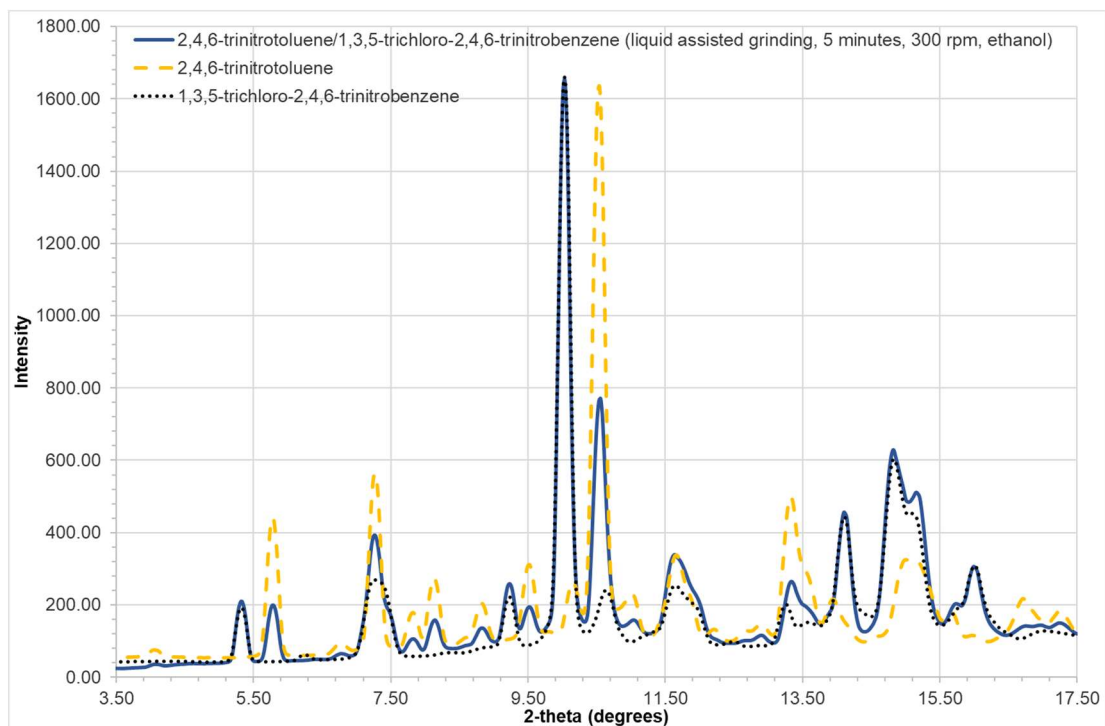


Figure B.119 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,3,5-trichloro-2,4,6-trinitrobenzene produced by liquid assisted grinding for 5 minutes at 300 rpm with ethanol.

B.15 2,4,6-trinitrotoluene/2,4,6-trinitroaniline

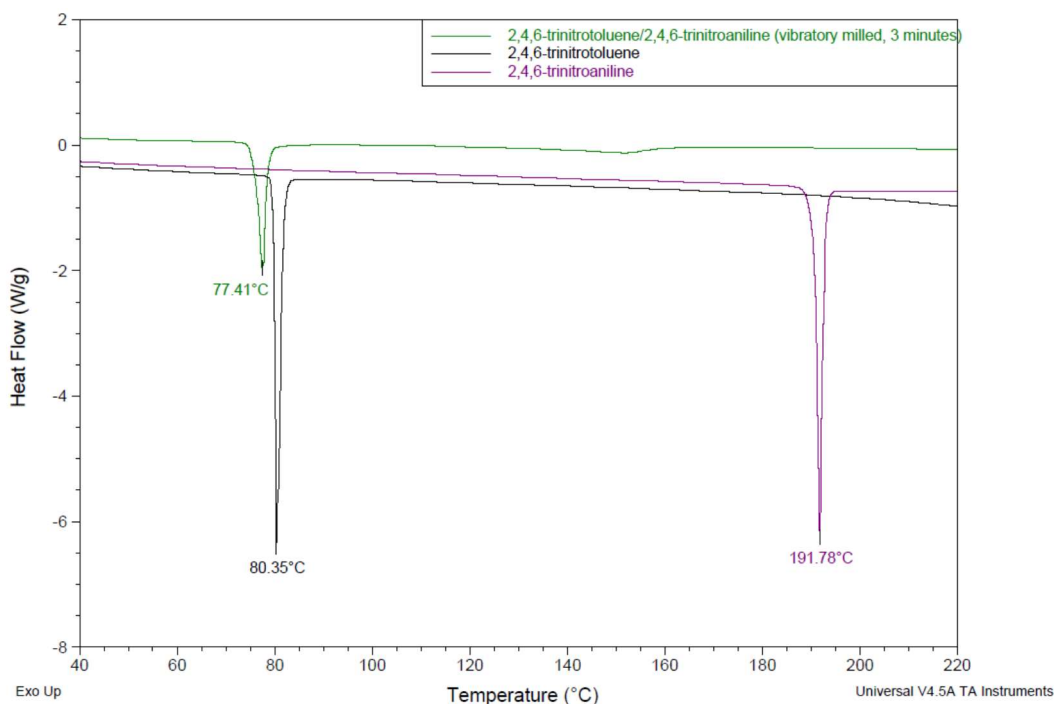


Figure B.120 – Thermal analysis of 2,4,6-trinitrotoluene/2,4,6-trinitroaniline produced by vibratory milled for 3 minutes.

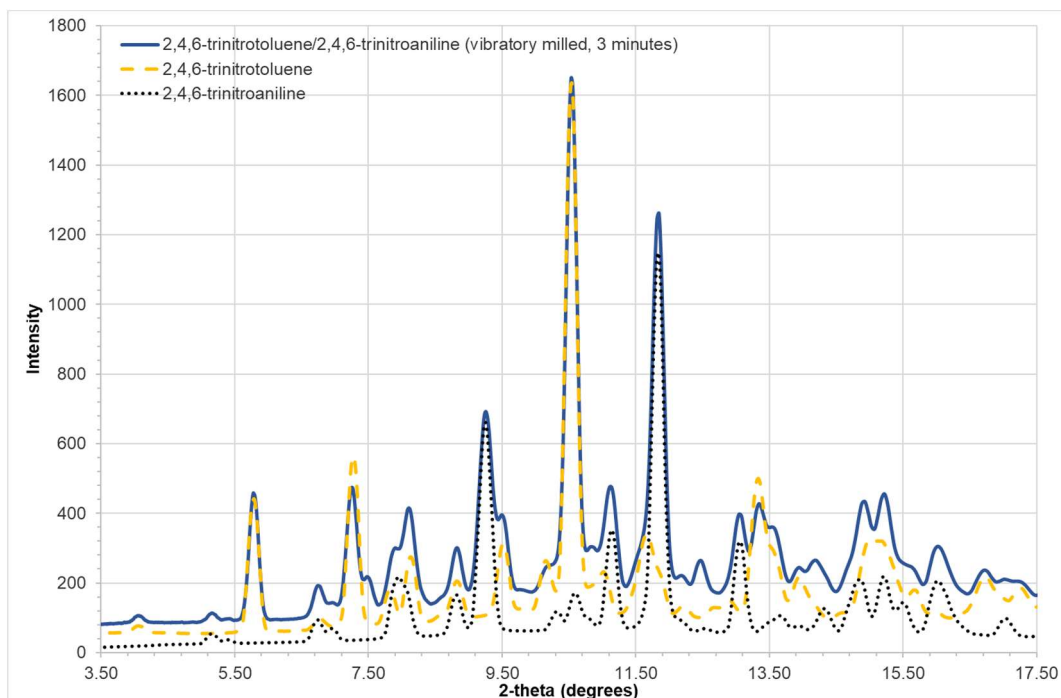


Figure B.121 - Powder x-ray pattern of 2,4,6-trinitrotoluene/2,4,6-trinitroaniline produced by vibratory milled for 3 minutes.

B.16 Molecular electrostatic potential

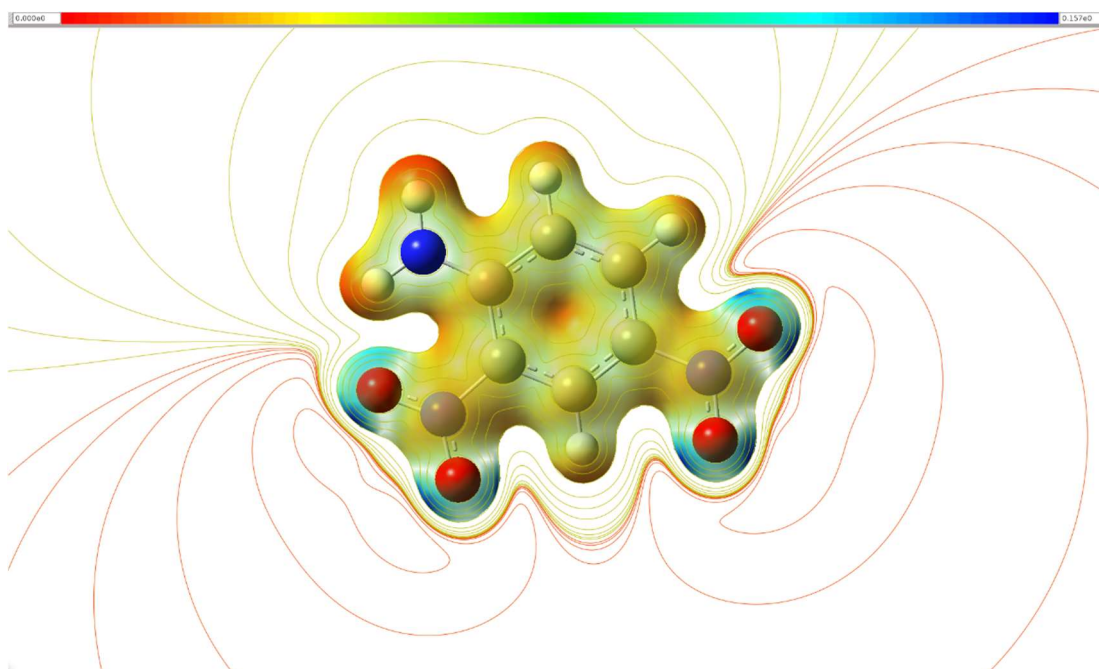


Figure B.122 - Molecular electrostatic potential of 2,4-dinitroaniline

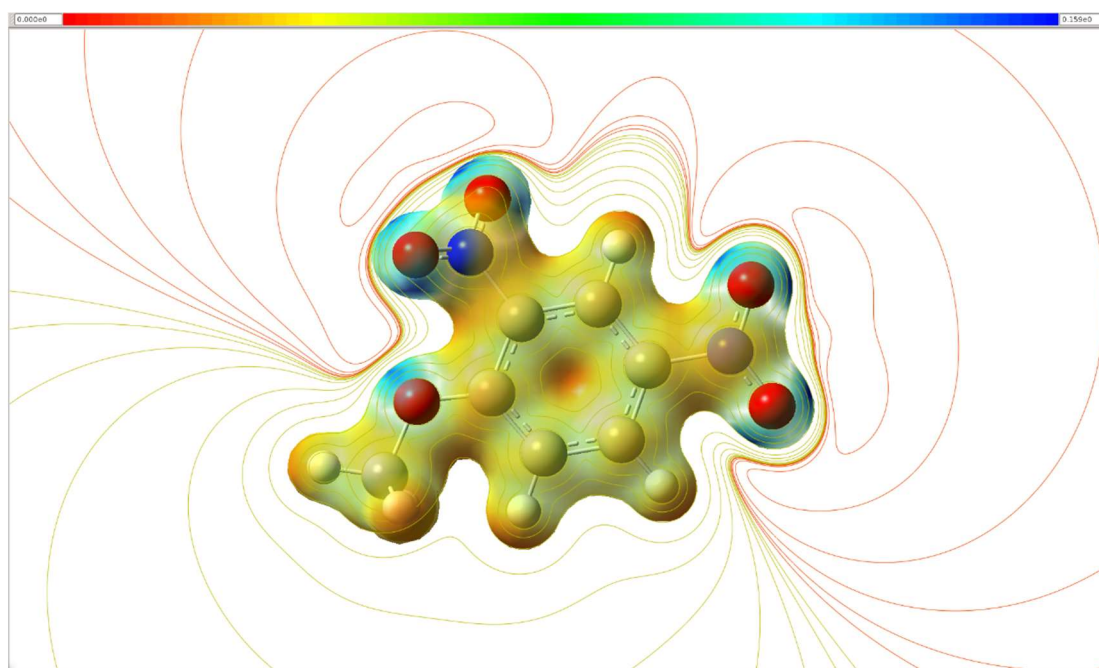


Figure B.123 - Molecular electrostatic potential of 2,4-dinitroanisole

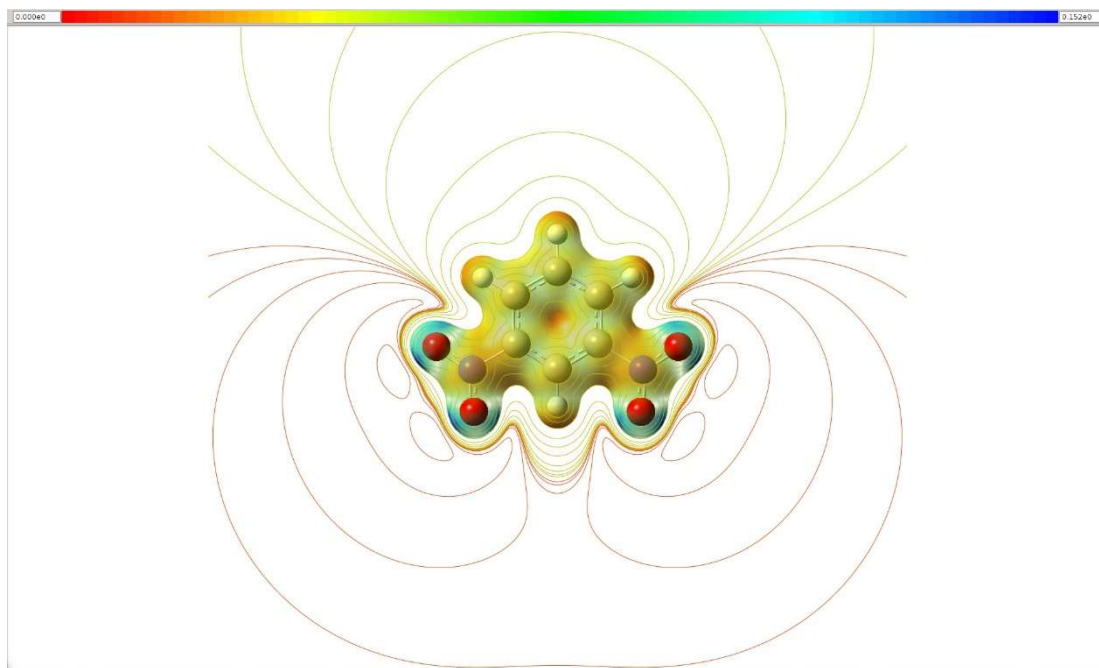


Figure B.124 - Molecular electrostatic potential of 2,4-dinitrobenzene

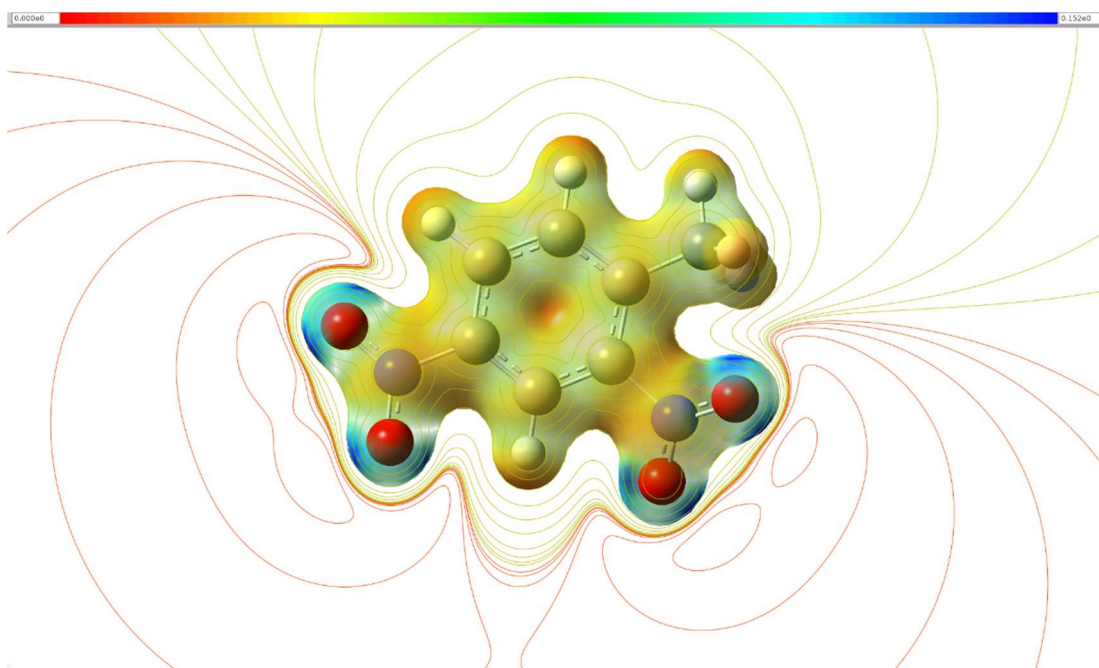


Figure B.125 - Molecular electrostatic potential of 2,4-dinitrotoluene

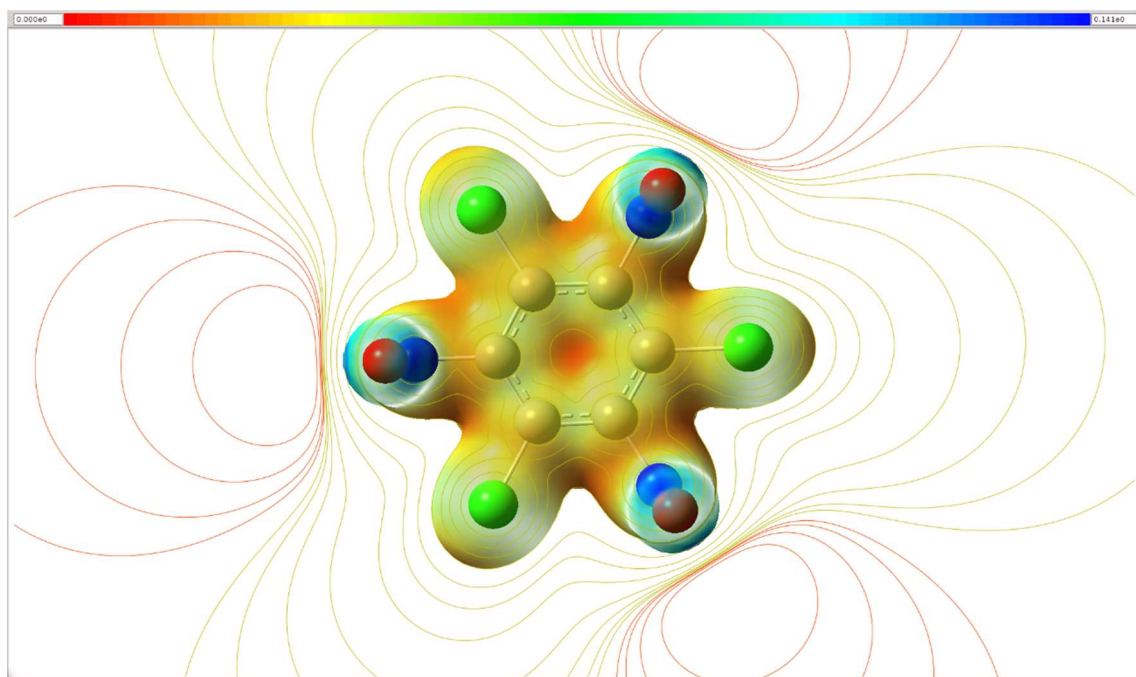


Figure B.126 - Molecular electrostatic potential of 1,3,5-trichloro-2,4,6-trinitrobenzene

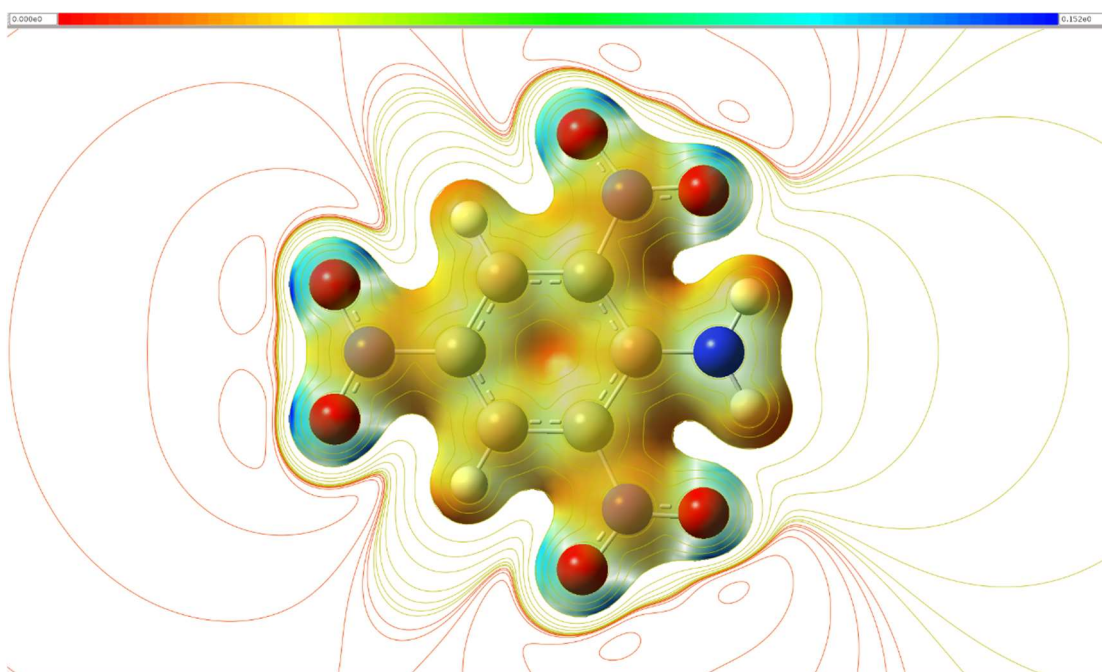


Figure B.127 - Molecular electrostatic potential of 2,4,6-trinitroaniline

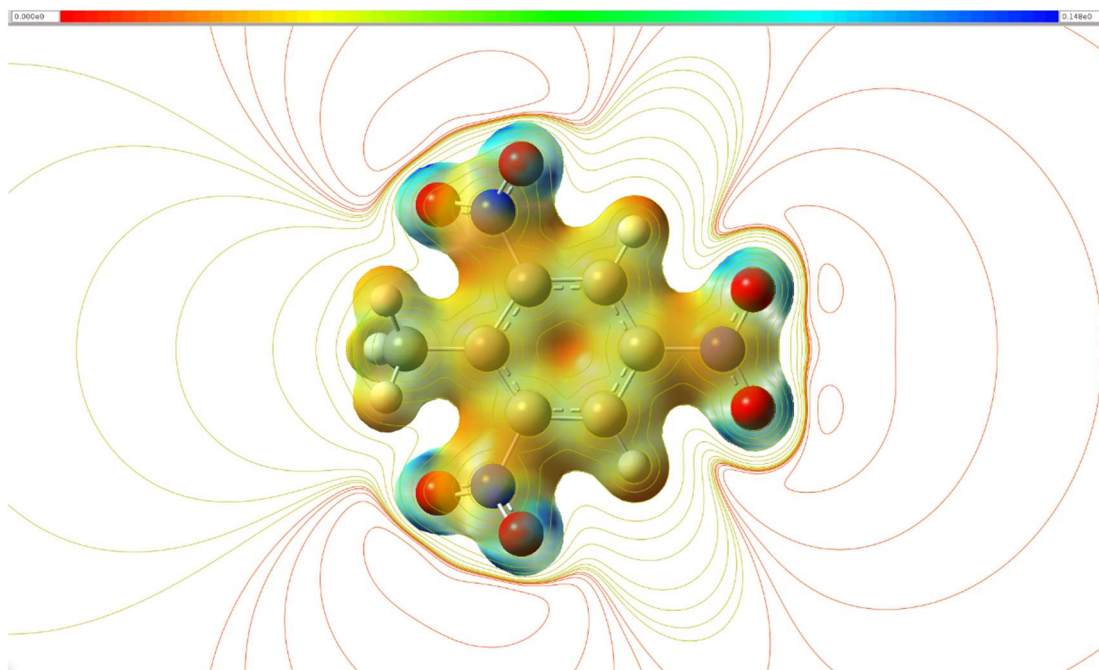


Figure B.128 - Molecular electrostatic potential of 2,4,6,-trinitrotoluene

C Results 3 – Manipulation of electrostatic potential and its effect on co-crystal formation

C.1 2-naphthol/pyrrolidine

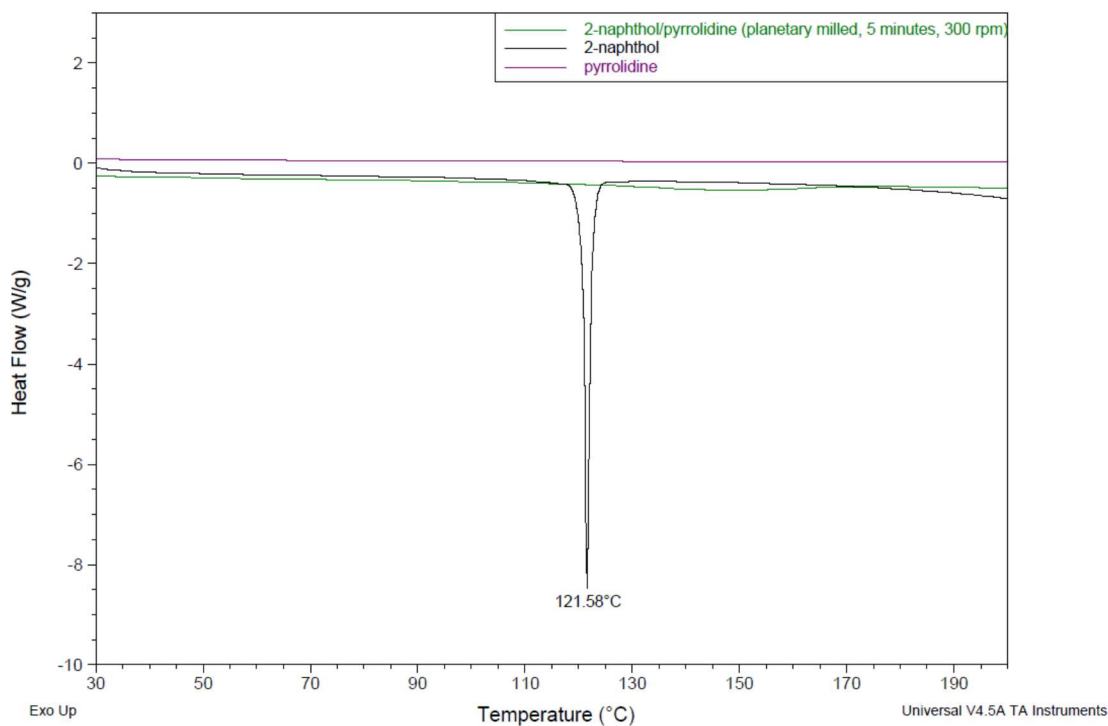


Figure C.1 - Thermal analysis of 2-naphthol/pyrrolidine produced by planetary milling for 5 minutes at 300 rpm. Pyrrolidine and the mixed system are liquids, therefore no melts are observed.

C.2 2-naphthol/3-pyrroline

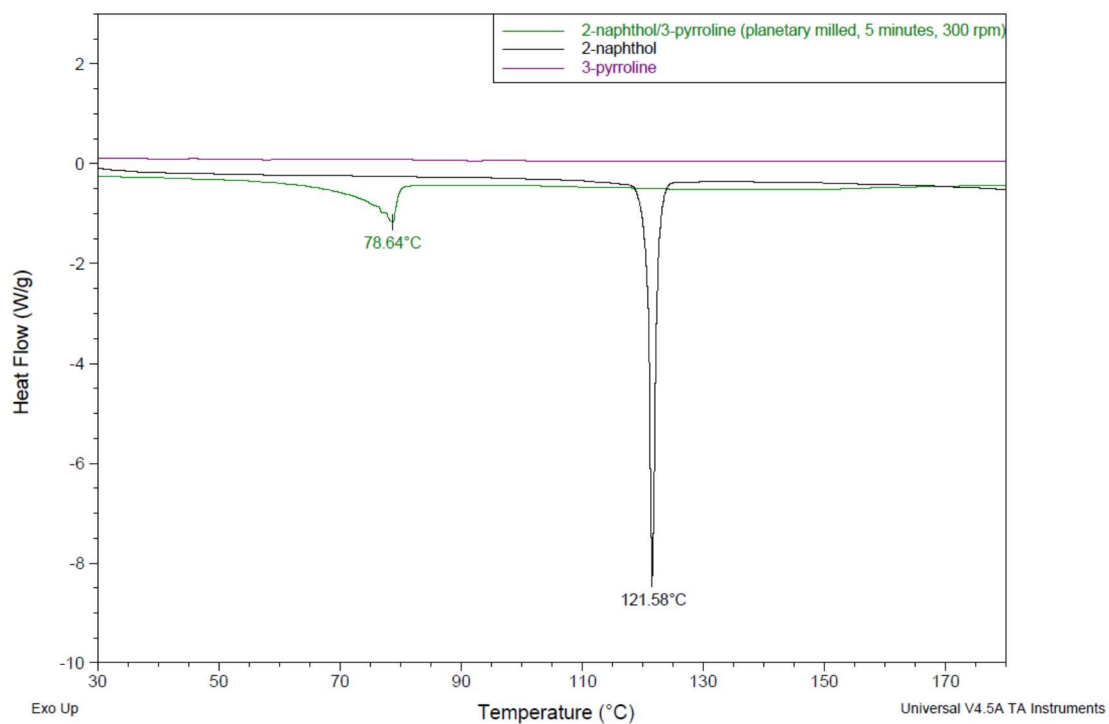


Figure C.2 - Thermal analysis of 2-naphthol/3-pyrroline produced by planetary milling for 5 minutes at 300 rpm. Pyrrole is a liquid, therefore no melt is observed.

C.3 2-naphthol/pyrrole

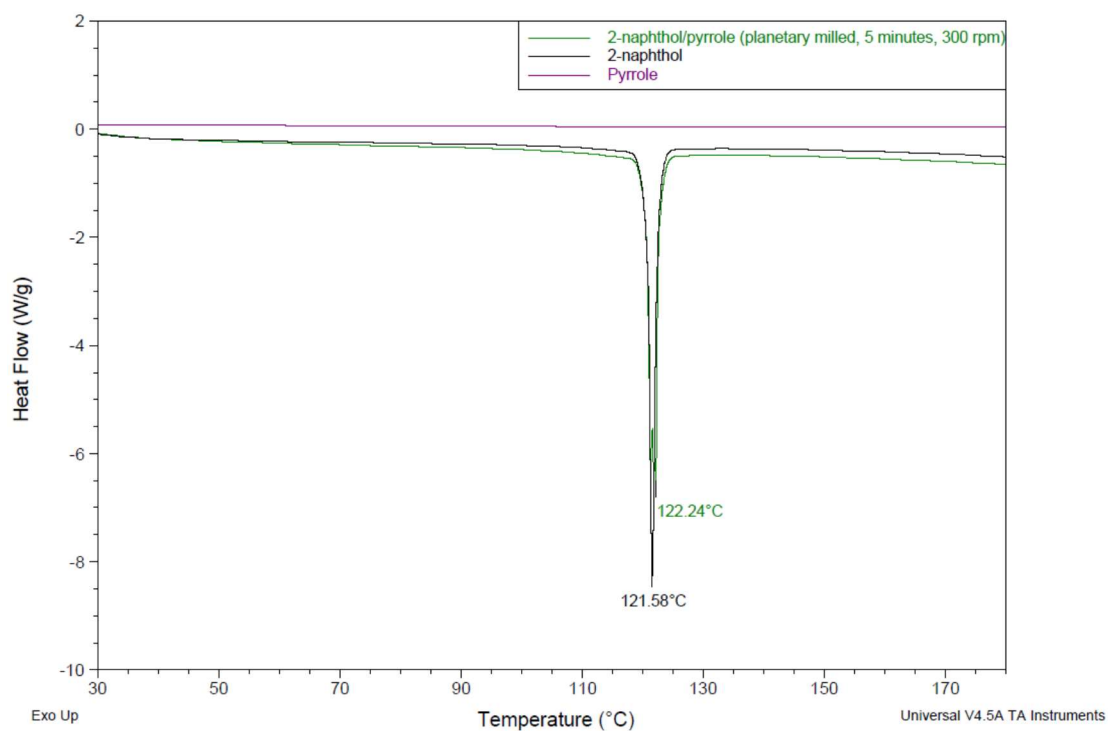


Figure C.3 – Thermal analysis of 2-naphthol/pyrrole produced by planetary milling for 5 minutes at 300 rpm. Pyrrole is a liquid, therefore no melt is observed.

C.4 2-naphthol/2-nitropyrrole

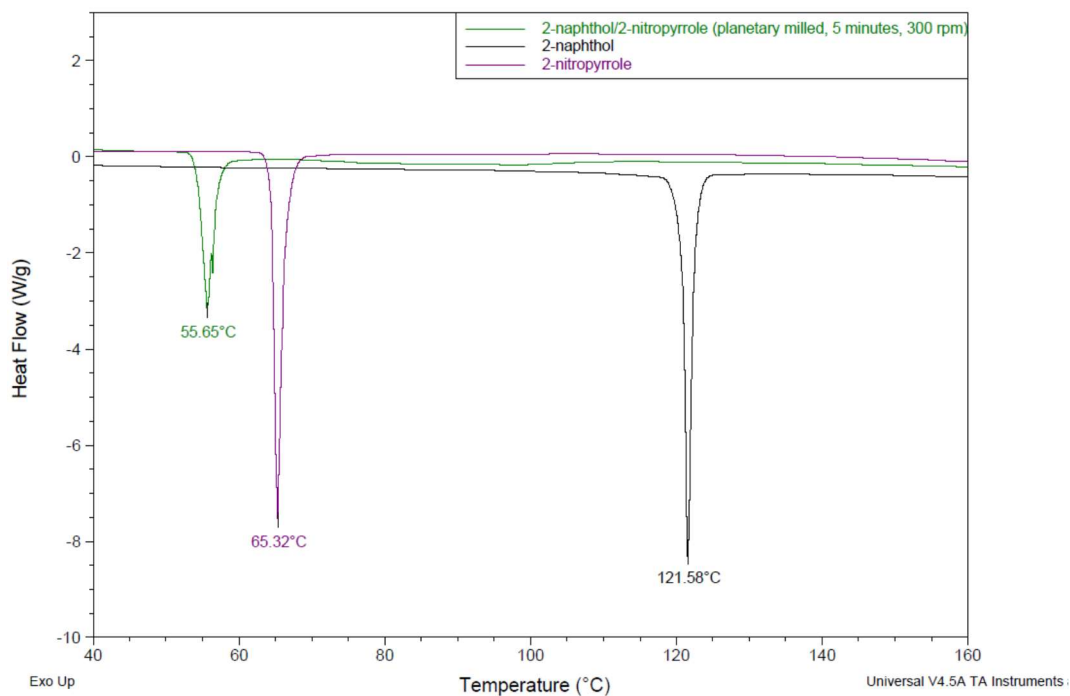


Figure C.4 – Thermal analysis of 2-naphthol/2-nitropyrrole produced by planetary milling for 5 minutes at 300 rpm.

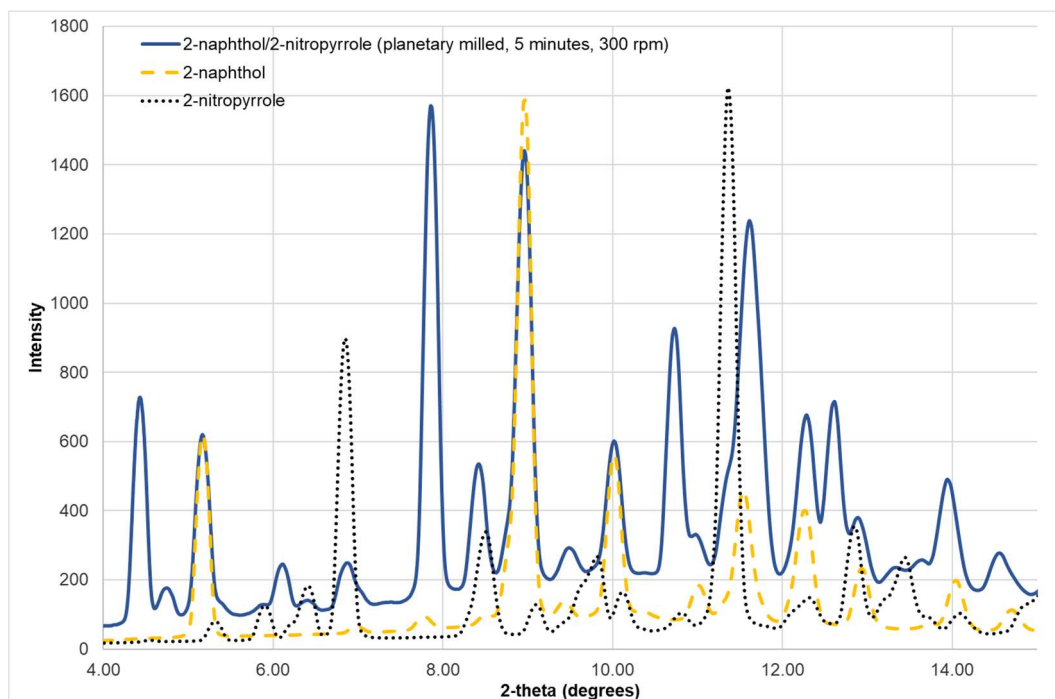


Figure C.5 - Powder x-ray pattern of 2-naphthol/2-nitropyrrole produced by planetary milling for 5 minutes at 300 rpm.

C.5 2-naphthol/2-methylpyrrole

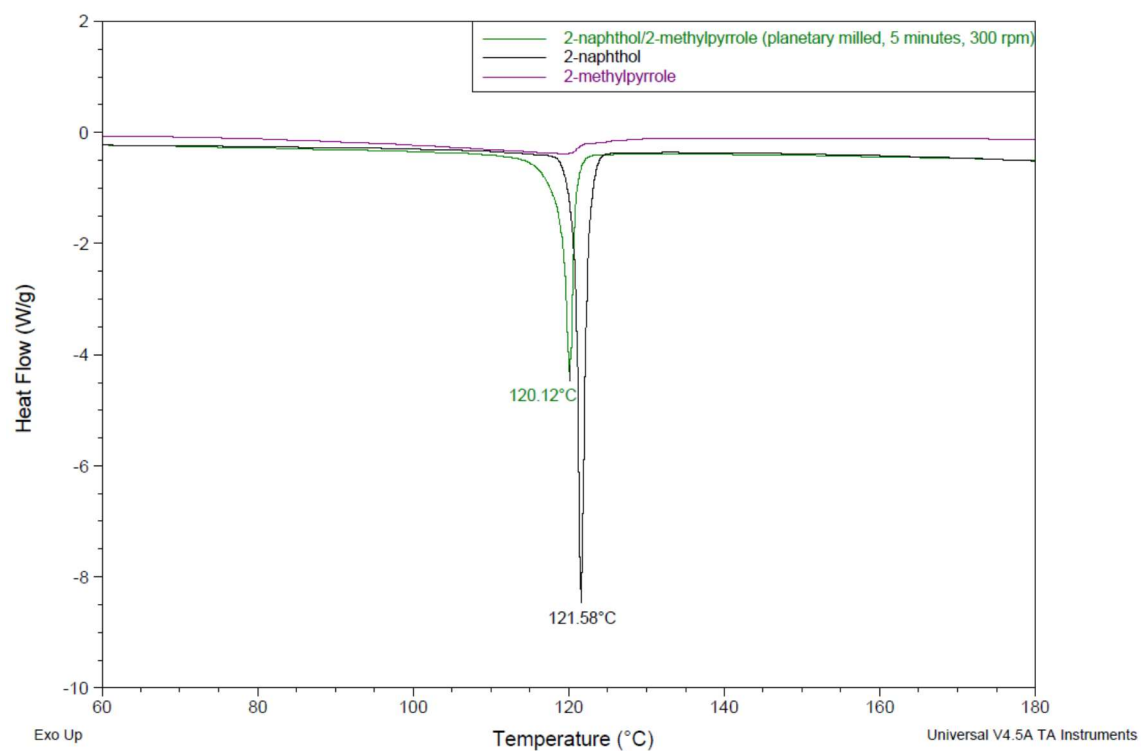


Figure C.6 - Thermal analysis of 2-naphthol/2-methylpyrrole produced by planetary milling for 5 minutes at 300 rpm. 2-methylpyrrole is a liquid and showed no melt.

C.6 2-naphthol/3-methylpyrrole

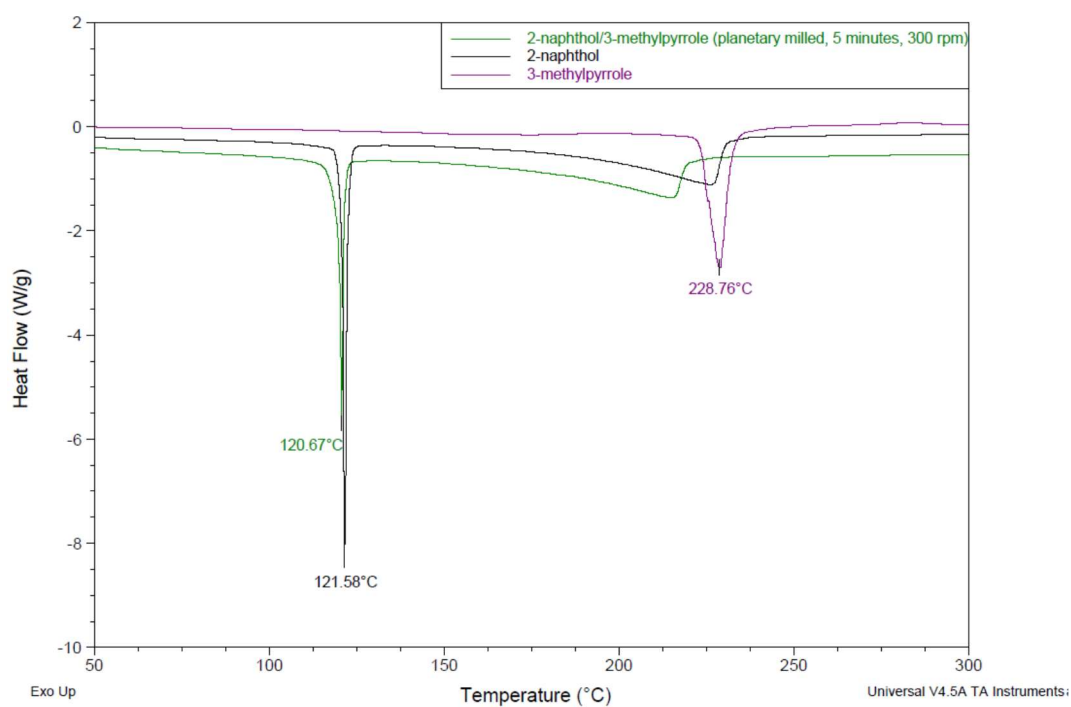


Figure C.7 - Thermal analysis of 2-naphthol/3-methylpyrrole produced by planetary milling for 5 minutes at 300 rpm.

C.7 2-naphthol/2,4-dimethylpyrrole

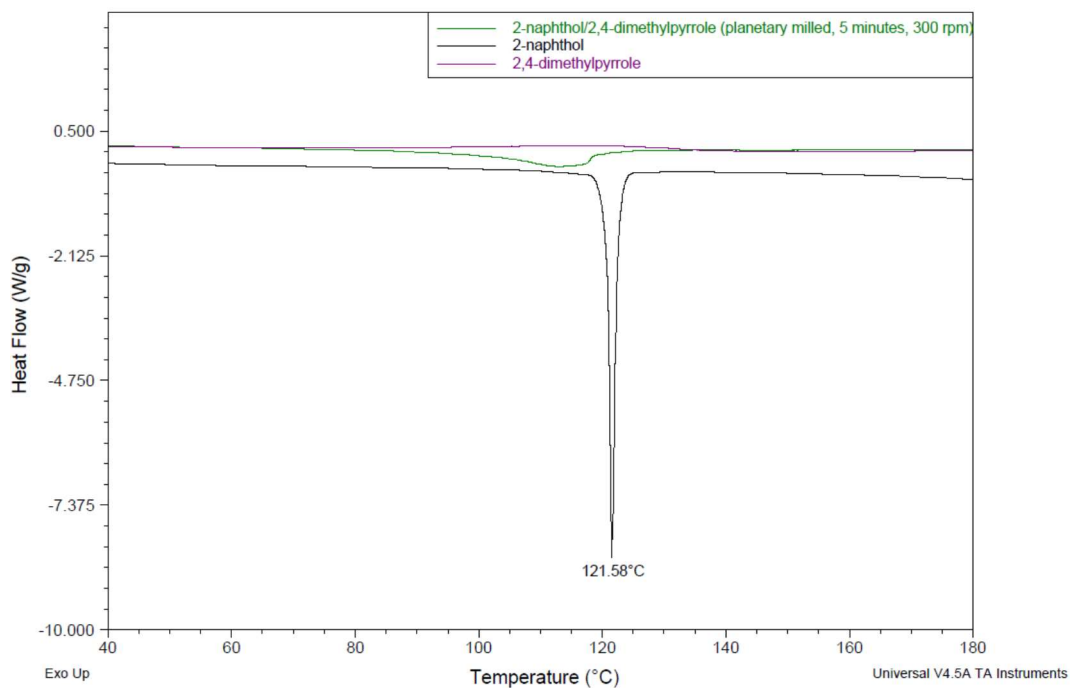


Figure C.8 - Thermal analysis of 2-naphthol/2,4-dimethylpyrrole produced by planetary milling for 5 minutes at 300 rpm. 2,4-dimethylpyrazole is a liquid and did not display a melt.

C.8 2-naphthol/2,5-dimethylpyrrole

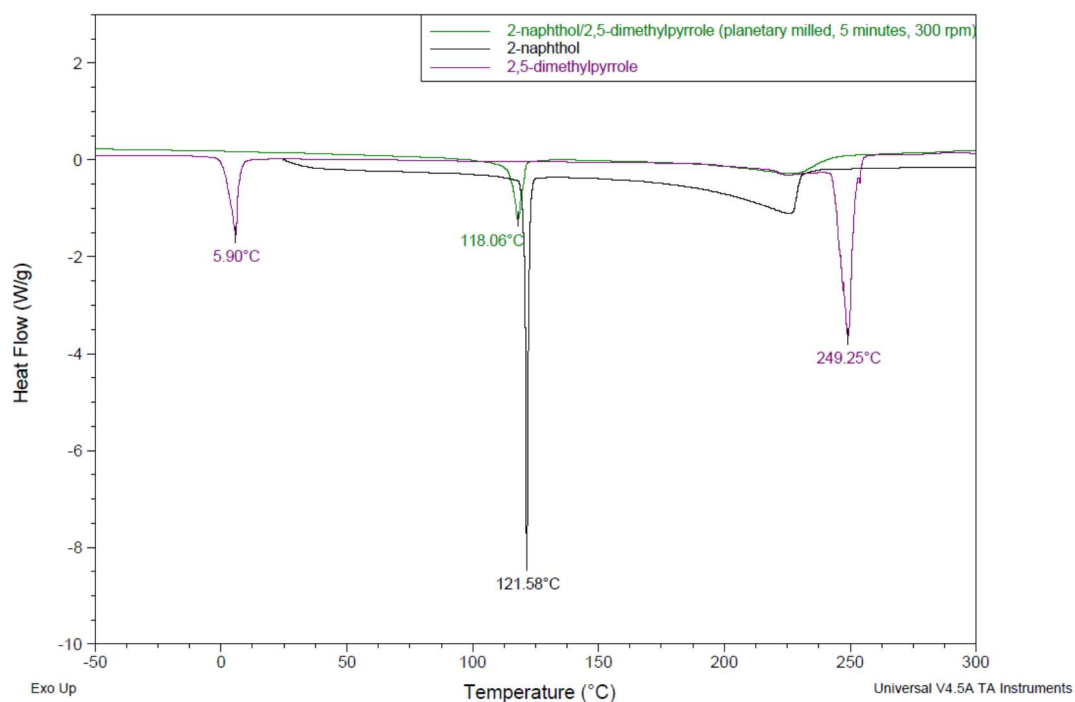


Figure C.9 - Thermal analysis of 2-naphthol/2,5-dimethylpyrrole produced by planetary milling for 5 minutes at 300 rpm.

C.9 2-naphthol/pyrazole

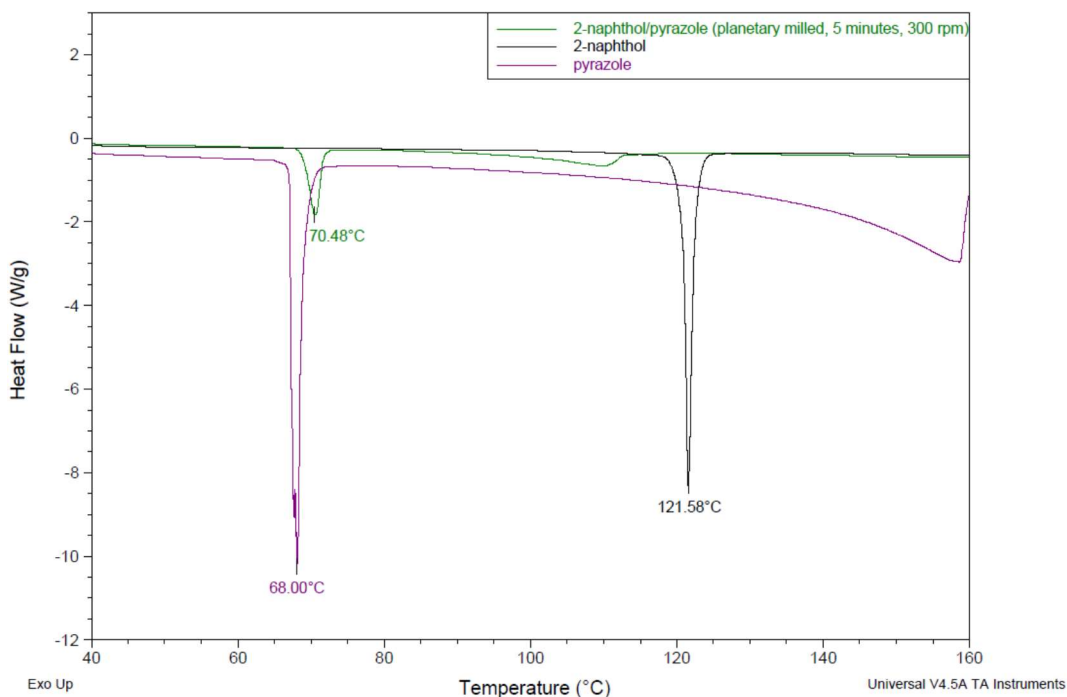


Figure C.10 – Thermal analysis of 2-naphthol/pyrazole produced by planetary milling for 5 minutes at 300 rpm.

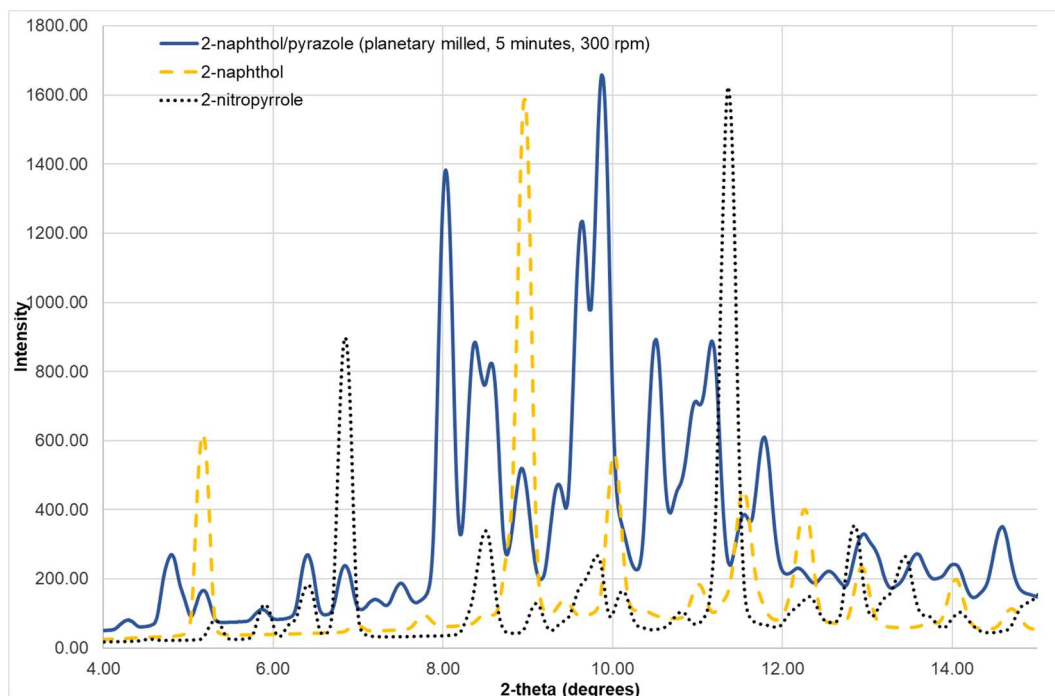


Figure C.11 - Powder x-ray pattern of 2-naphthol/pyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.10 2-naphthol/3-nitropyrazole

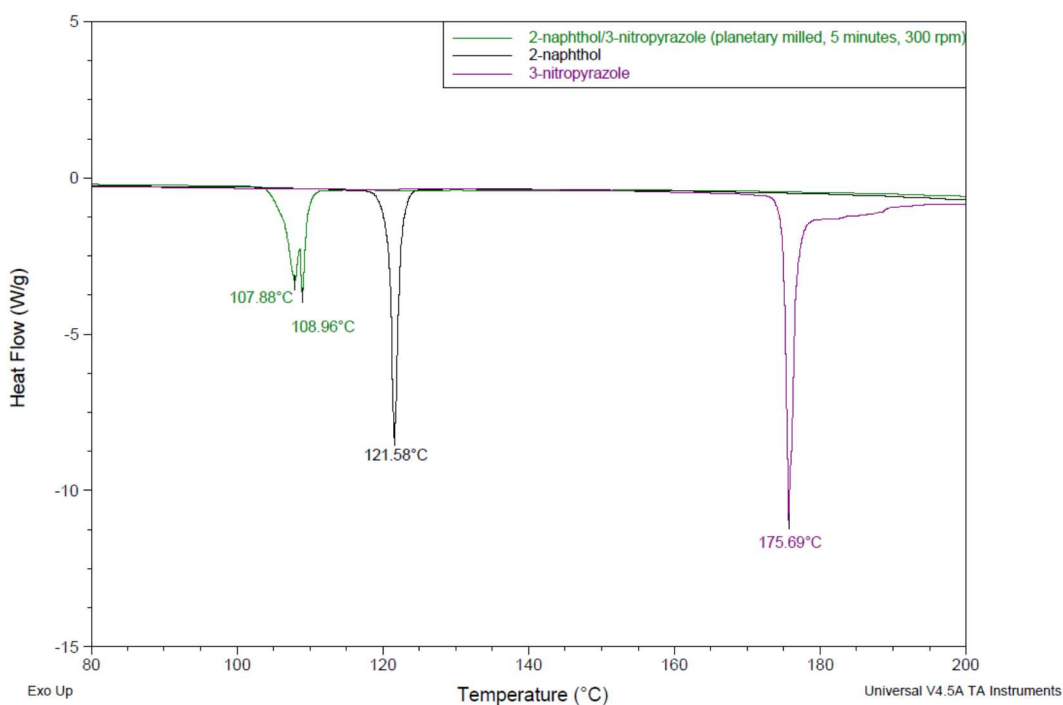


Figure C.12 - Thermal analysis of 2-naphthol/3-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

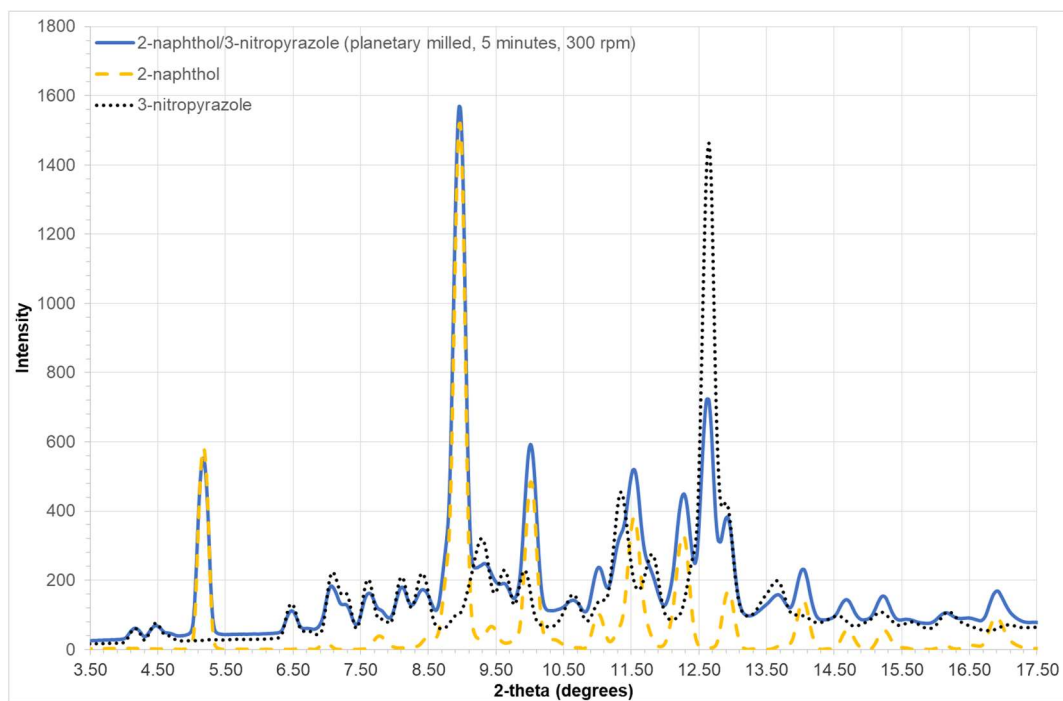


Figure C.13 – Powder x-ray pattern of 2-naphthol/3-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.11 2-naphthol/4-nitropyrazole

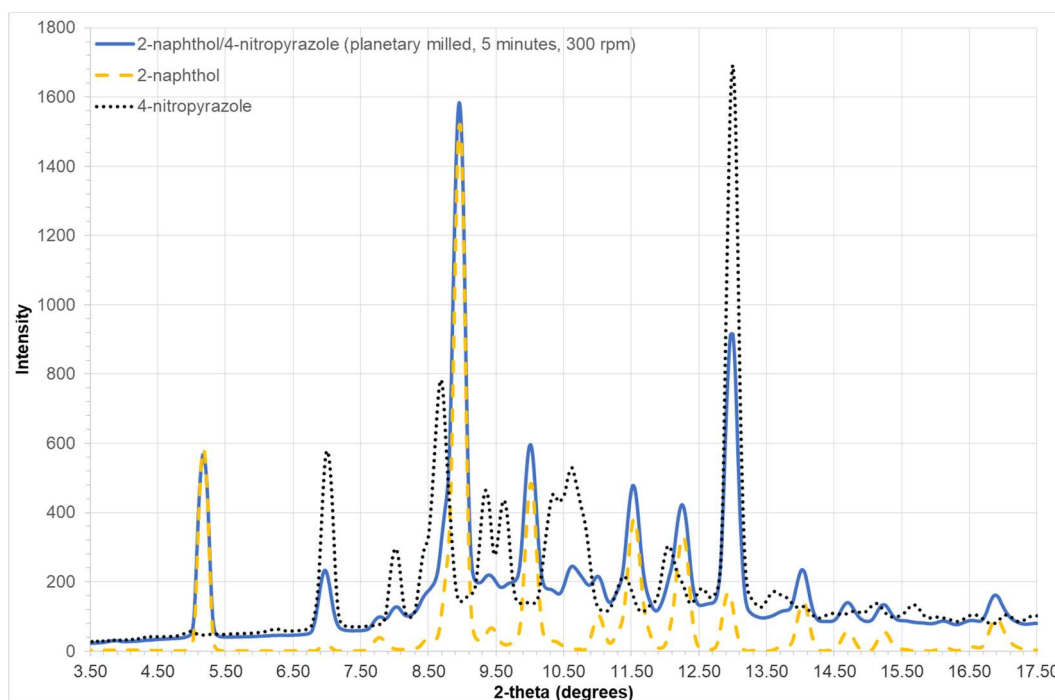


Figure C.14 - Powder x-ray pattern of 2-naphthol/4-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.12 2-naphthol/5-methylpyrazole

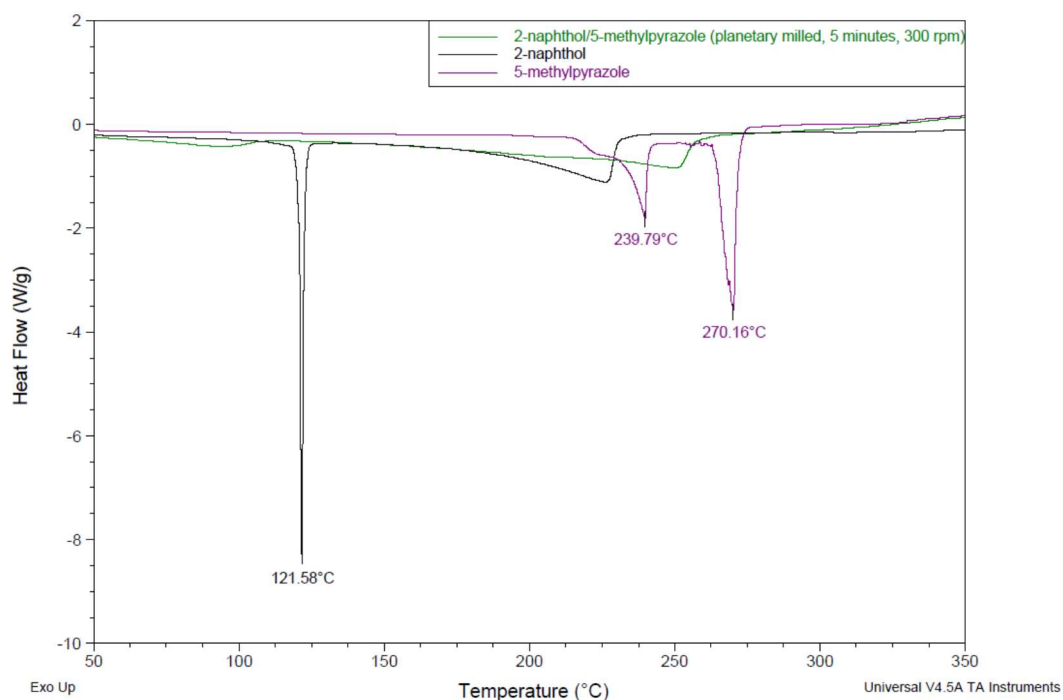


Figure C.15 - Thermal analysis of 2-naphthol/5-methylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.13 2-naphthol/pyrazol-4-amine

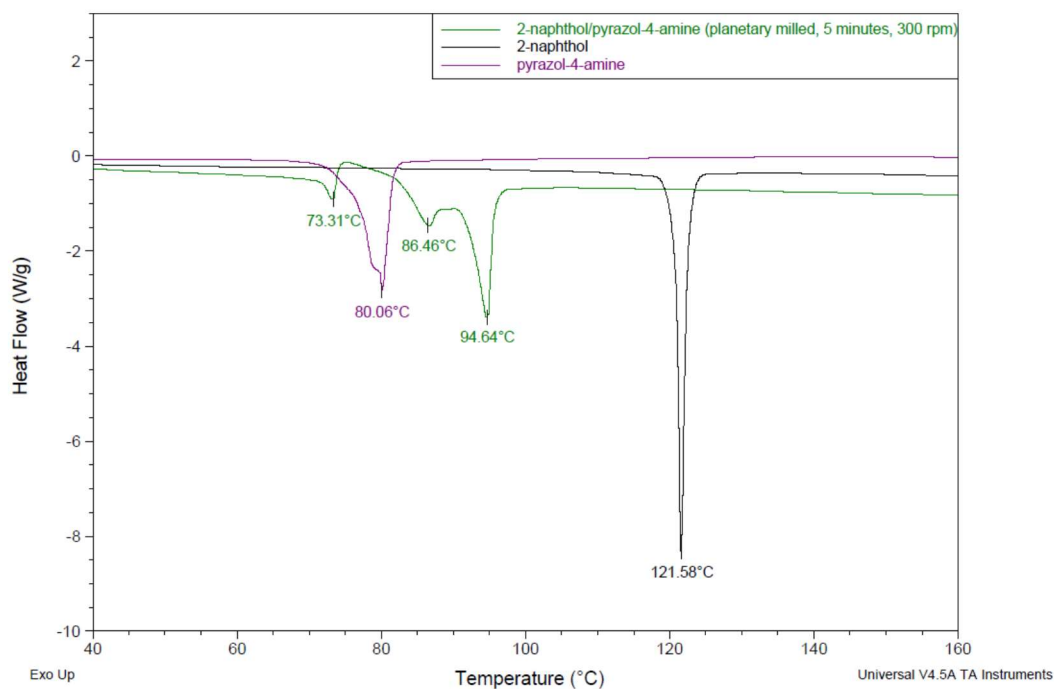


Figure C.16 - Thermal analysis of 2-naphthol/pyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

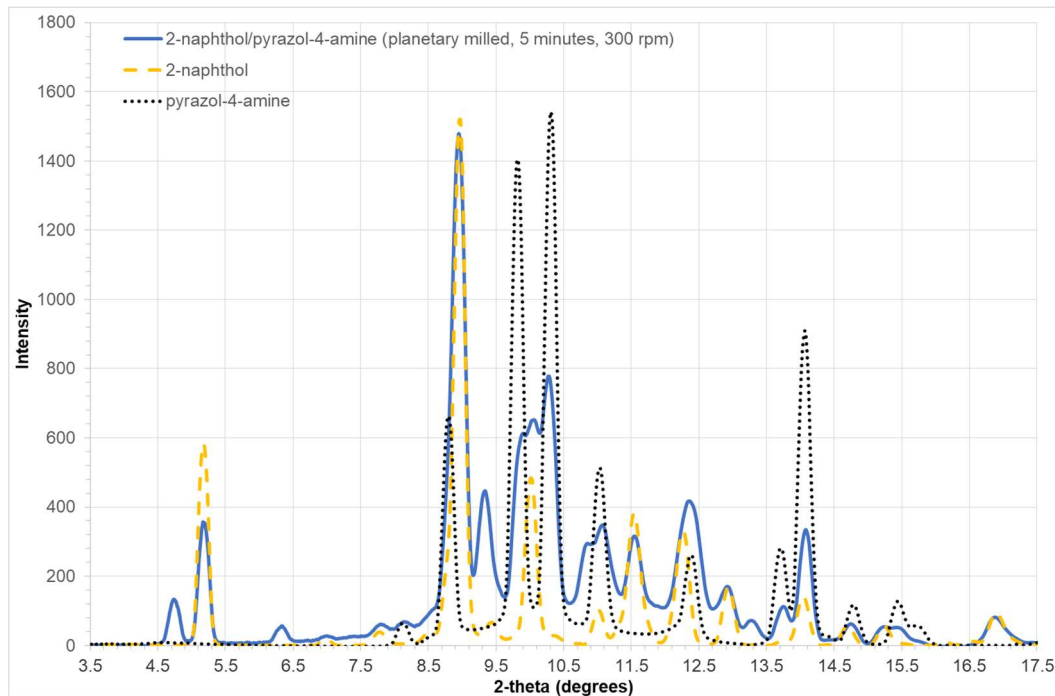


Figure C.17 – Powder x-ray pattern of 2-naphthol/pyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

C.14 2-naphthol/3-bromopyrazole

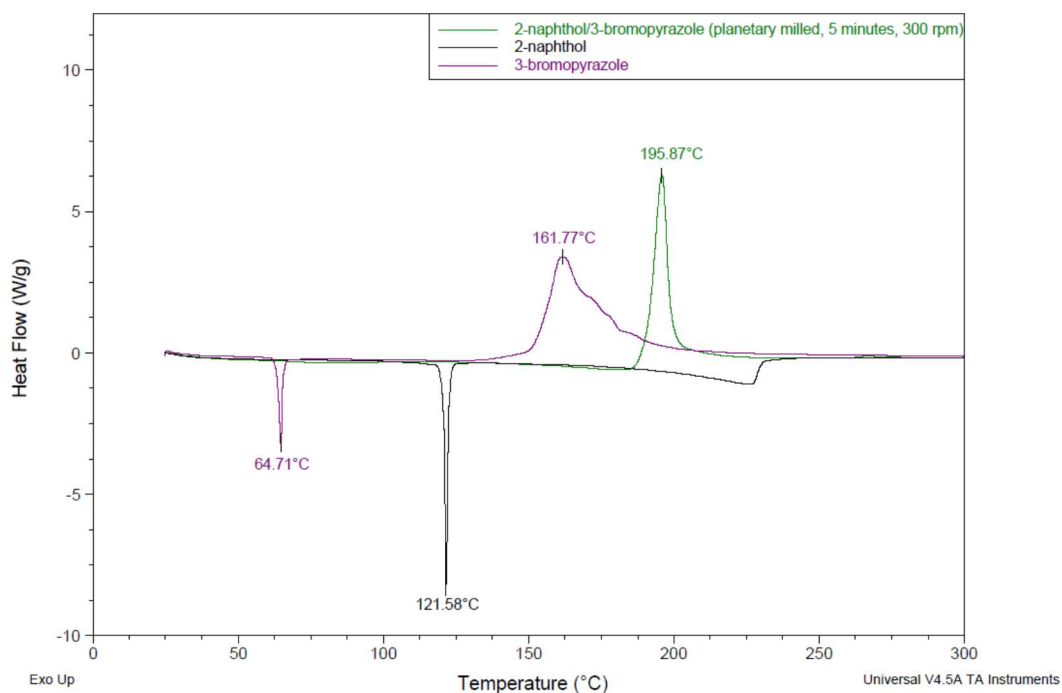


Figure C.18 - Thermal analysis of 2-naphthol/3-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

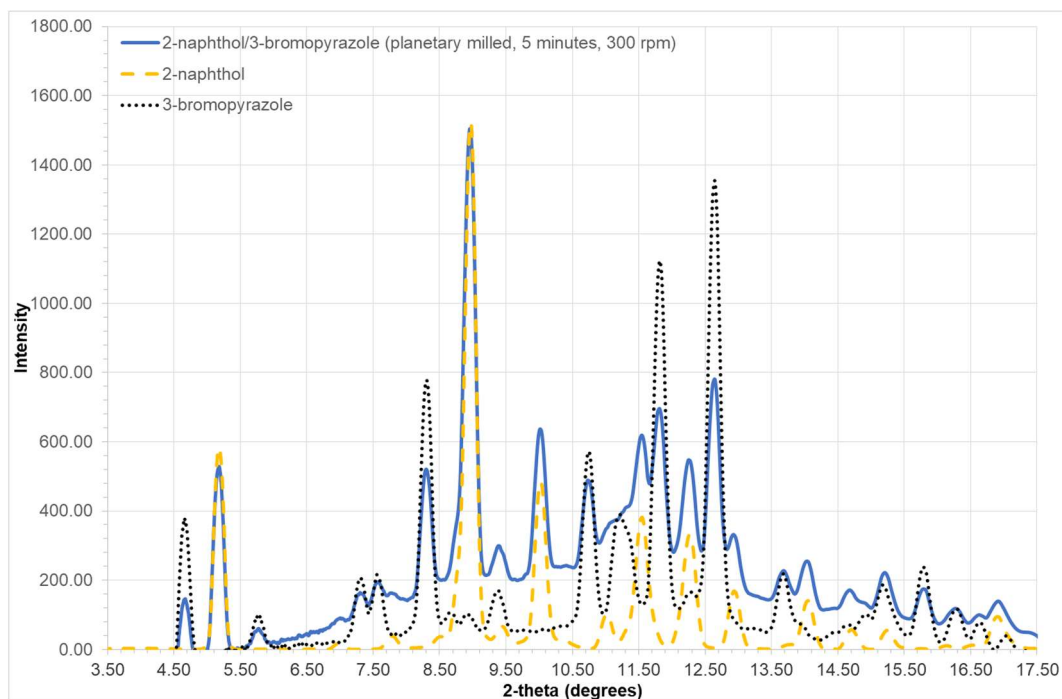


Figure C.19 – Powder x-ray pattern of 2-naphthol/3-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.15 2-naphthol/4-bromopyrazole

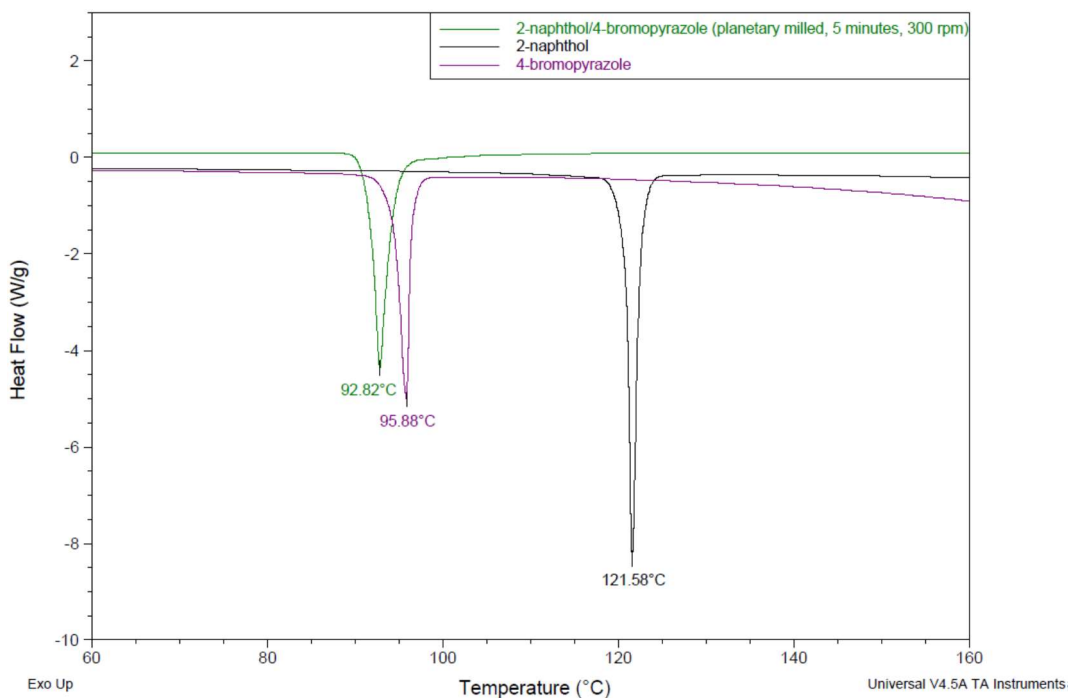


Figure C.20 - Thermal analysis of 2-naphthol/4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

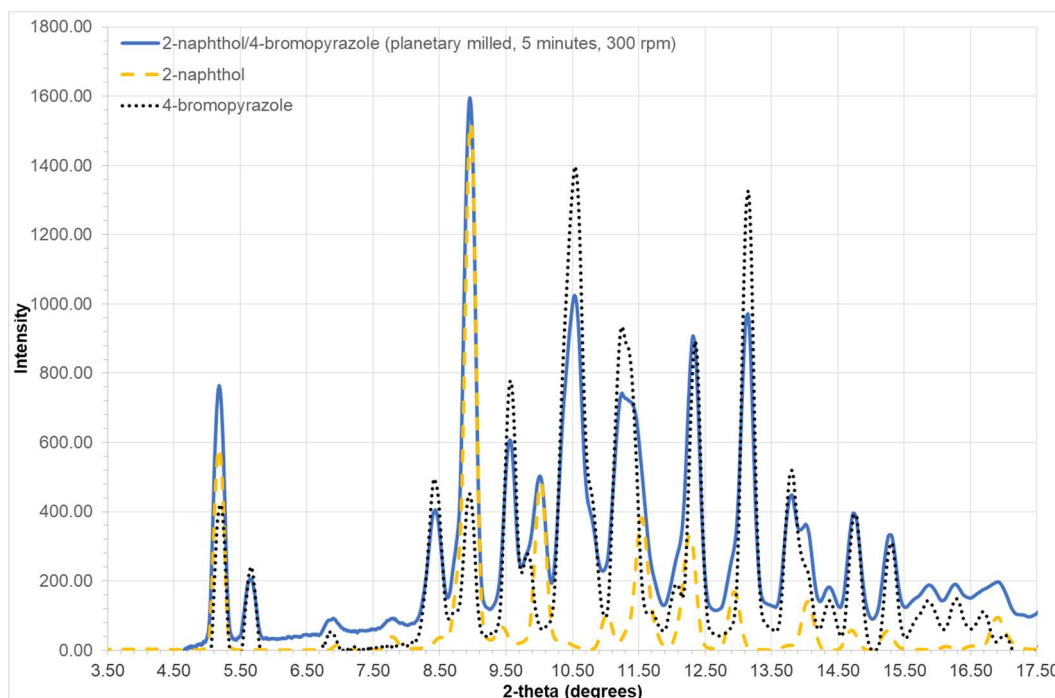


Figure C.21 – Powder x-ray pattern of 2-naphthol/4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.16 2-naphthol/3,4-dimethylpyrazole

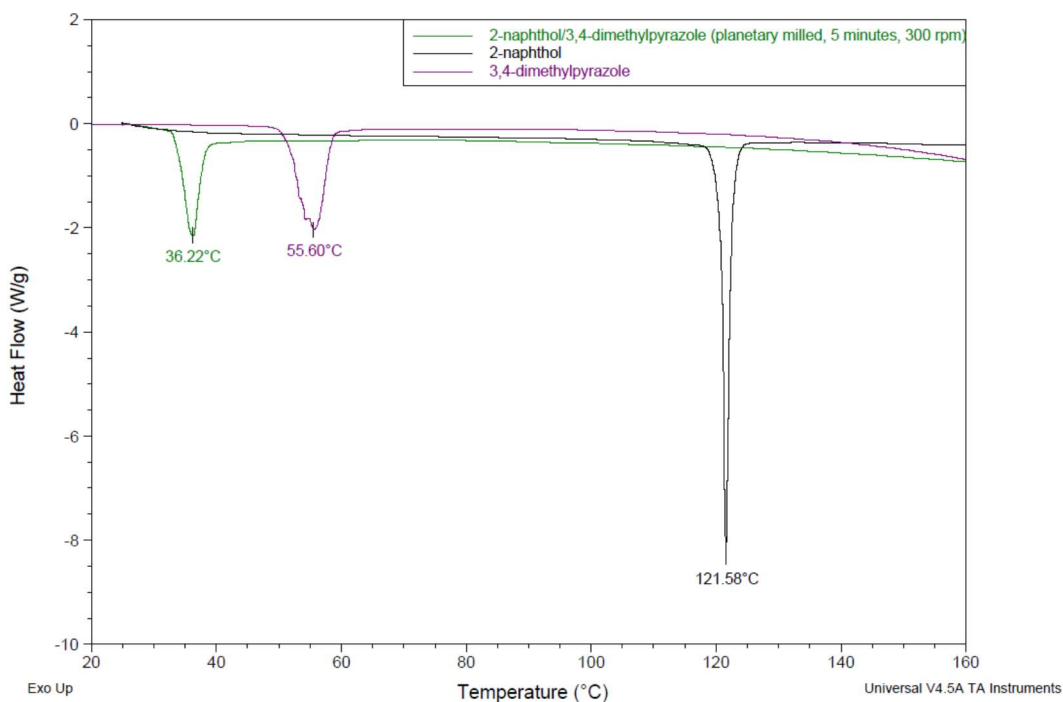


Figure C.22 - Thermal analysis of 2-naphthol/3,4-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

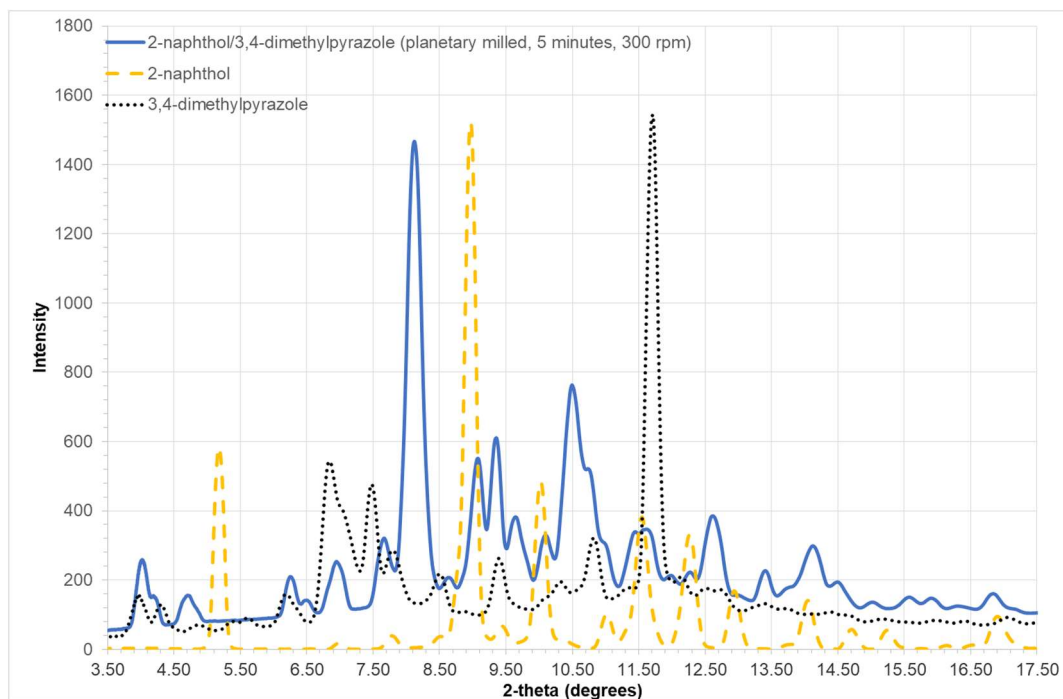


Figure C.23 – Powder x-ray pattern of 2-naphthol/3,4-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.17 2-naphthol/3,5-dimethylpyrazole

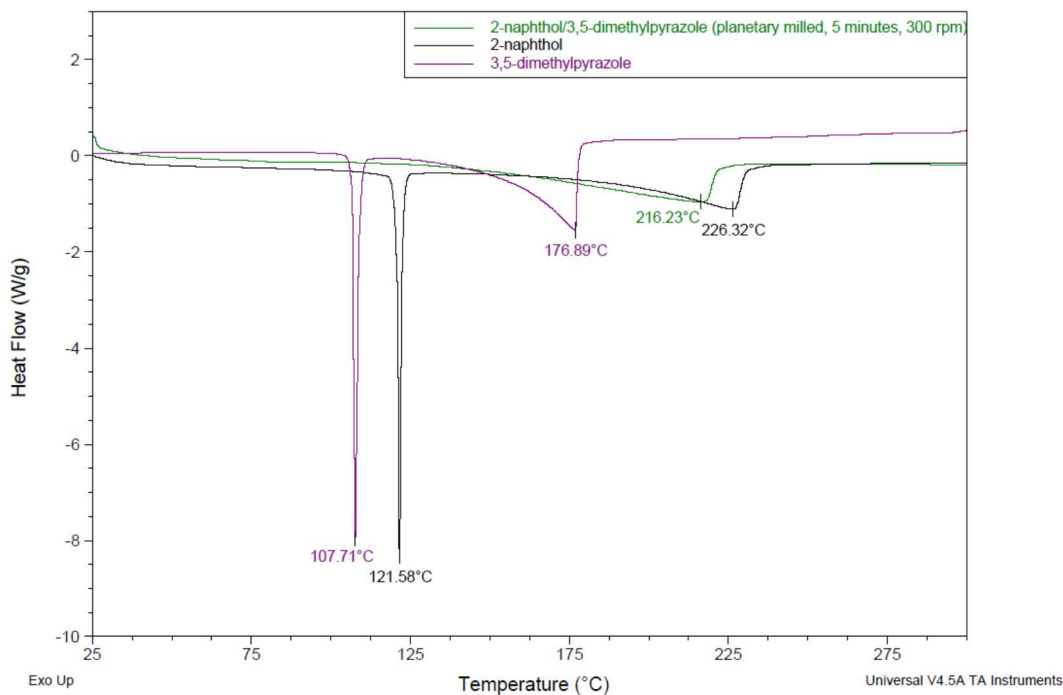


Figure C.24 - Thermal analysis of 2-naphthol/3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm. No melt is observed for the mixed system

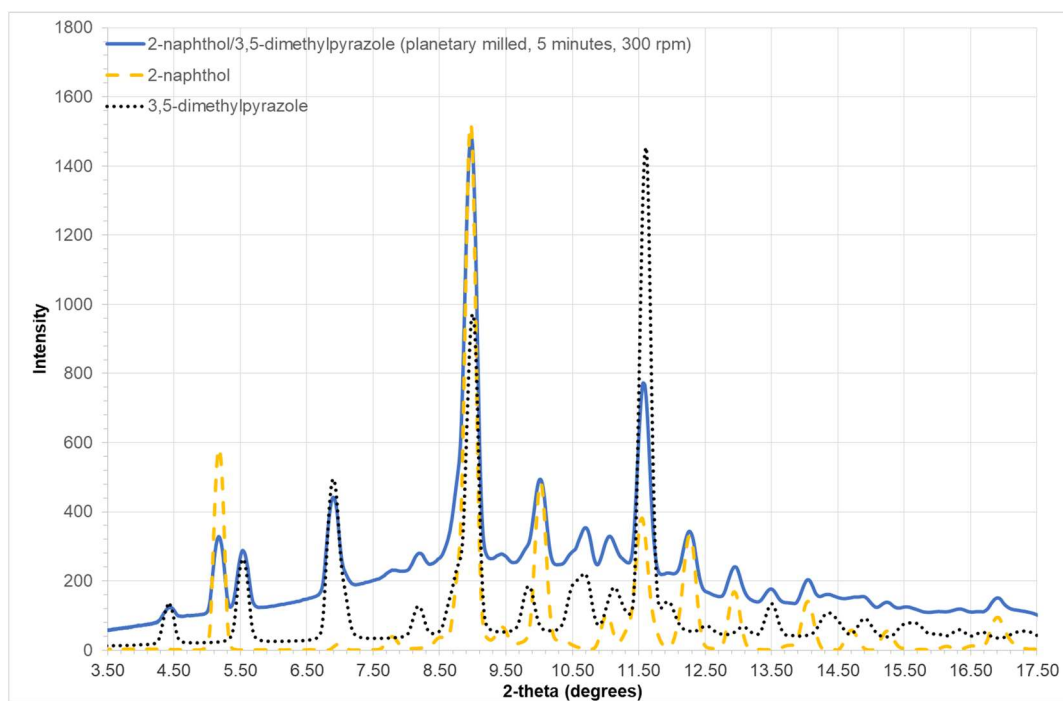


Figure C.25 – Powder x-ray pattern of 2-naphthol/3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.18 2-naphthol/3,4,5-tribromopyrazole

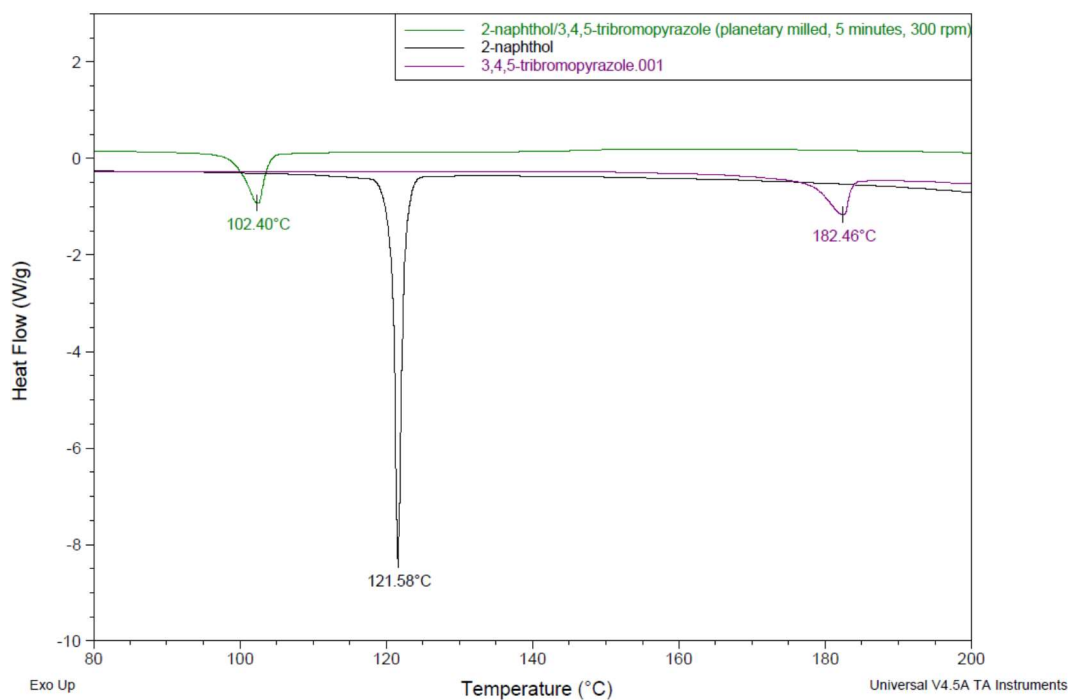


Figure C.26 - Thermal analysis of 2-naphthol/3,4,5-tribromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

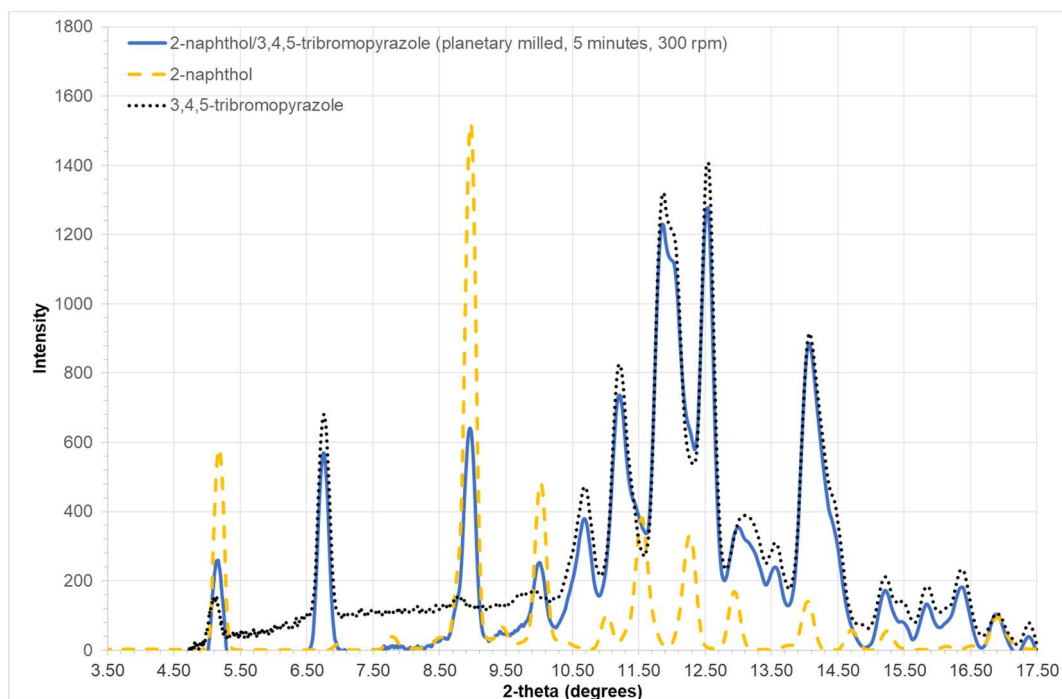


Figure C.27 – Powder x-ray pattern of 2-naphthol/3,4,5-tribromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.19 2-naphthol/3-methyl-5-nitropyrazole

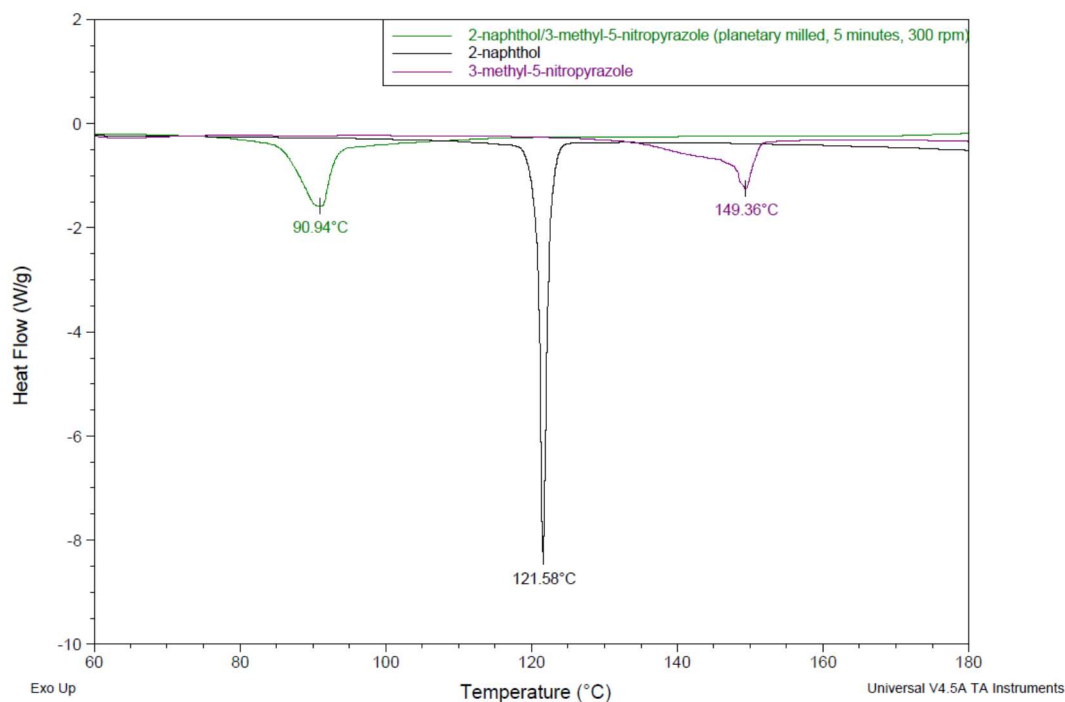


Figure C.28 - Thermal analysis of 2-naphthol/3-methyl-5-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

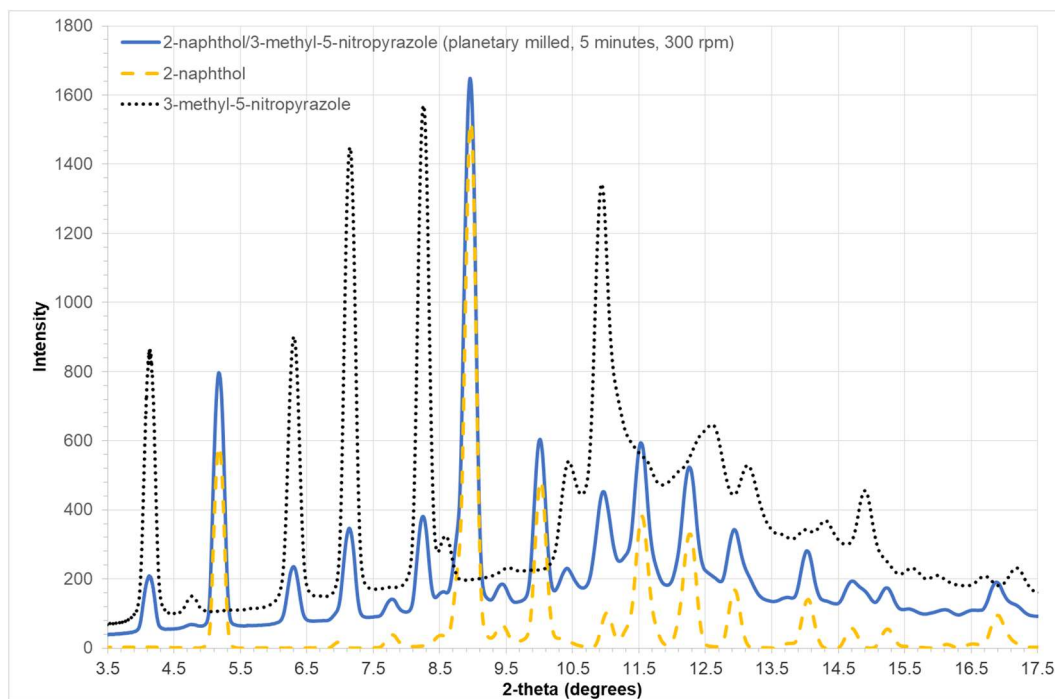


Figure C.29 – Powder x-ray pattern of 2-naphthol/3-methyl-5-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.20 2-naphthol/5-methylpyrazol-3-amine

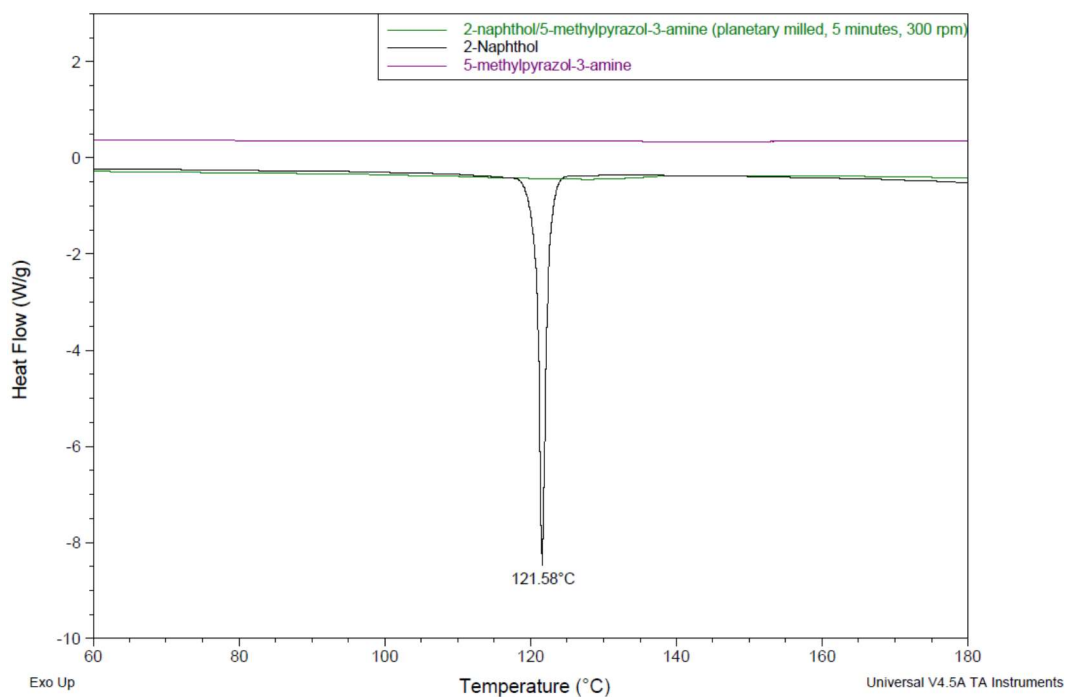


Figure C.30 - Thermal analysis of 2-naphthol/5-methylpyrazol-3-amine produced by planetary milling for 5 minutes at 300 rpm. Both 5-methylpyrazol-3-amine and the mixed system are liquids and did not display melts.

C.21 2-naphthol/4-bromopyrazol-3-amine

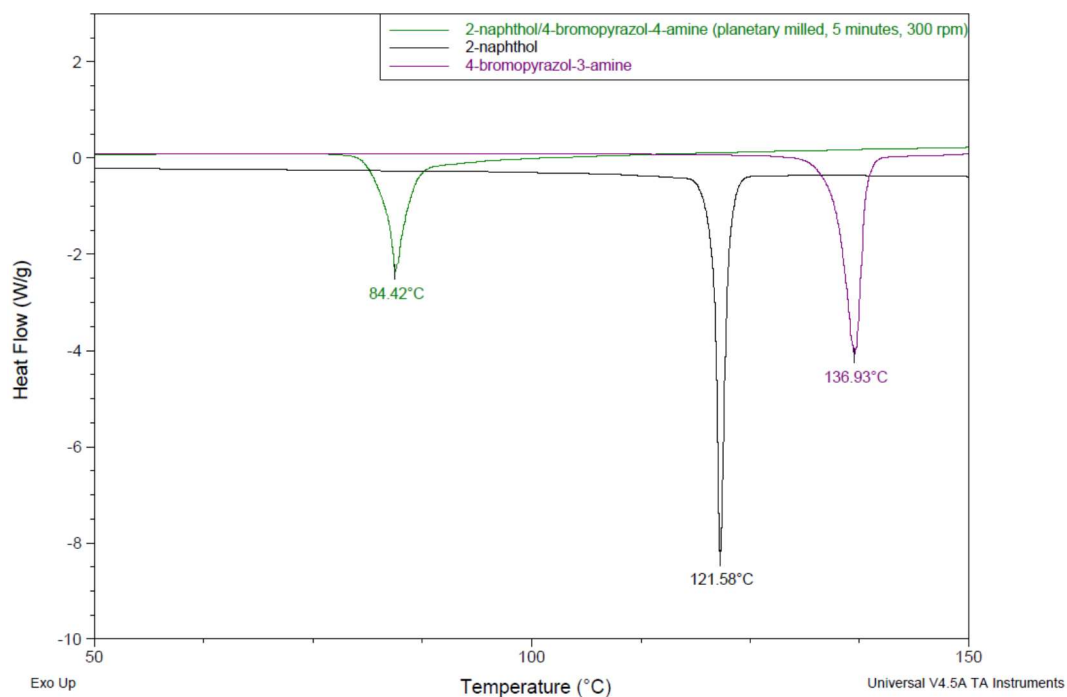


Figure C.31 - Thermal analysis of 2-naphthol/4-bromopyrazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

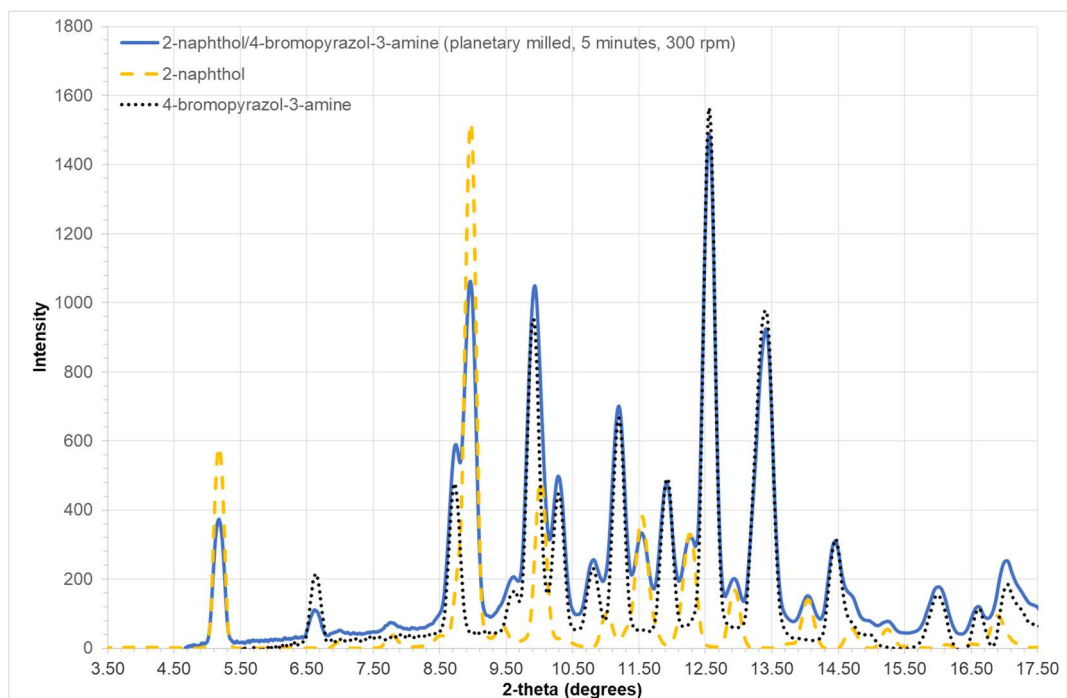


Figure C.32 – Powder x-ray pattern of 2-naphthol/4-bromopyrazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

C.22 2-naphthol/3-bromopyrazol-5-amine

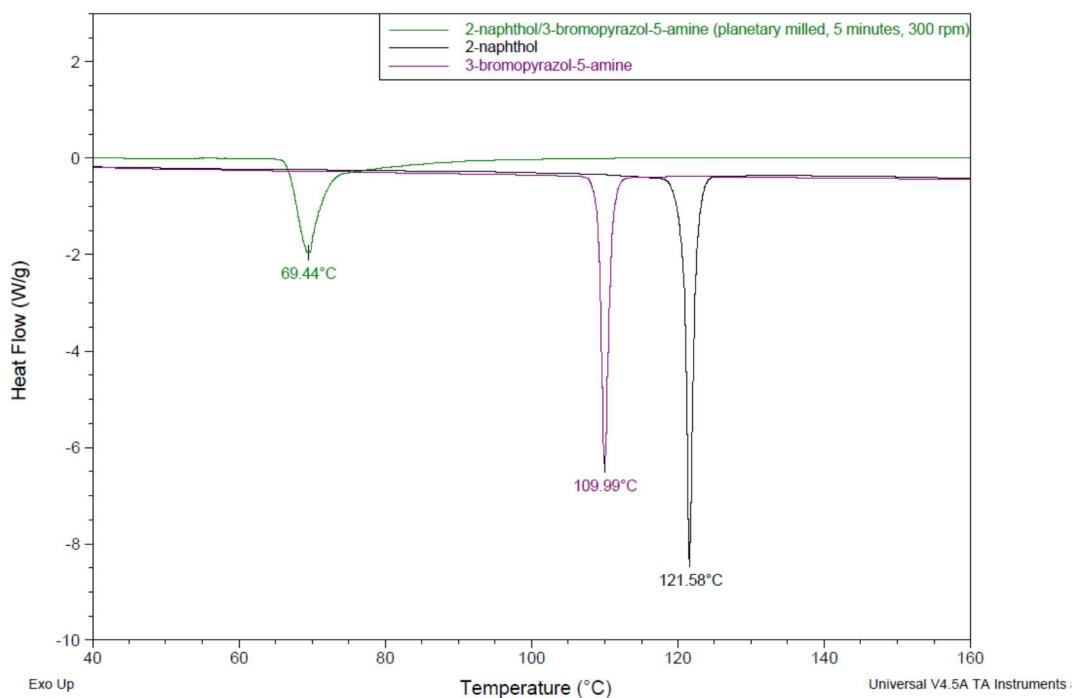


Figure C.33 - Thermal analysis of 2-naphthol/3-bromopyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

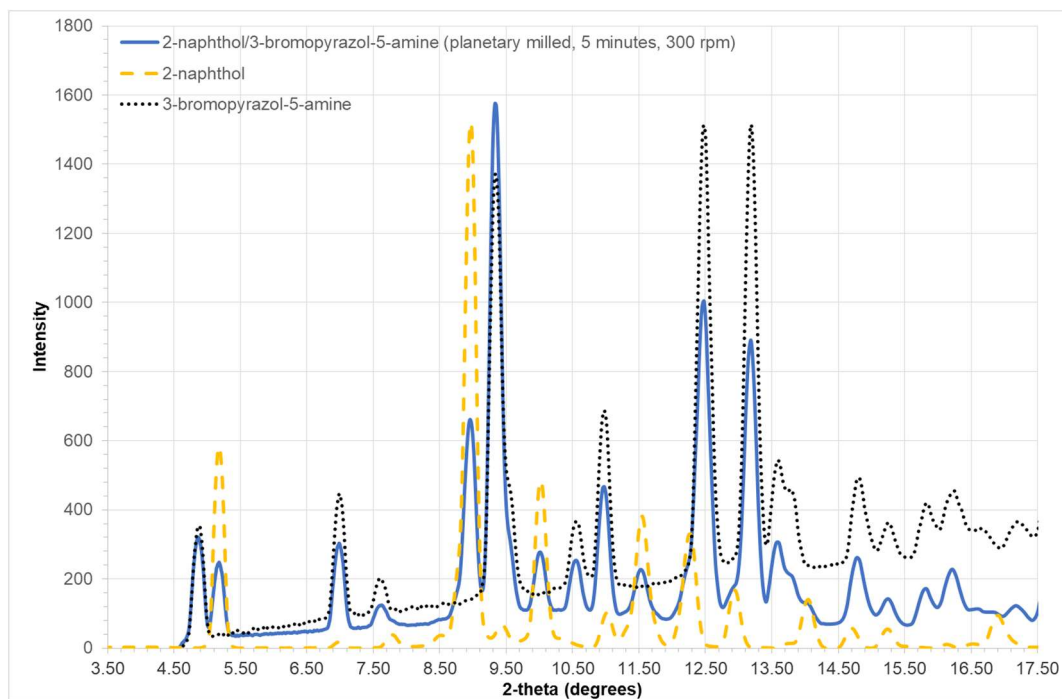


Figure C.34 – Powder x-ray pattern of 2-naphthol/3-bromopyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

C.23 2-naphthol/3,5-dimethylpyrazol-4-amine

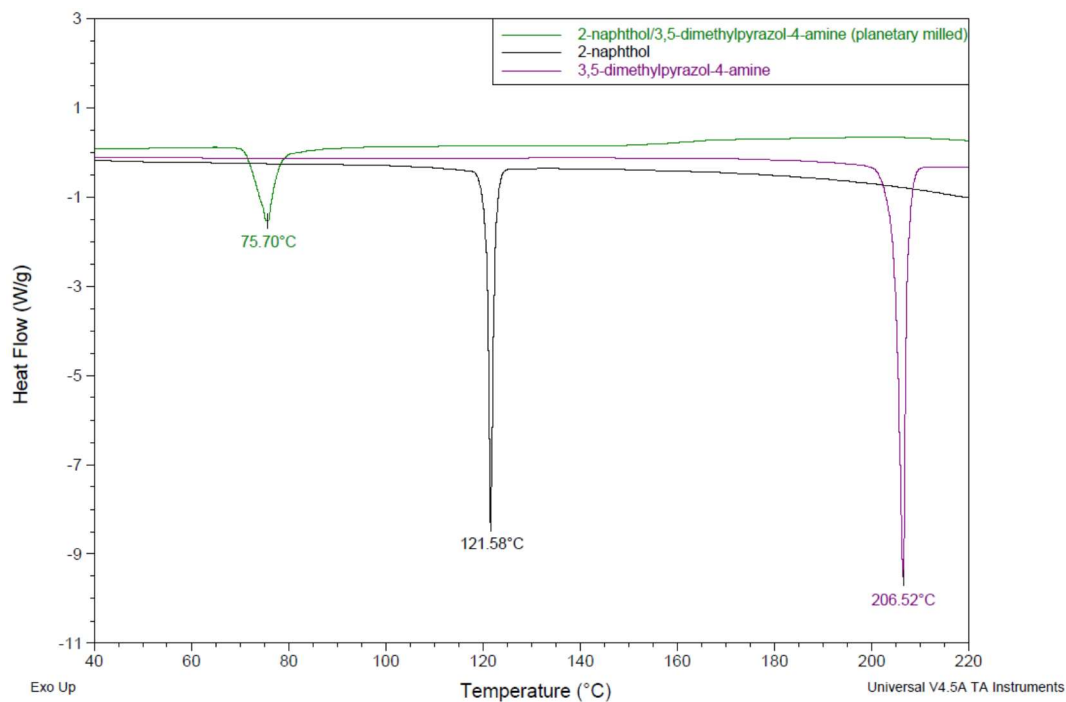


Figure C.35 - Thermal analysis of 2-naphthol/3,5-dimethylpyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

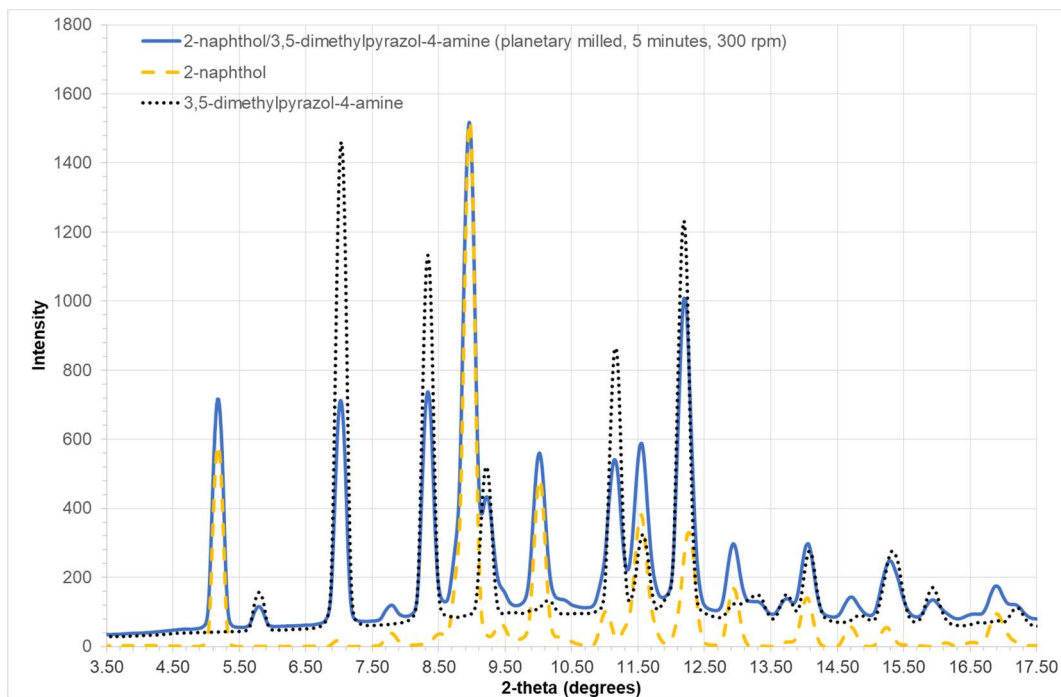


Figure C.36 – Powder x-ray pattern of 2-naphthol/3,5-dimethylpyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

C.24 2-naphthol/3,4-dimethylpyrazol-5-amine

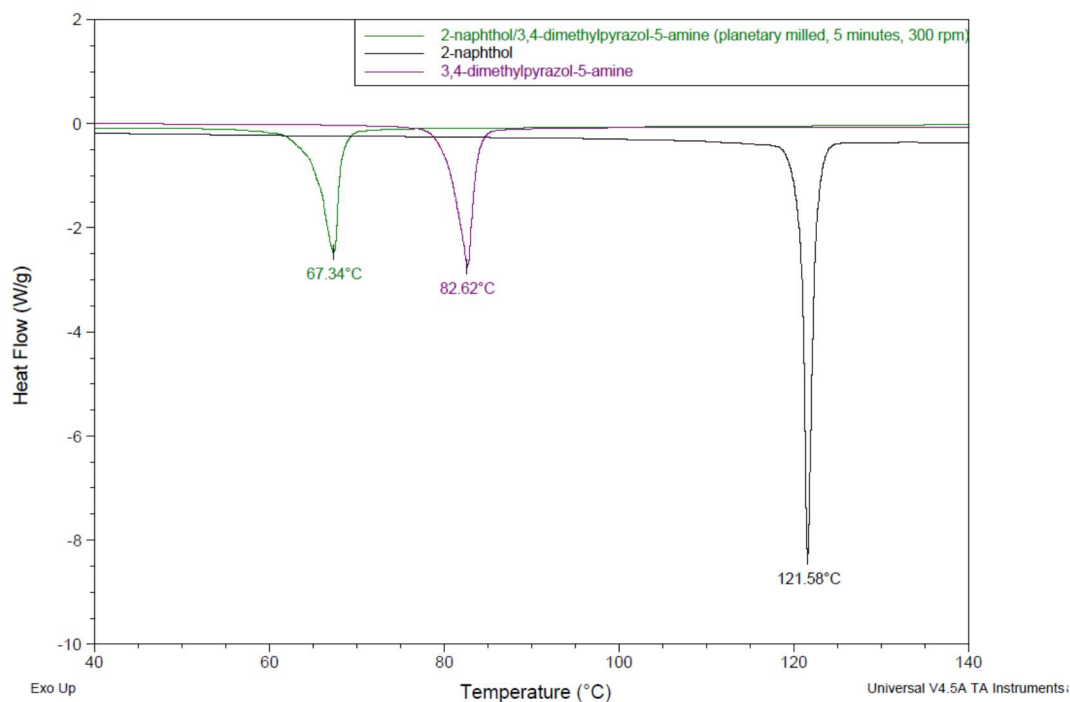


Figure C.37 - Thermal analysis of 2-naphthol/3,4-dimethylpyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

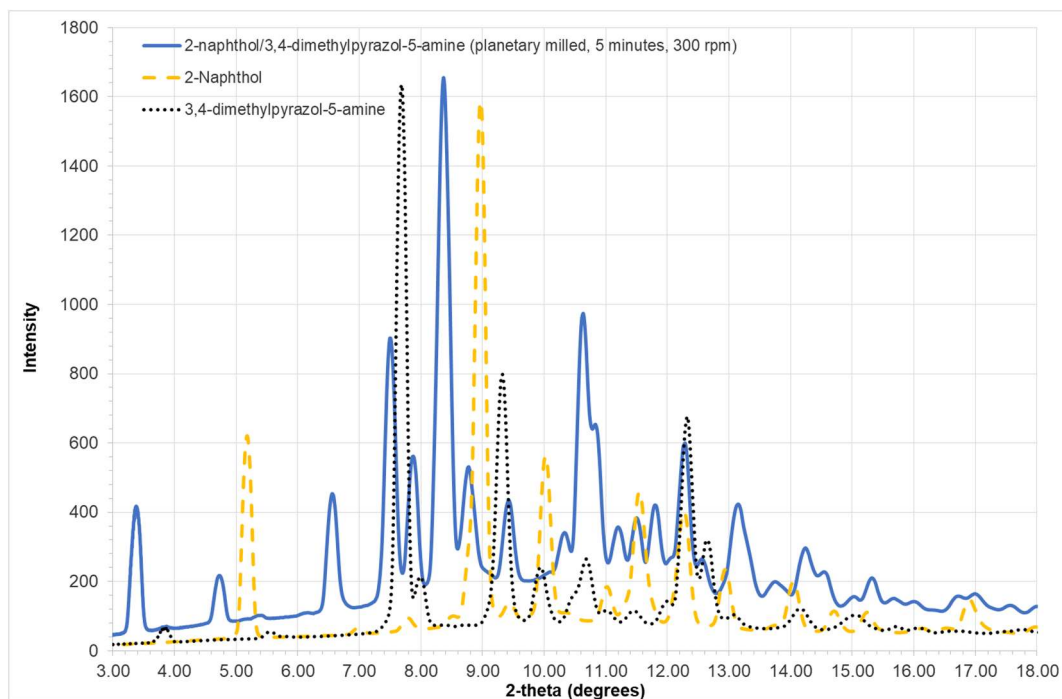


Figure C.38 – Powder x-ray pattern of 2-naphthol/3,4-dimethylpyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

C.25 2-naphthol/3-methyl-4-bromopyrazole

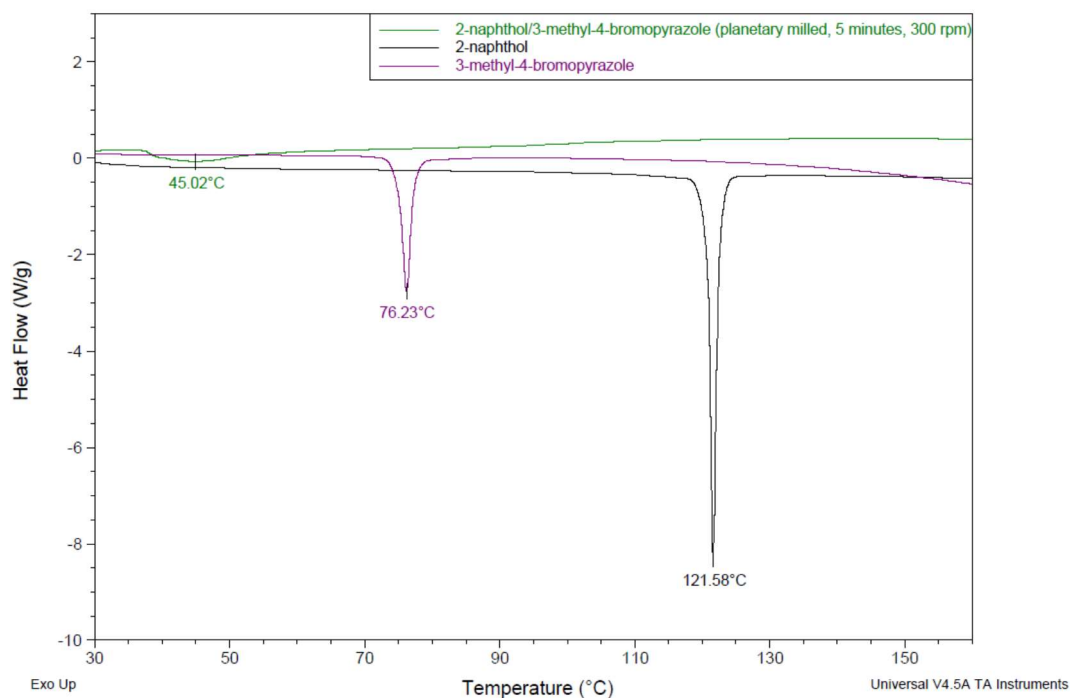


Figure C.39 - Thermal analysis of 2-naphthol/3-methyl-4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

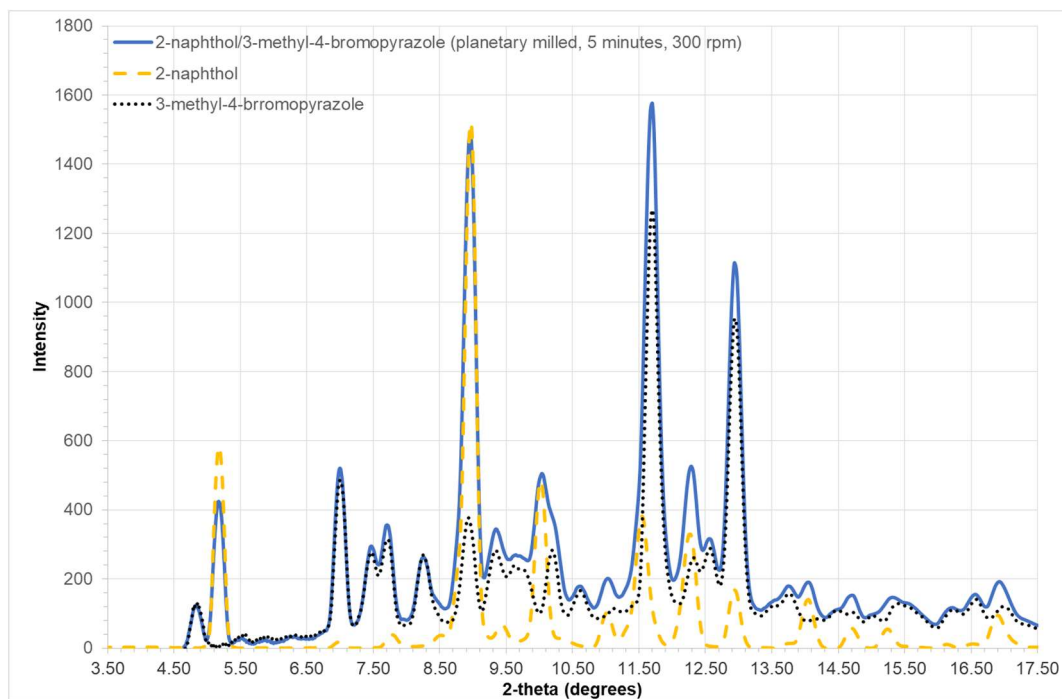


Figure C.40 – Powder x-ray pattern of 2-naphthol/3-methyl-4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.26 2-naphthol/3-bromo-5-methylpyrazole

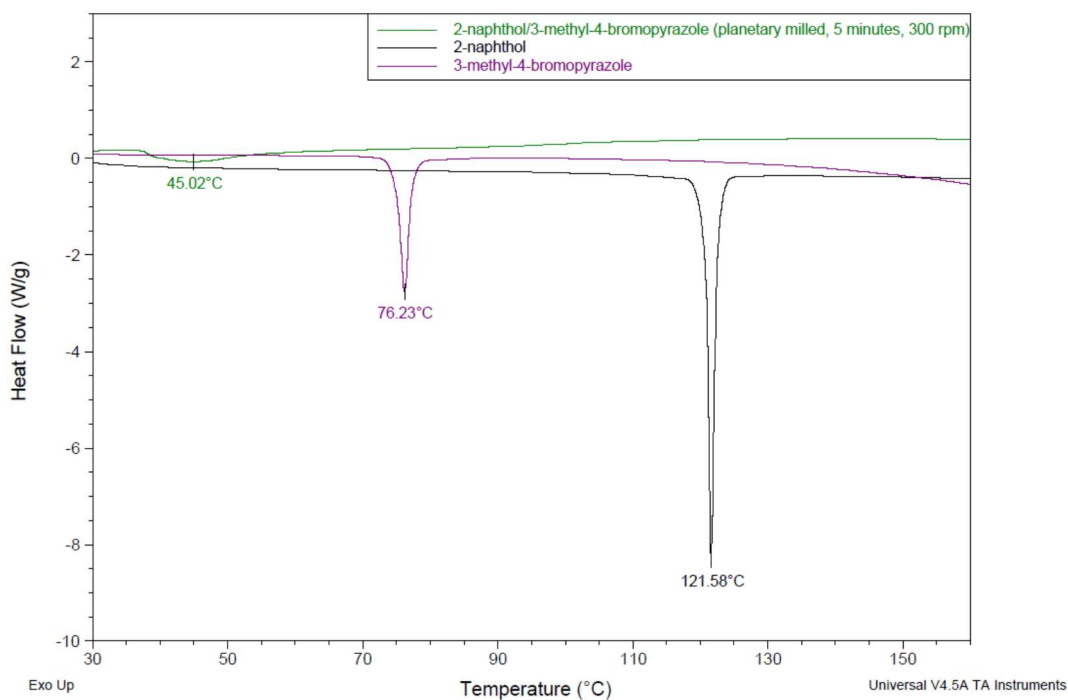


Figure C.41 - Thermal analysis of 2-naphthol/3-bromo-5-methylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

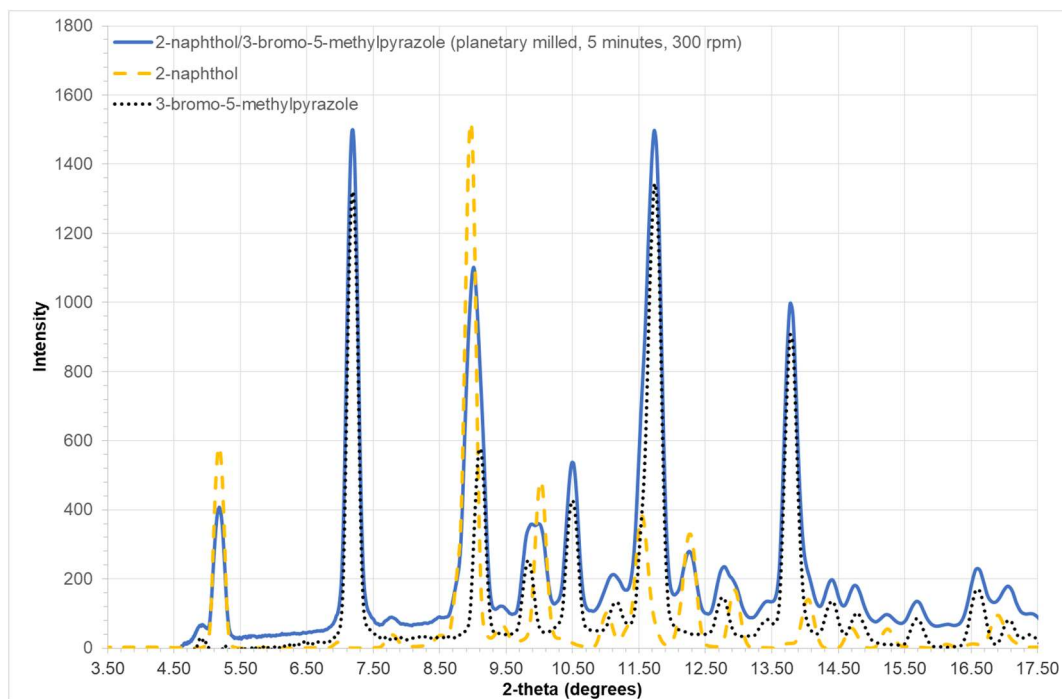


Figure C.42 – Powder x-ray pattern of 2-naphthol/3-bromo-5-methylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.27 2-naphthol/4-bromo-3,5-dimethylpyrazole

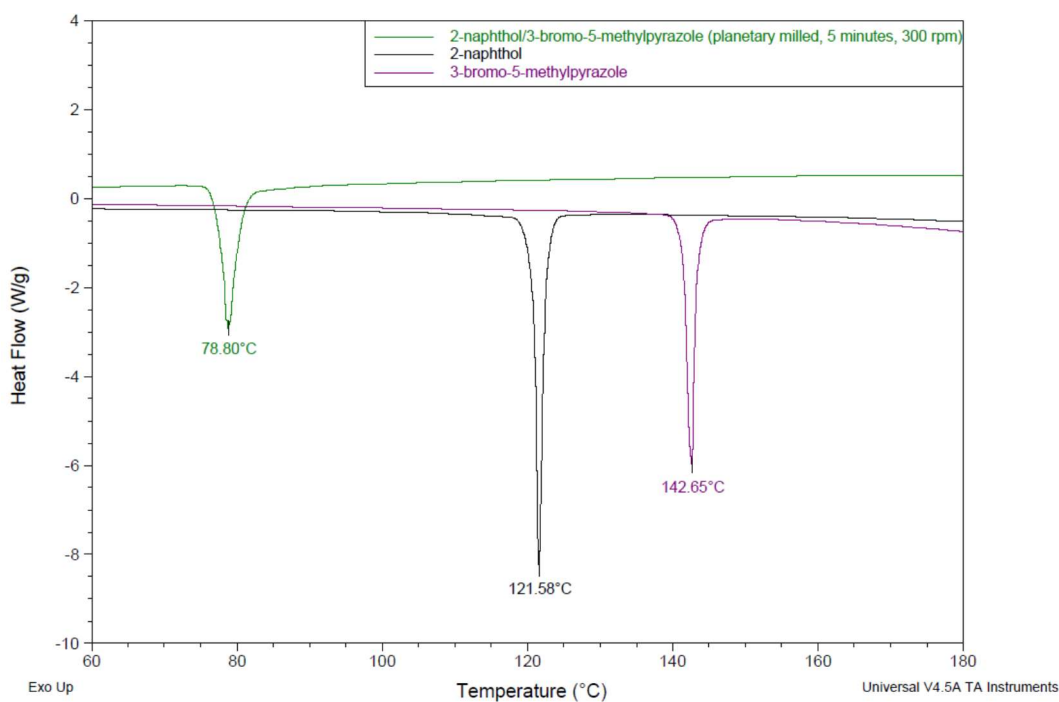


Figure C.43 - Thermal analysis of 2-naphthol/4-bromo-3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

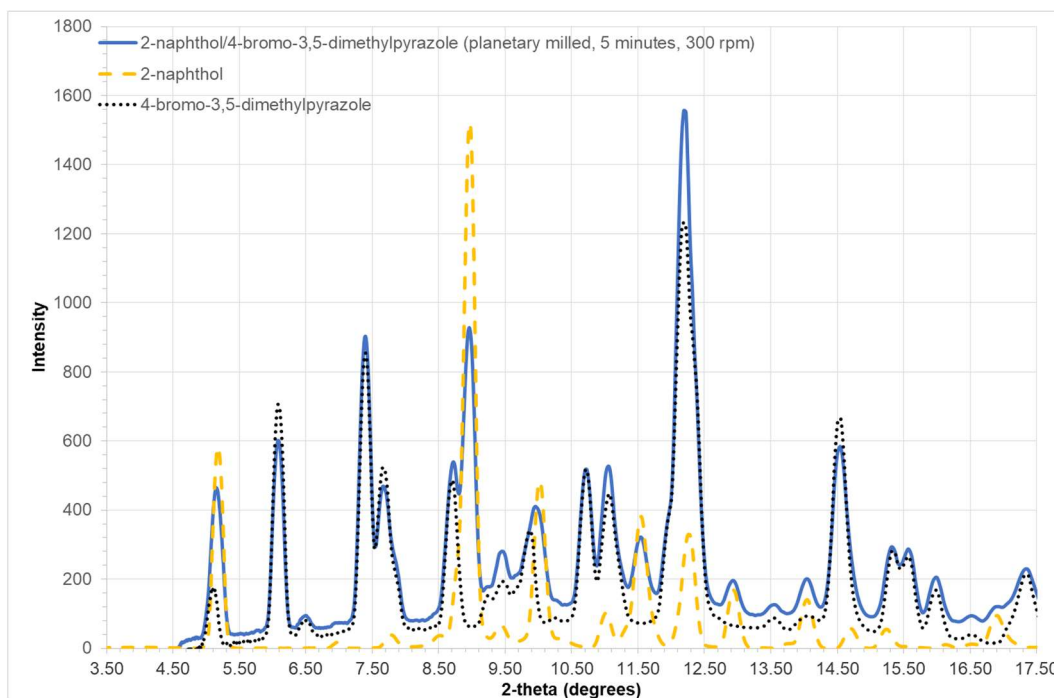


Figure C.44 – Powder x-ray pattern of 2-naphthol/4-bromo-3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

C.28 2-naphthol/imidazole

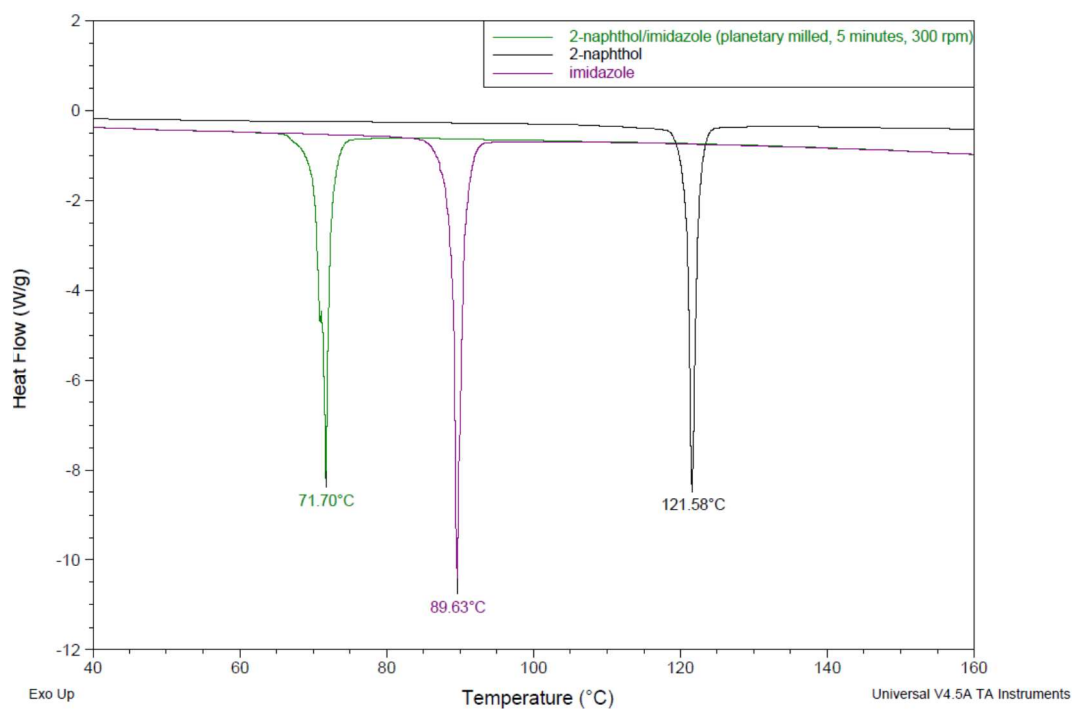


Figure C.45 - Thermal analysis of 2-naphthol/imidazole produced by planetary milling for 5 minutes at 300 rpm.

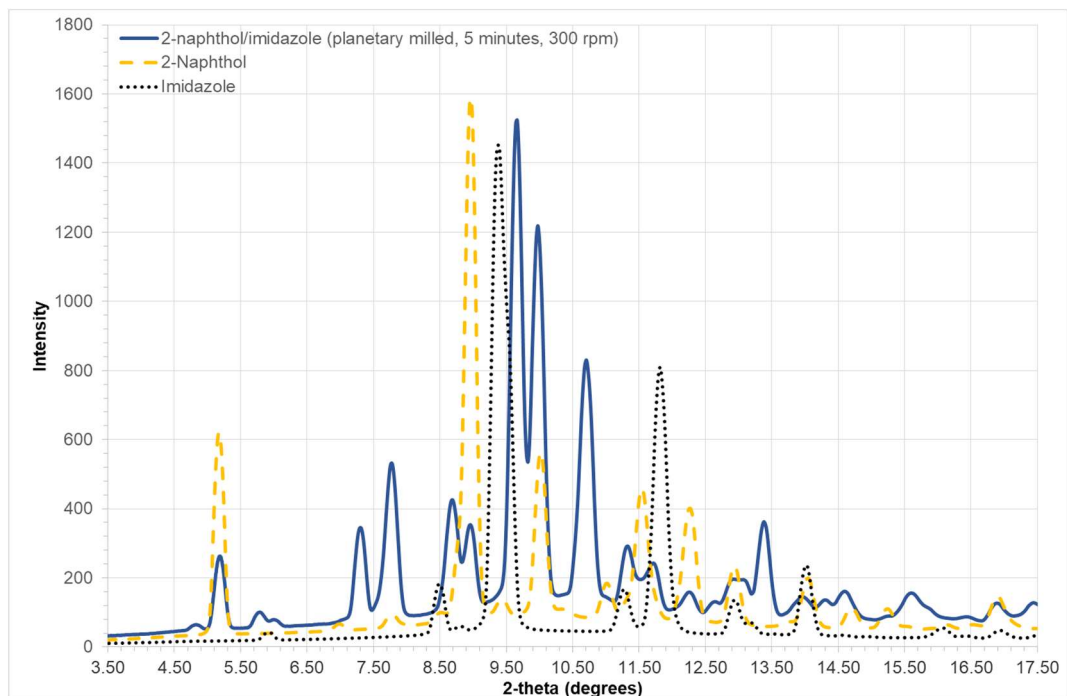


Figure C.46 – Powder x-ray pattern of 2-naphthol/imidazole produced by planetary milling for 5 minutes at 300 rpm.

C.29 2-naphthol/2-nitroimidazole

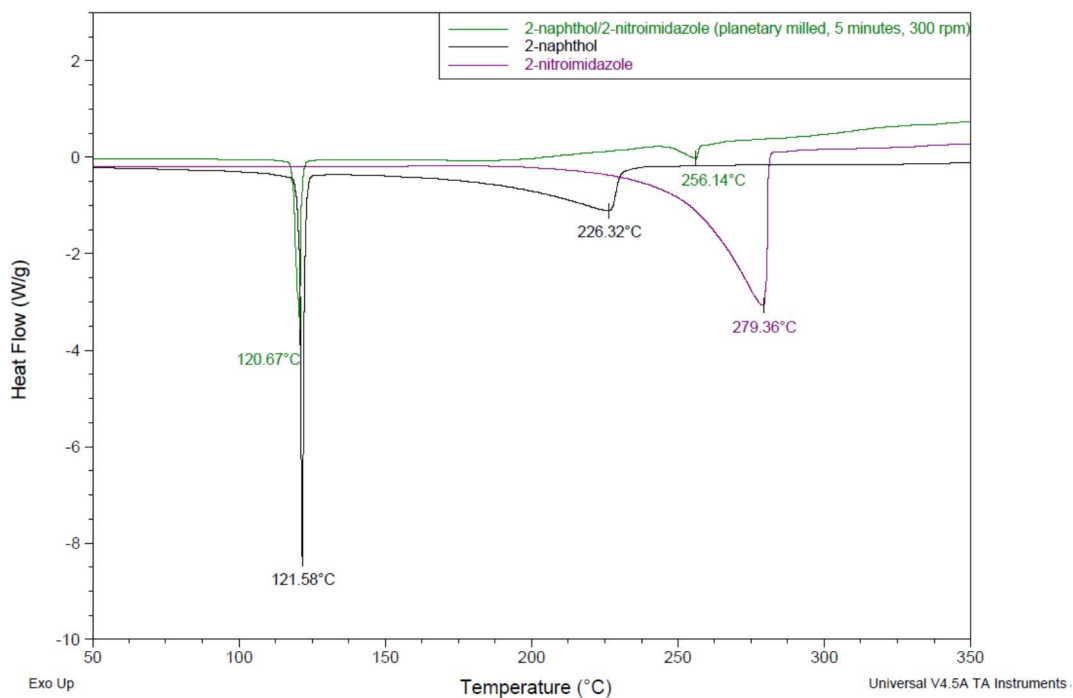


Figure C.47 - Thermal analysis of 2-naphthol/2-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

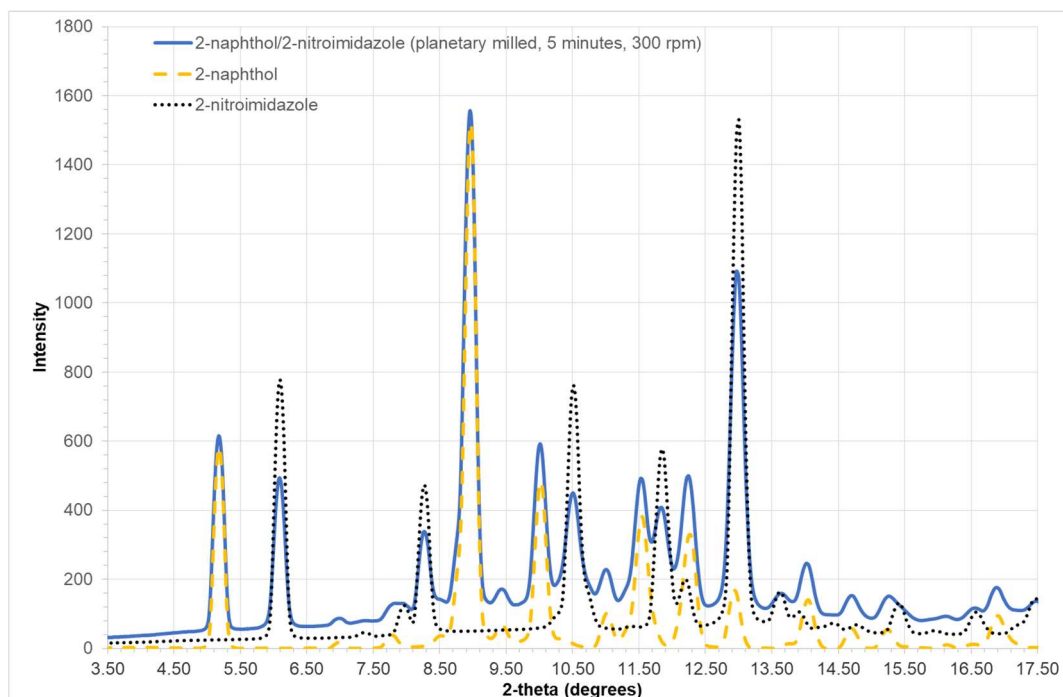


Figure C.48 – Powder x-ray pattern of 2-naphthol/2-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.30 2-naphthol/2-methylimidazole

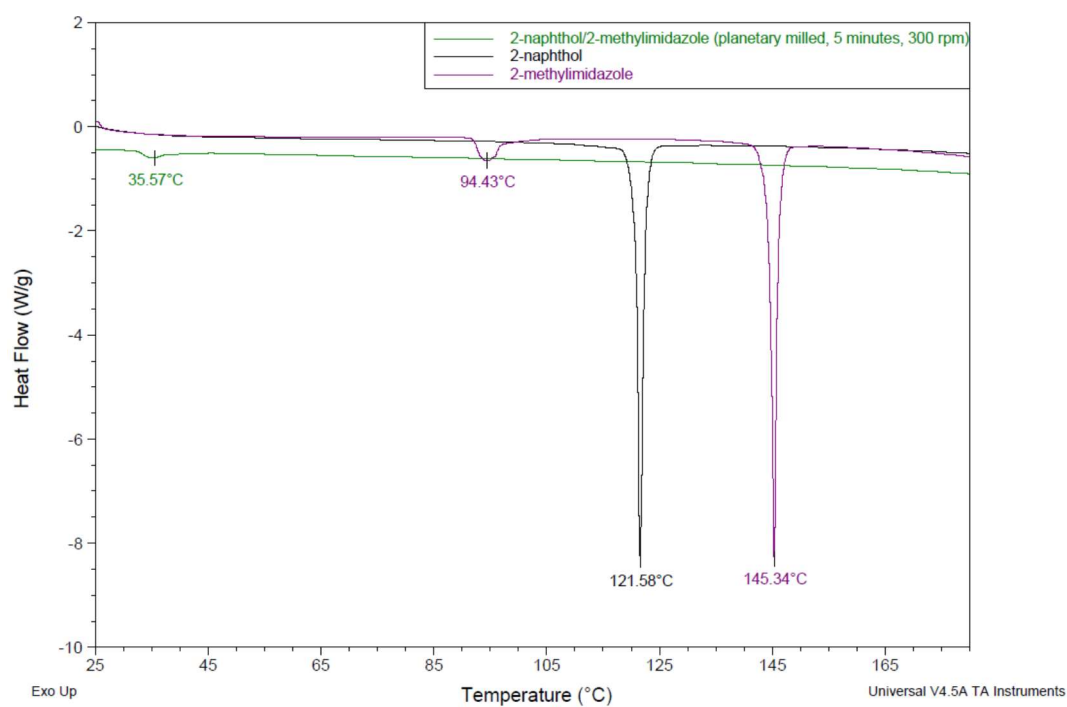


Figure C.49 - Thermal analysis of 2-naphthol/2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.31 2-naphthol/4-methylimidazole

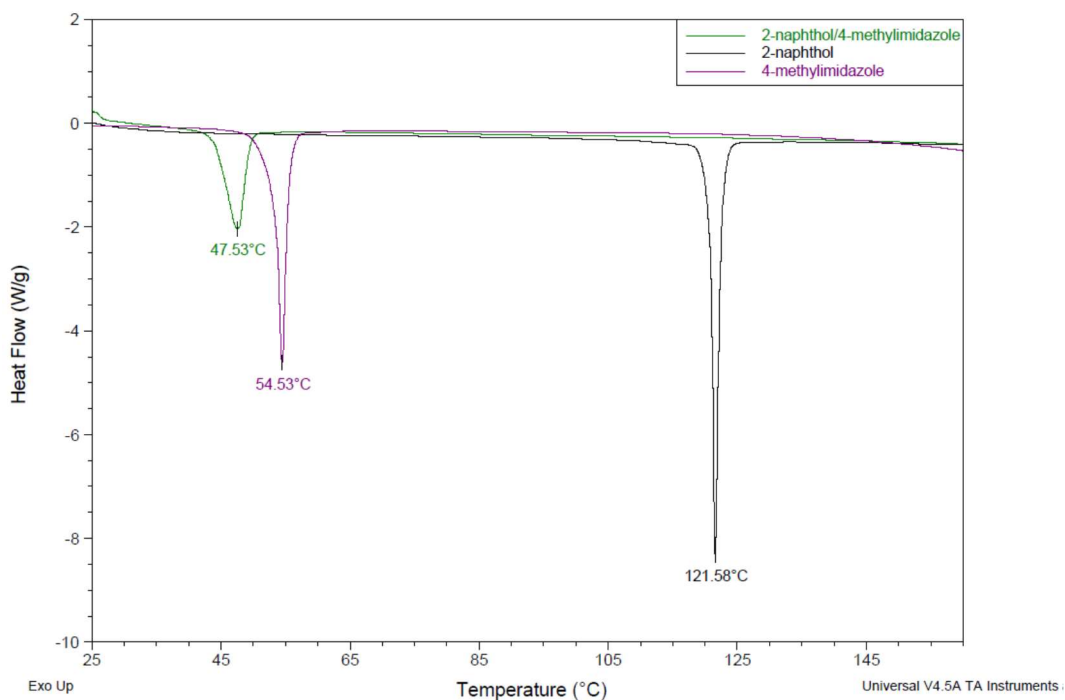


Figure C.50 - Thermal analysis of 2-naphthol/4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

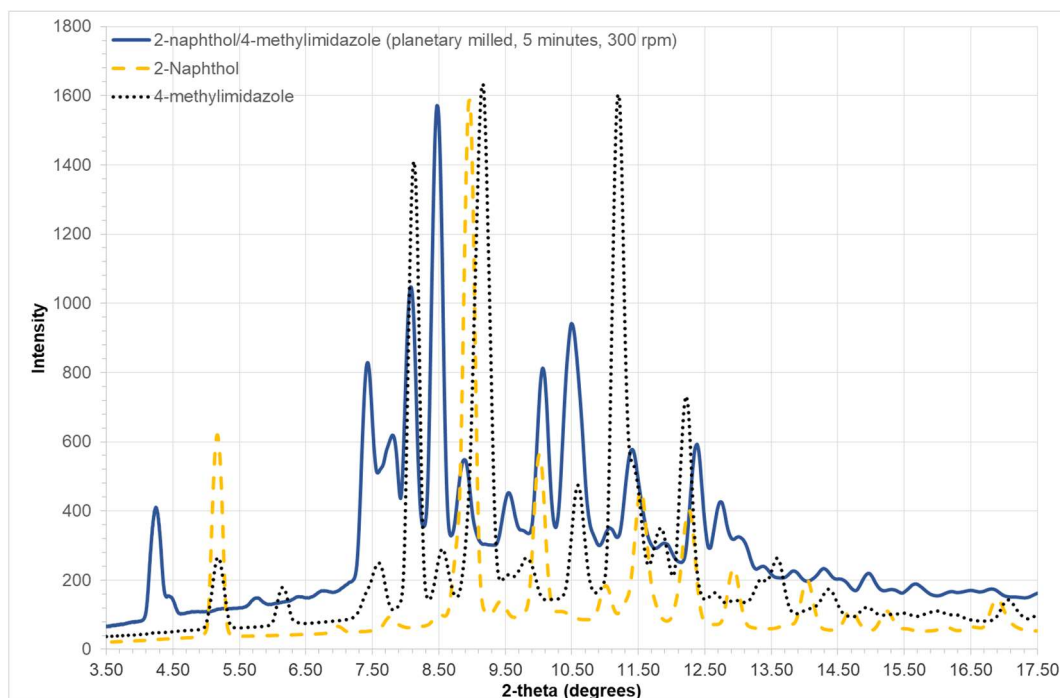


Figure C.51 – Powder x-ray pattern of 2-naphthol/4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.32 2-naphthol/imidazol-2-amine

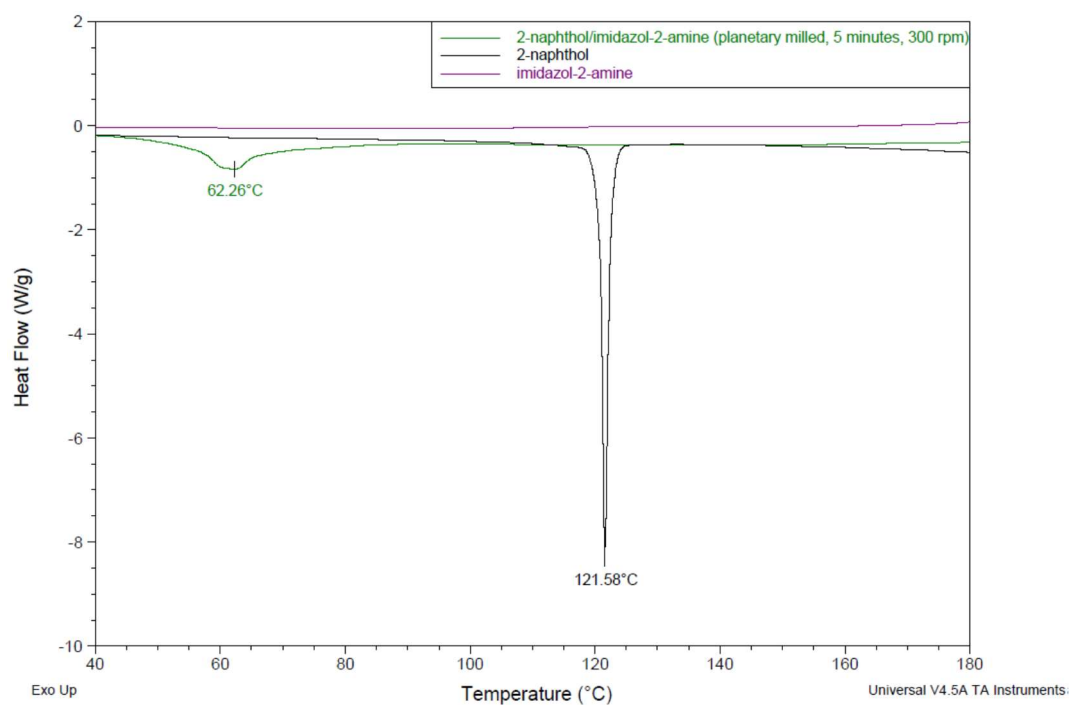


Figure C.52 - Thermal analysis of 2-naphthol/imidazol-2-amine produced by planetary milling for 5 minutes at 300 rpm. Imidazol-2-amine is a liquid and did not display a melt.

C.33 2-naphthol/2-bromoimidazole

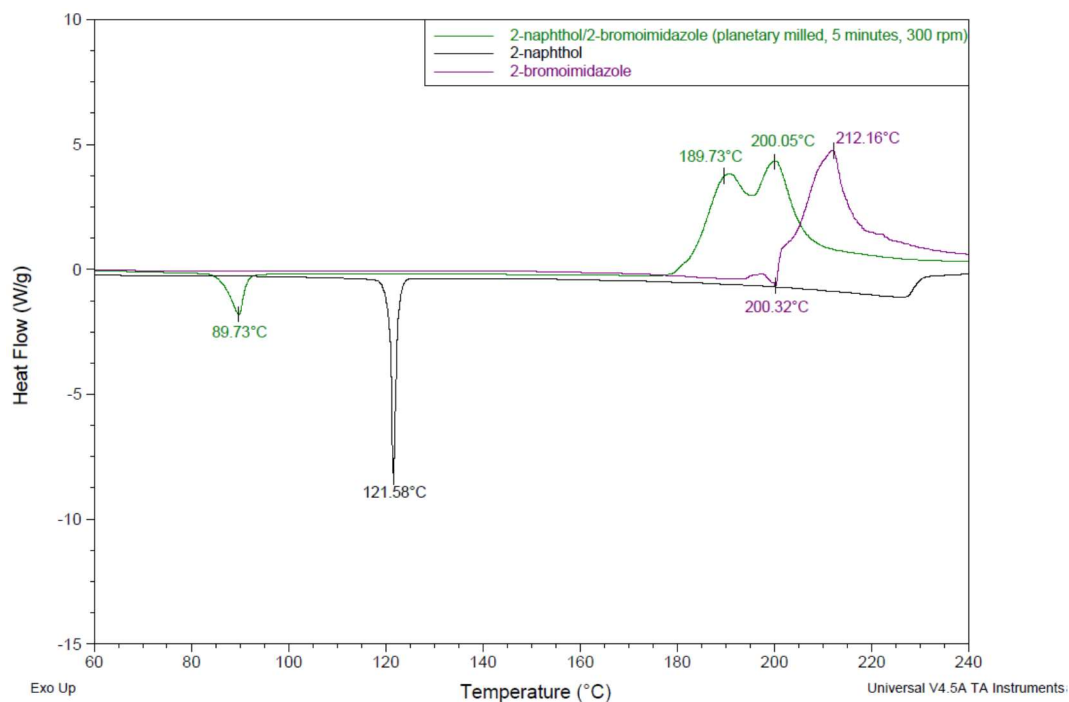


Figure C.53 - Thermal analysis of 2-naphthol/2-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

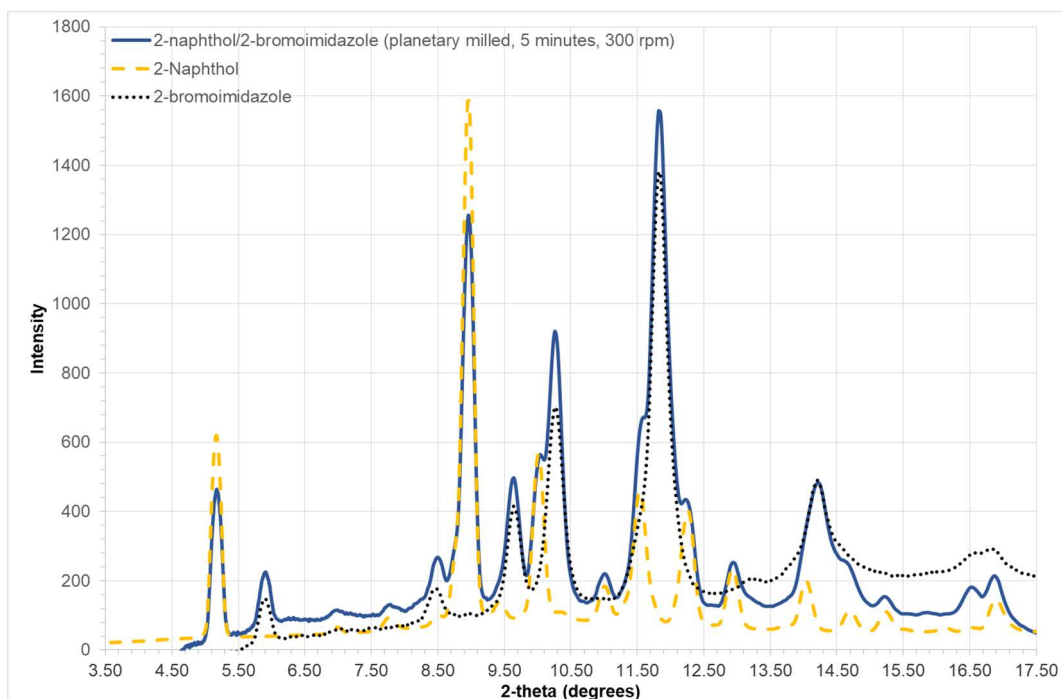


Figure C.54 – Powder x-ray pattern of 2-naphthol/2-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.34 2-naphthol/4-bromoimidazole

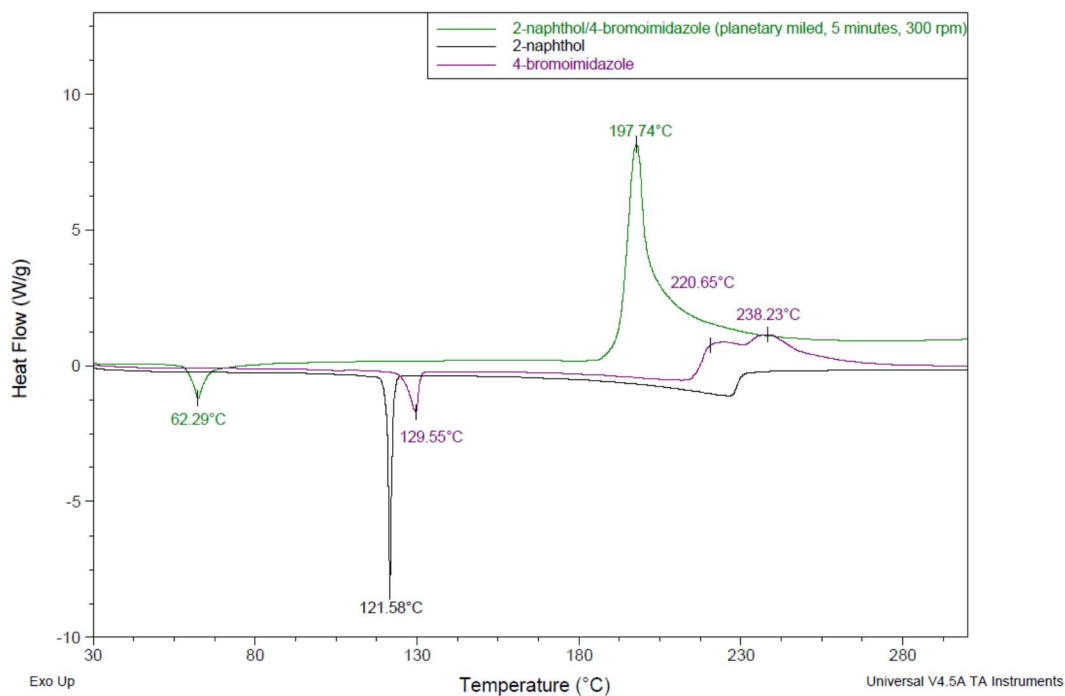


Figure C.55 - Thermal analysis of 2-naphthol/4-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

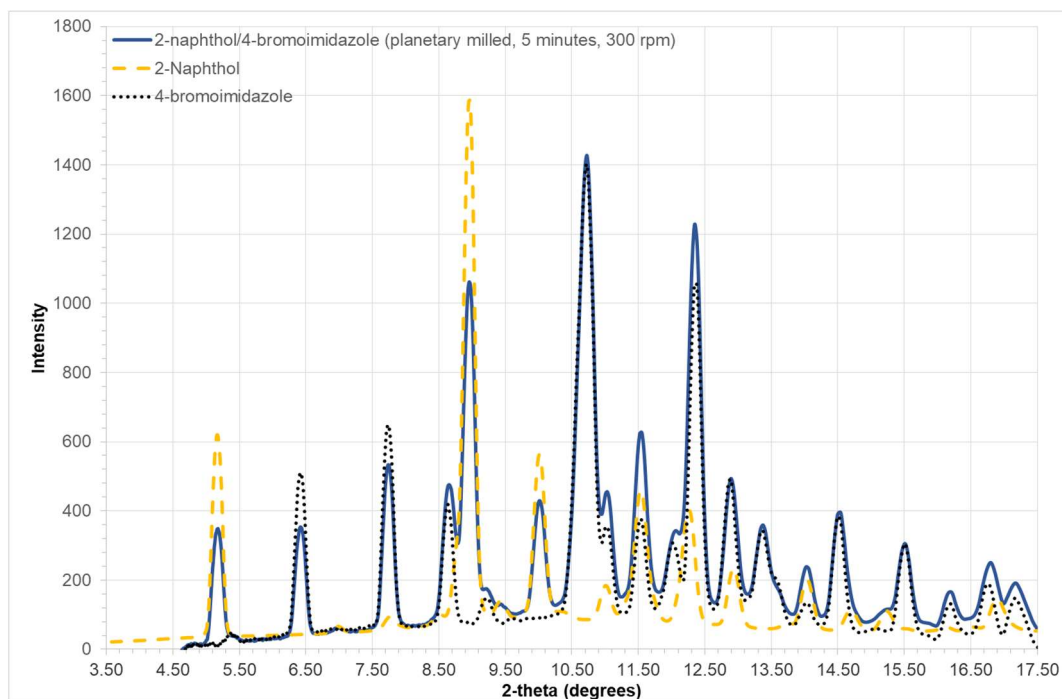


Figure C.56 – Powder x-ray pattern of 2-naphthol/4-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.35 2-naphthol/2,4-dimethylimidazole

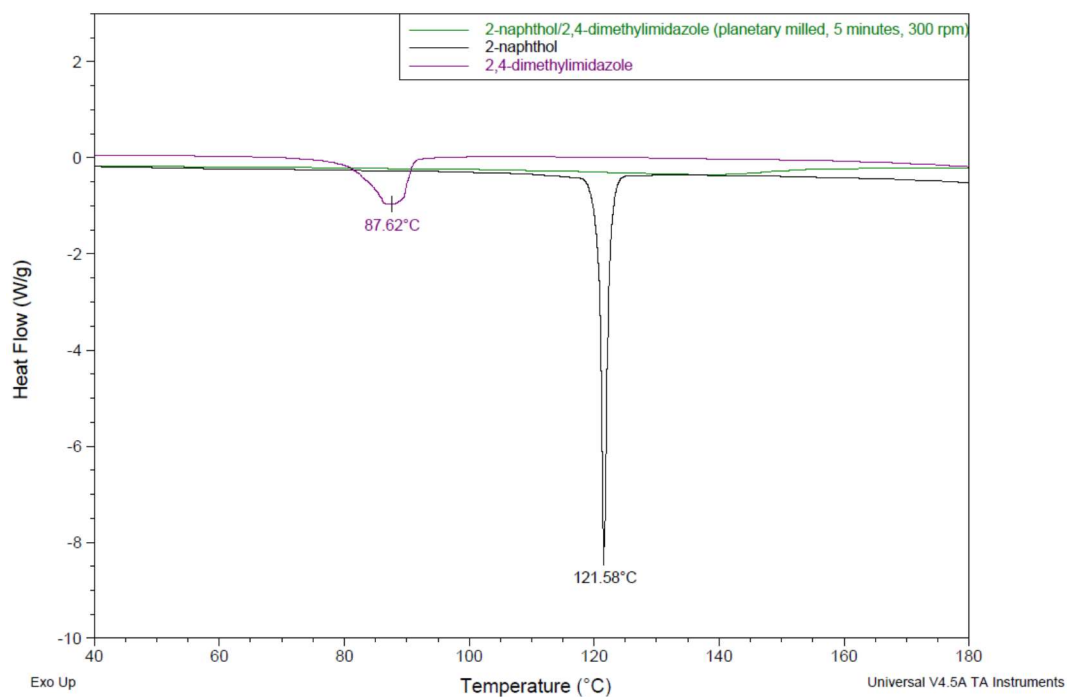


Figure C.57 - Thermal analysis of 2-naphthol/2,4-dimethylimidazole produced by planetary milling for 5 minutes at 300 rpm. The mixed system is a liquid and did not display a melt.

C.36 2-naphthol/4,5-dinitroimidazole

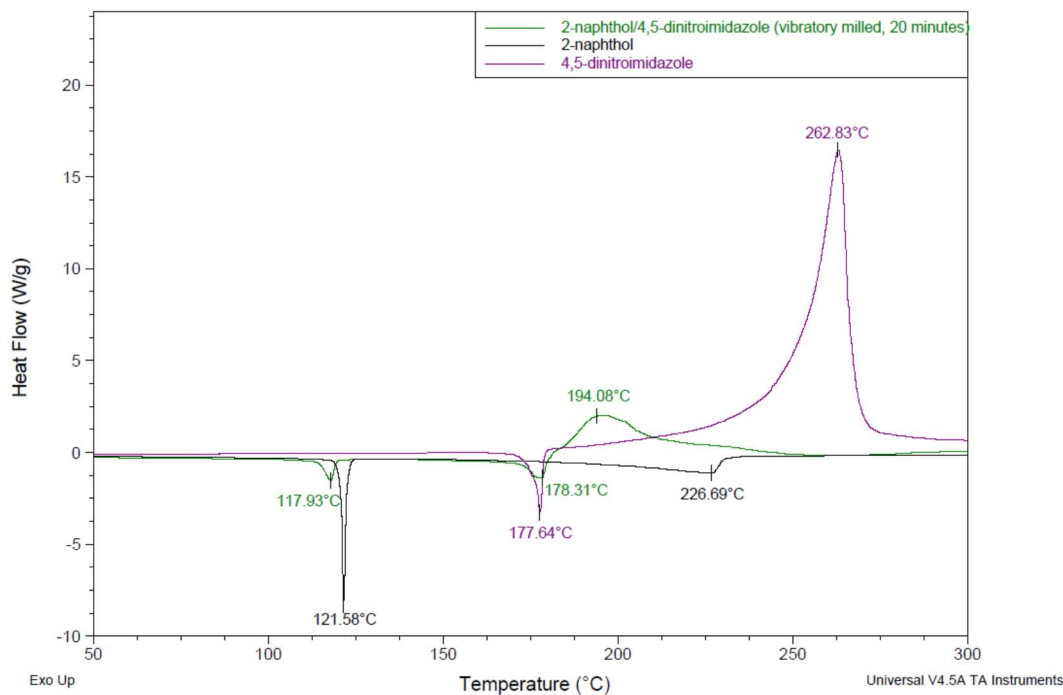


Figure C.58 - Thermal analysis of 2-naphthol/4,5-dinitroimidazole produced by vibratory milling for 20 minutes.

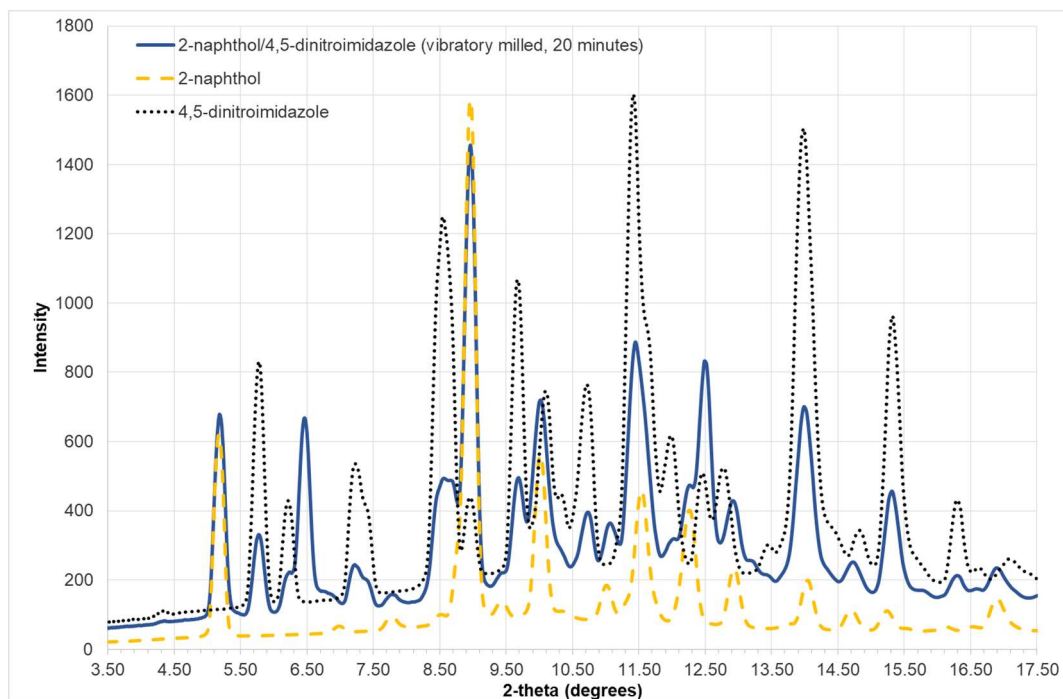


Figure C.59 – Powder x-ray pattern of 2-naphthol/4,5-dinitroimidazole produced by vibratory milling for 20 minutes.

C.37 2-naphthol/4,5-dichlororimidazole

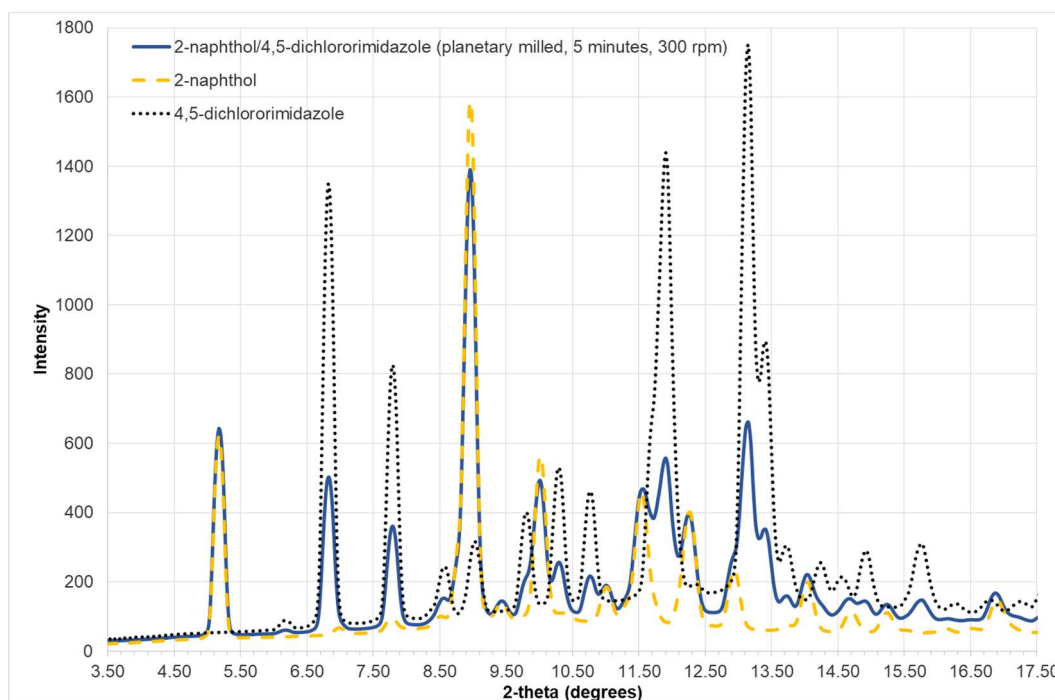


Figure C.60 - Powder x-ray pattern of 2-naphthol/4,5-dichlororimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.38 2-naphthol/2,4,5-tribromoimidazole

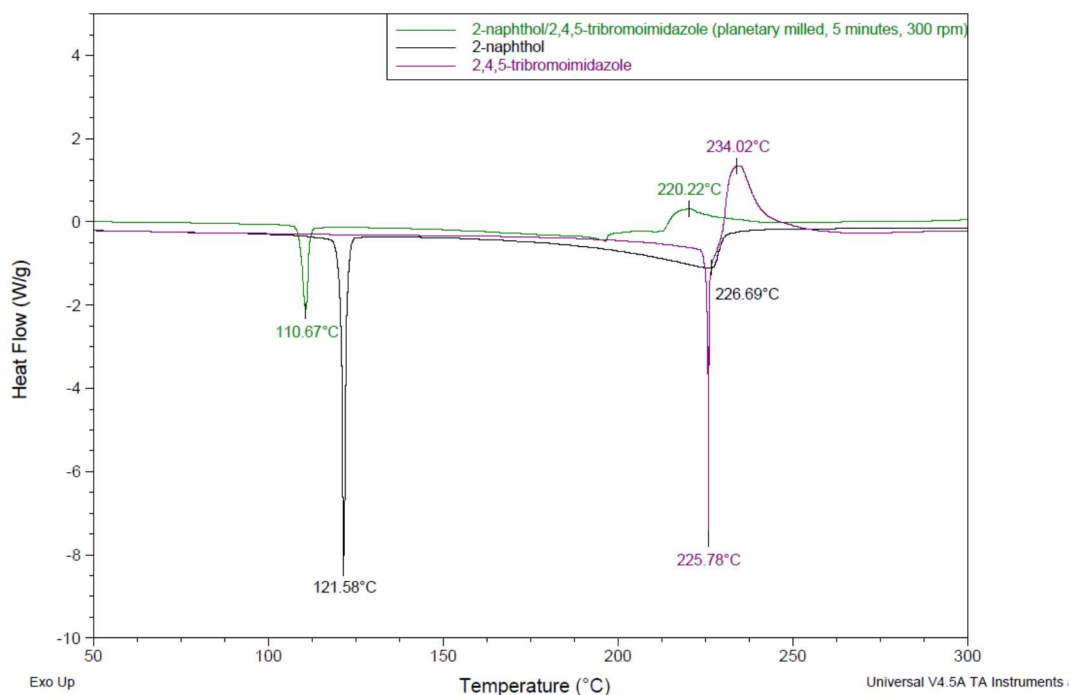


Figure C.61 – Thermal analysis of 2-naphthol/2,4,5-tribromolimidazole produced by planetary milling for 5 minutes at 300 rpm.

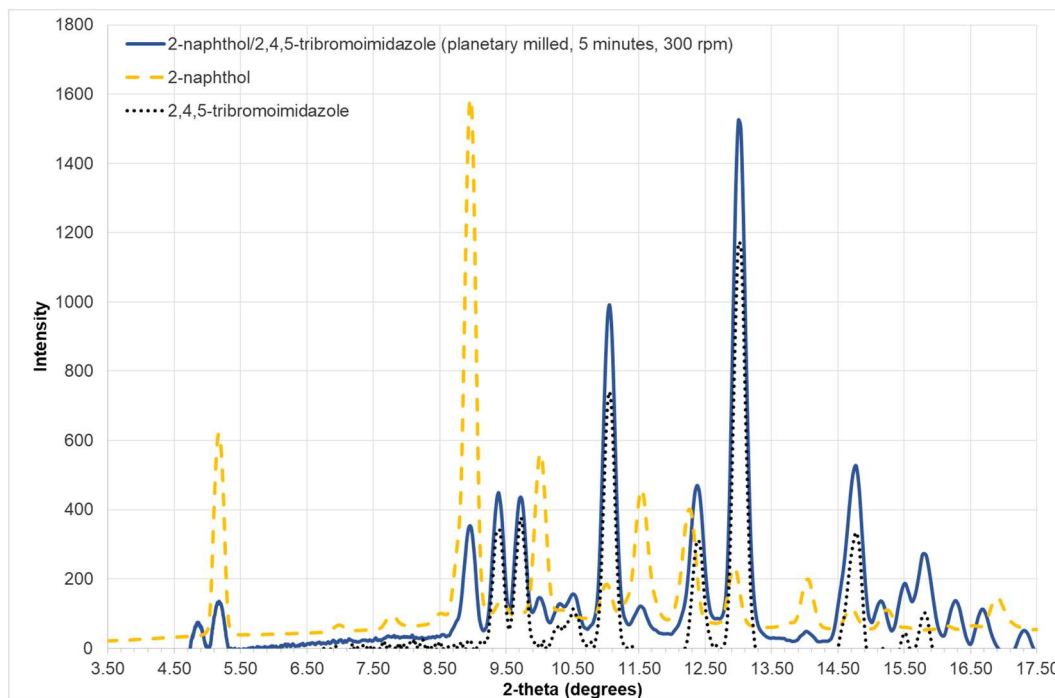


Figure C.62 - Powder x-ray pattern of 2-naphthol/2,4,5-tribromolimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.39 2-naphthol/2-methyl-5-nitroimidazole

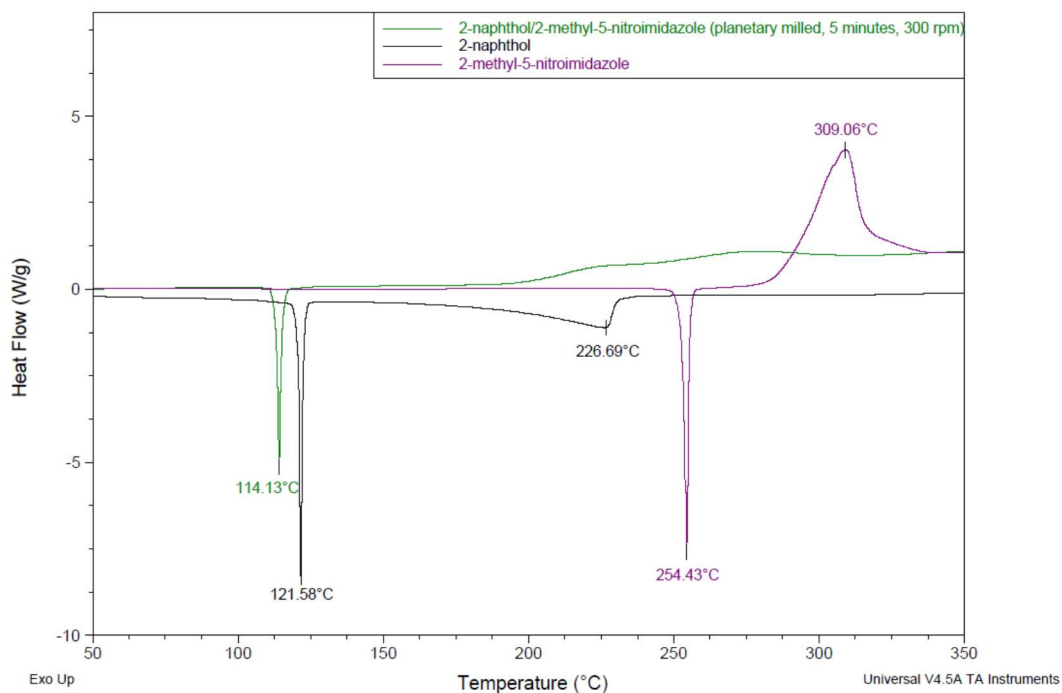


Figure C.63 - Thermal analysis of 2-naphthol/2-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

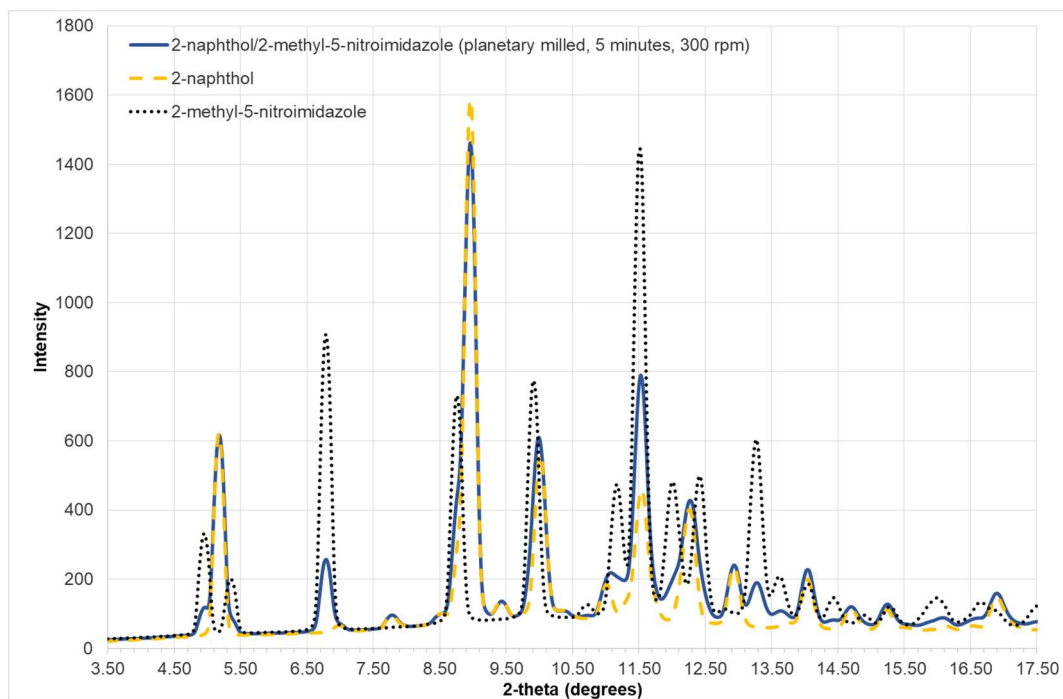


Figure C.64 – Powder x-ray pattern of 2-naphthol/2-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.40 2-naphthol/4-methyl-5-nitroimidazole

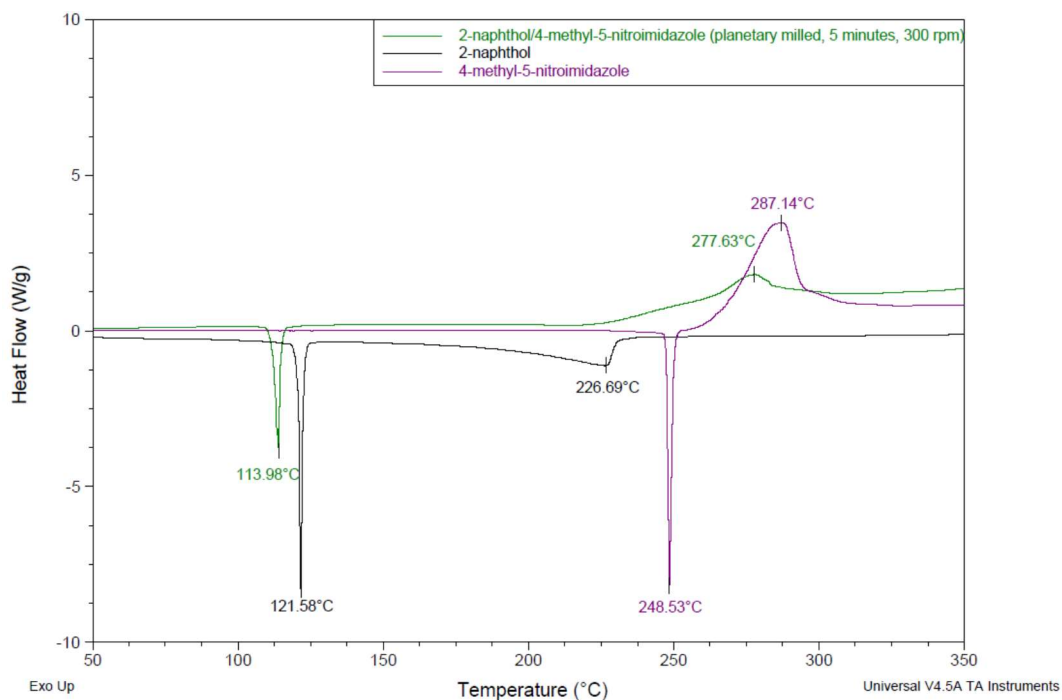


Figure C.65 - Thermal analysis of 2-naphthol/4-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

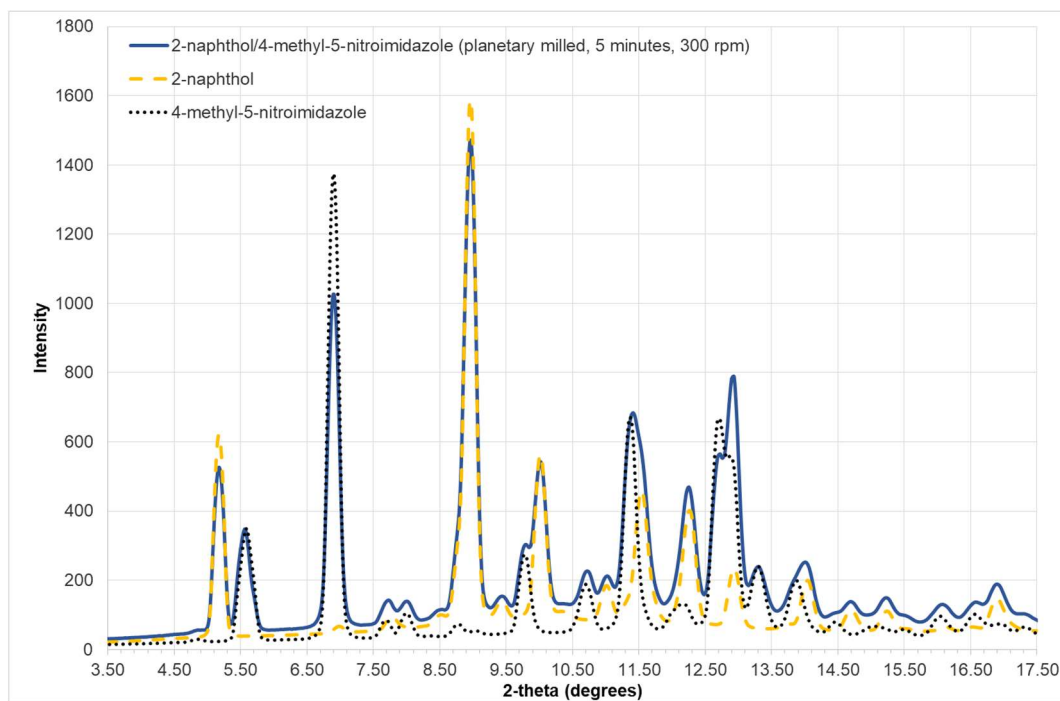


Figure C.66 – Powder x-ray pattern of 2-naphthol/4-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.41 2-naphthol/2-bromo-5-nitroimidazole

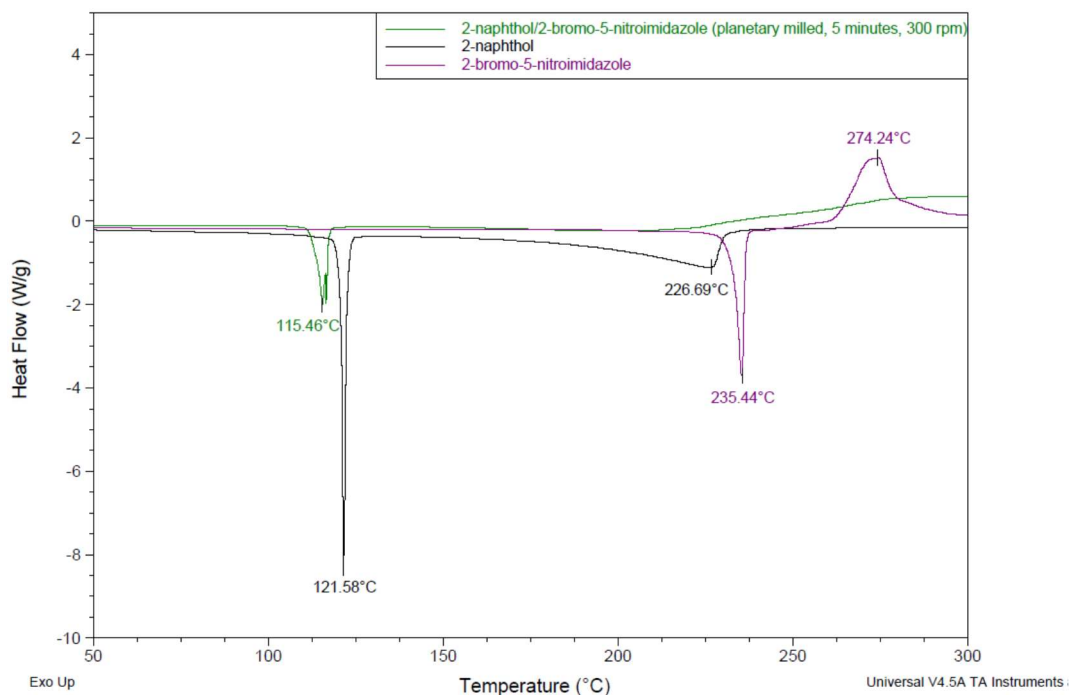


Figure C.67 - Thermal analysis of 2-naphthol/2-bromo-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

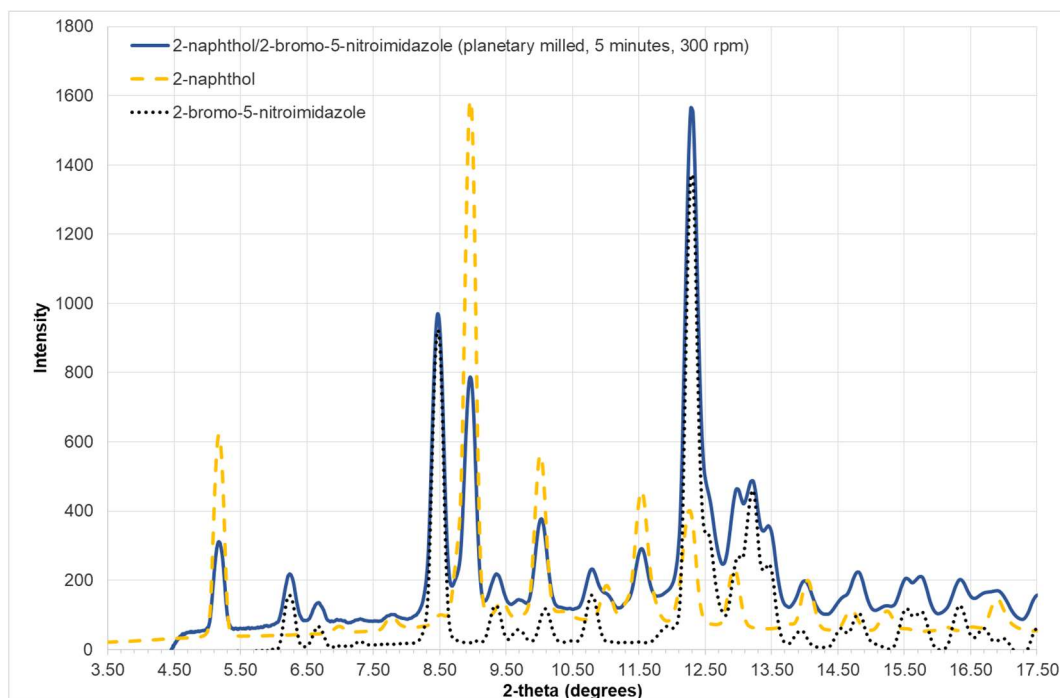


Figure C.68 – Powder x-ray pattern of 2-naphthol/2-bromo-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.42 2-naphthol/4-bromo-2-methylimidazole

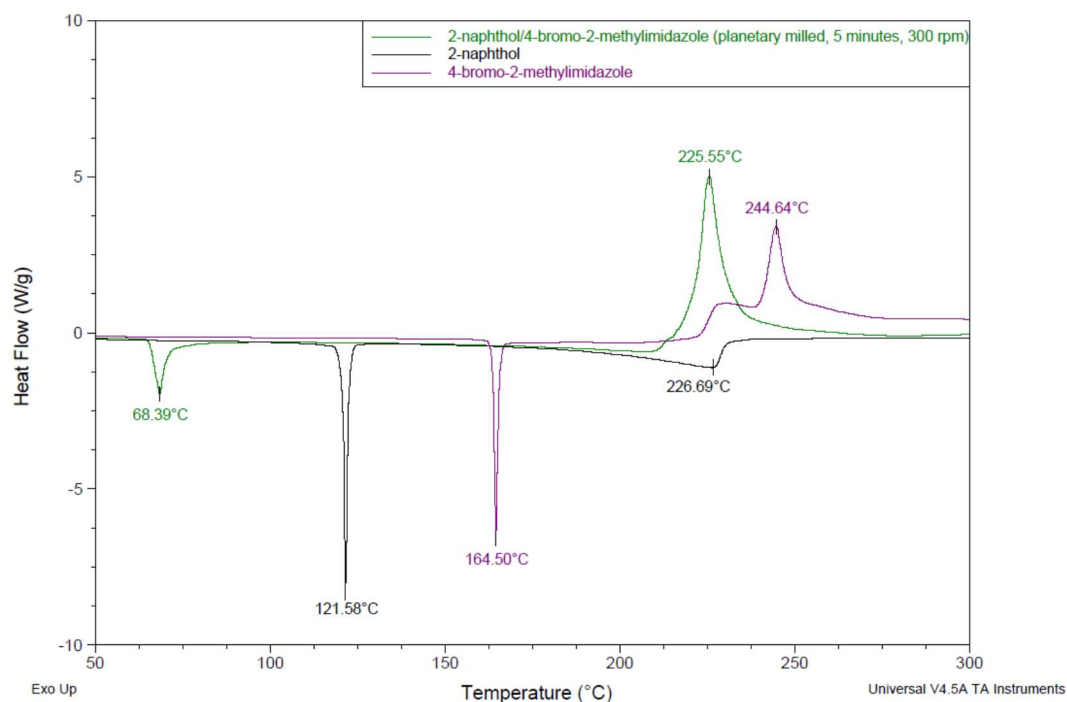


Figure C.69 – Thermal analysis of 2-naphthol/4-bromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

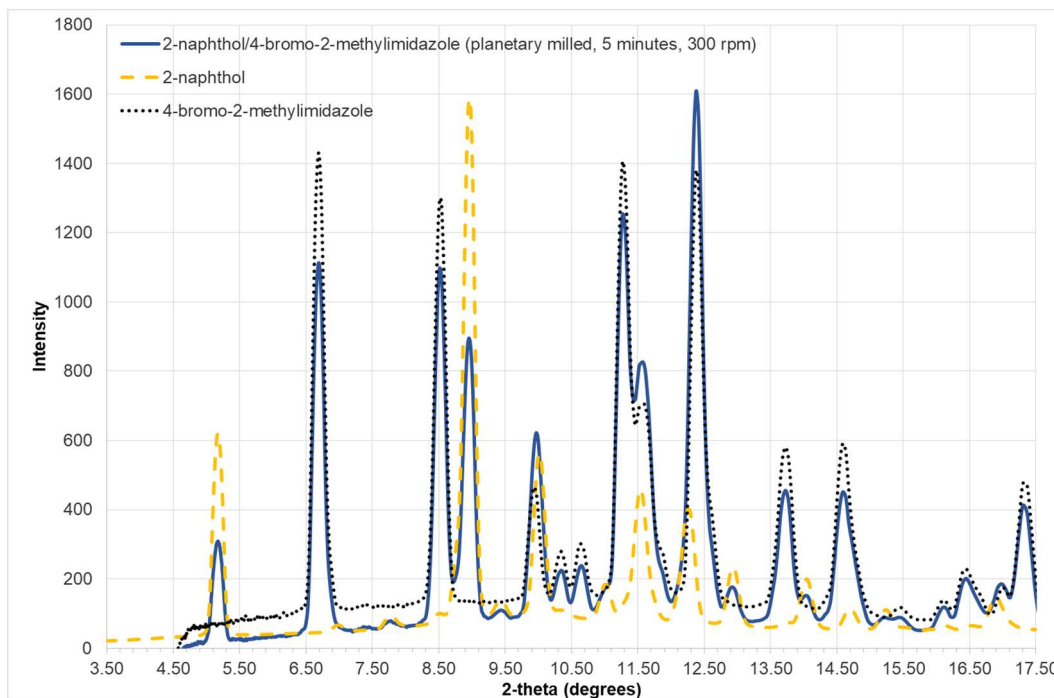


Figure C.70 - Powder x-ray pattern of 2-naphthol/4-bromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.43 2-naphthol/5-bromo-4-methylimidazole

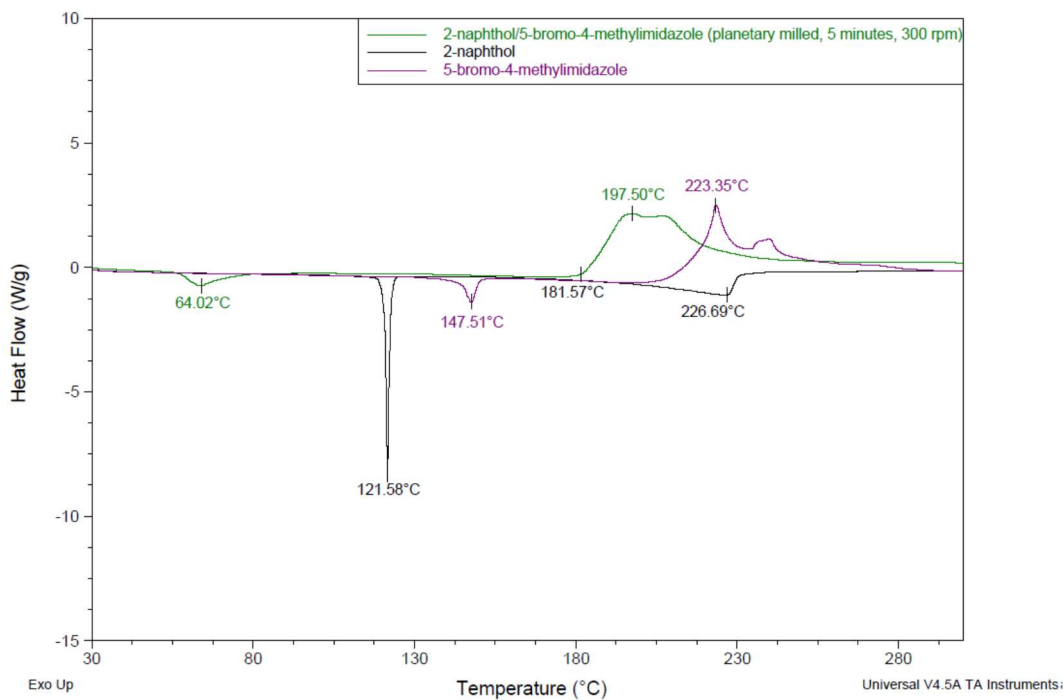


Figure C.71 - Thermal analysis of 2-naphthol/5-bromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

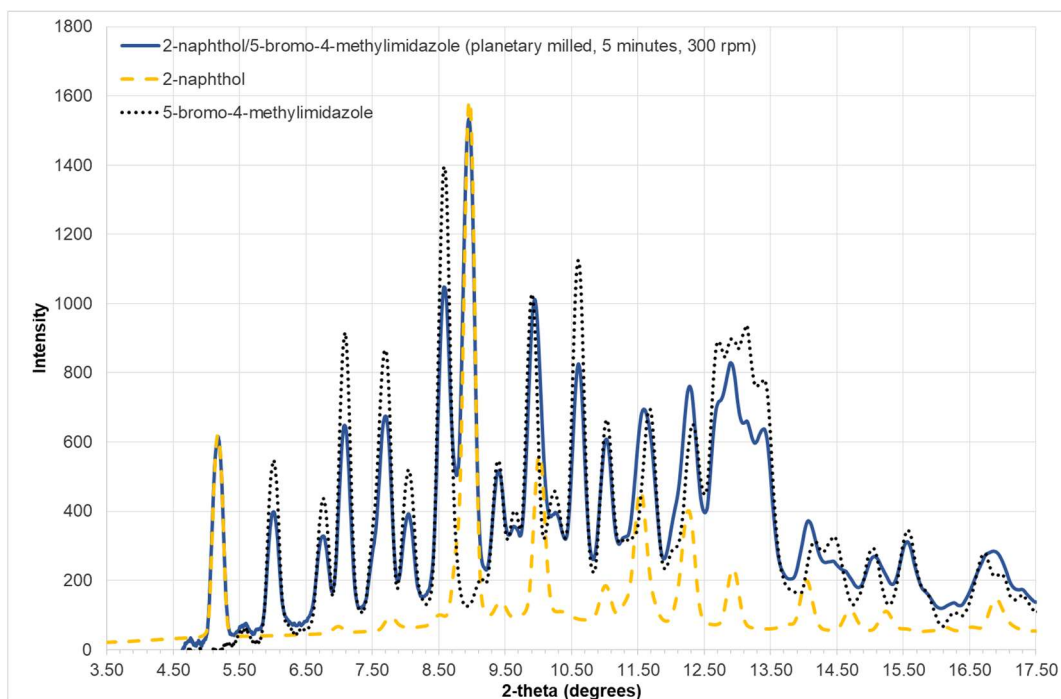


Figure C.72 – Powder x-ray pattern of 2-naphthol/5-bromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.44 2-naphthol/4,5-dibromo-2-methylimidazole

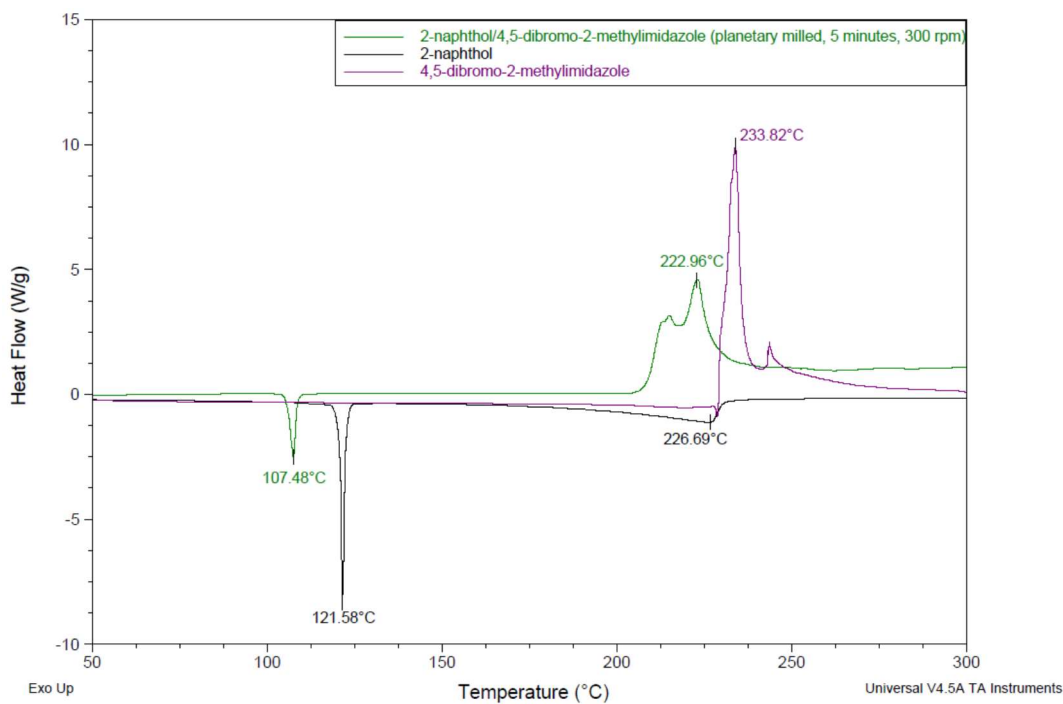


Figure C.73 - Thermal analysis of 2-naphthol/4,5-dibromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

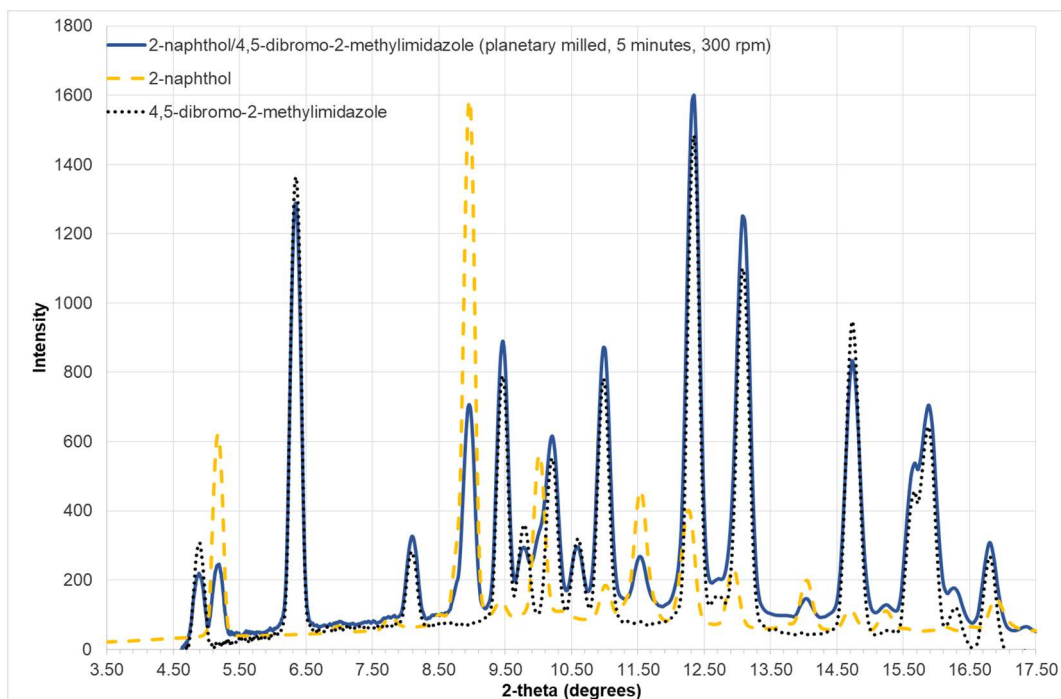


Figure C.74 – Powder x-ray pattern of 2-naphthol/4,5-dibromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.45 2-naphthol/2,5-dibromo-4-methylimidazole

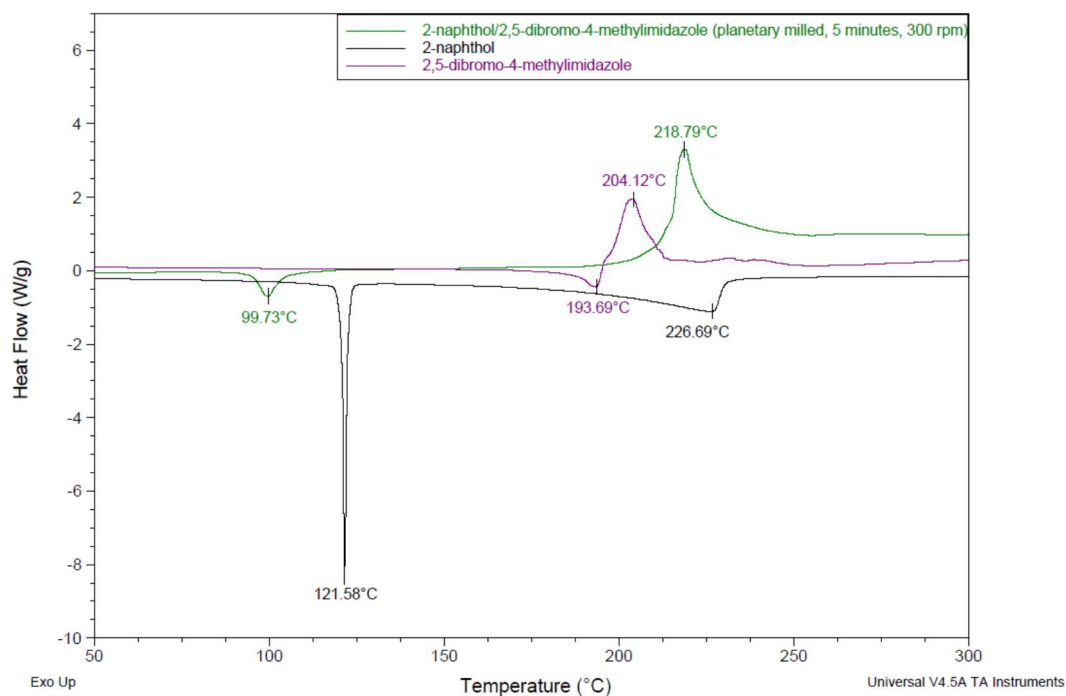


Figure C.75 - Thermal analysis of 2-naphthol/2,5-dibromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

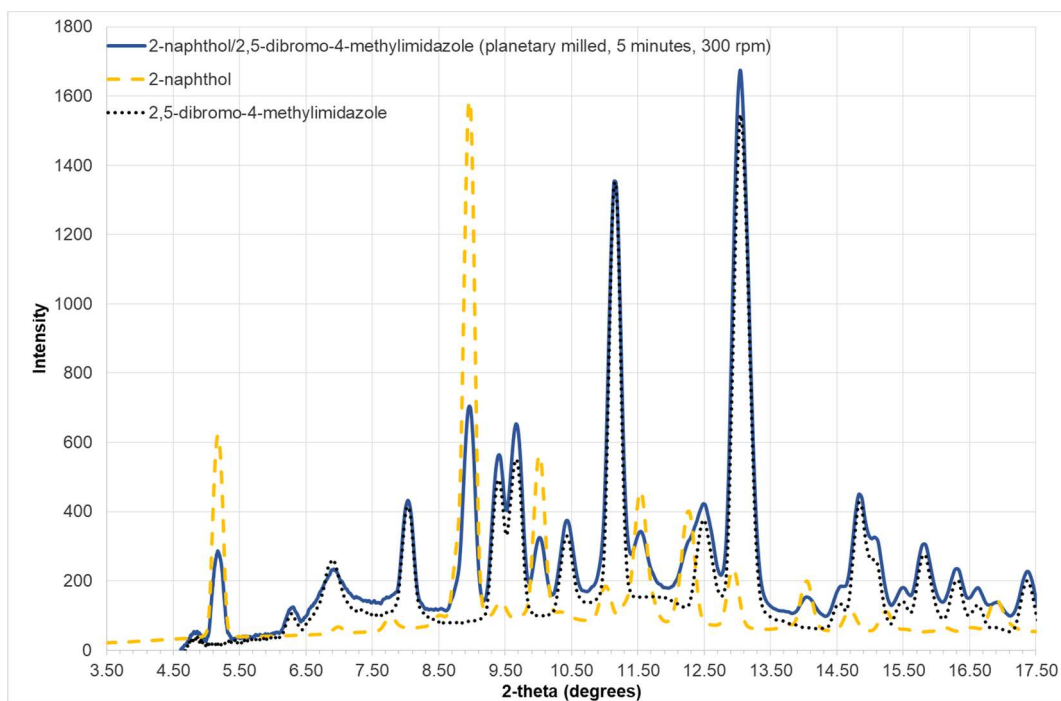


Figure C.76 – Powder x-ray pattern of 2-naphthol/2,5-dibromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

C.46 2-naphthol/1,2,3-triazole

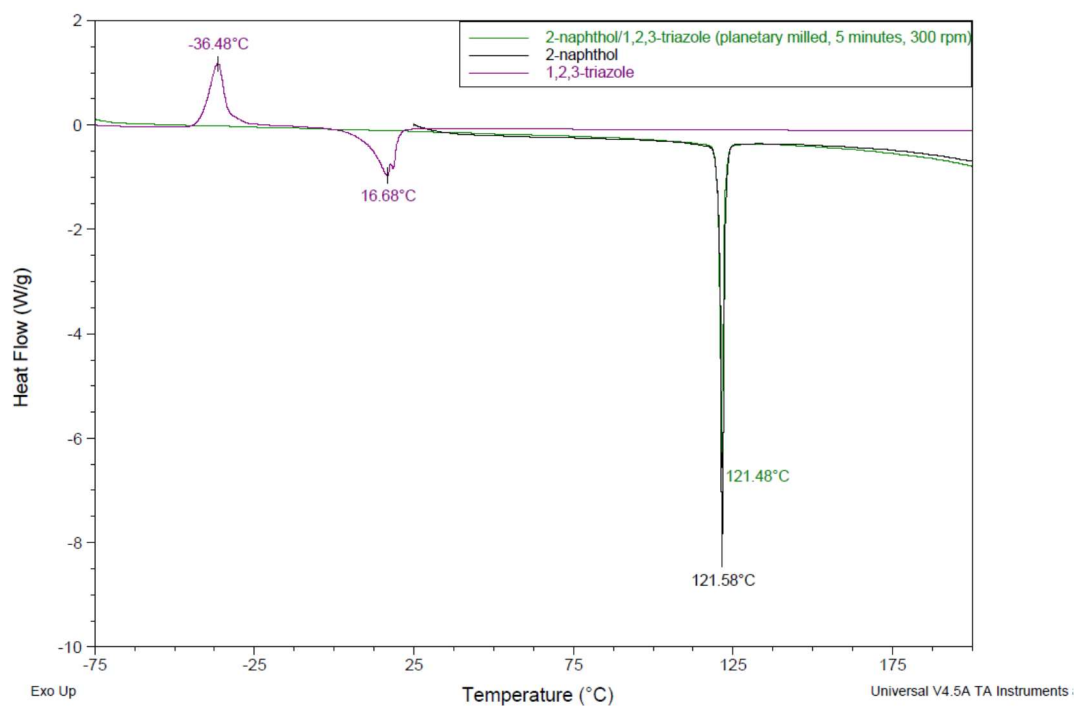


Figure C.77 - Thermal analysis of 2-naphthol/1,2,3-triazole produced by planetary milling for 5 minutes at 300 rpm.

C.47 2-naphthol/5-nitro-1,2,3-triazole

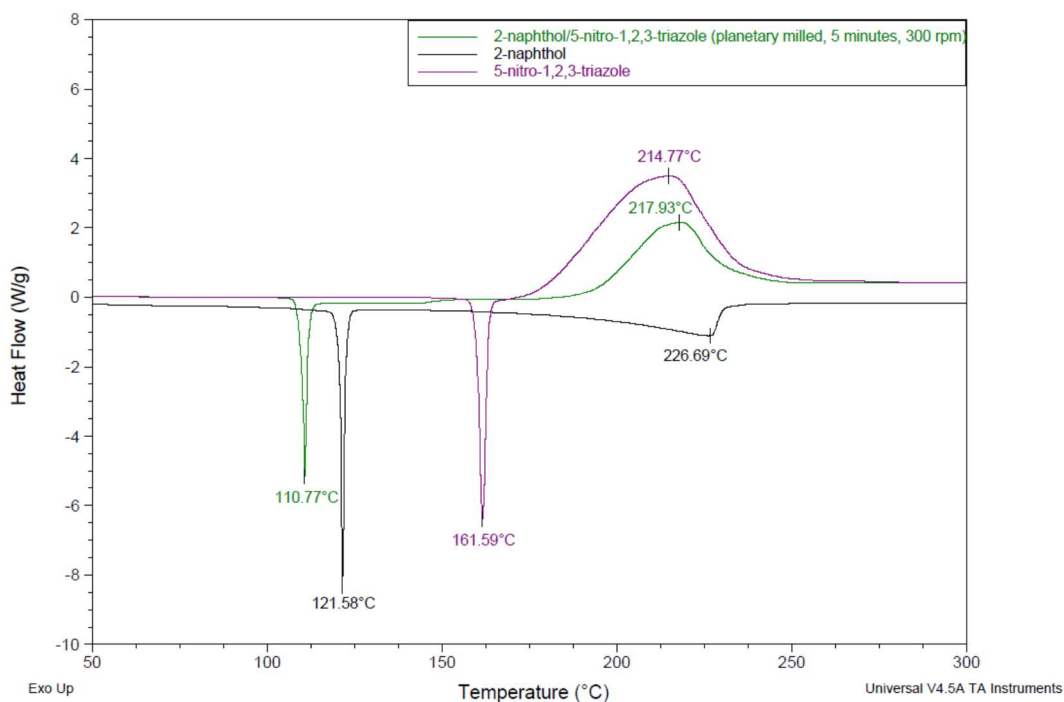


Figure C.78 - Thermal analysis of 2-naphthol/5-nitro-1,2,3-triazole produced by planetary milling for 5 minutes at 300 rpm.

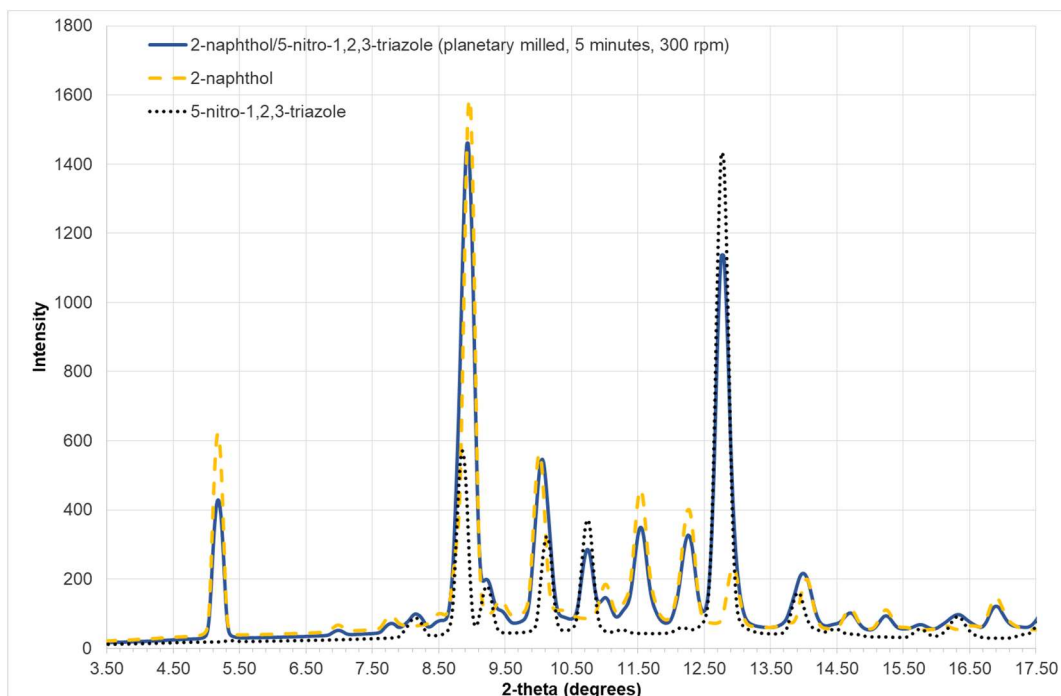


Figure C.79 – Powder x-ray pattern of 2-naphthol/5-nitro-1,2,3-triazole produced by planetary milling for 5 minutes at 300 rpm.

C.48 2-naphthol/1,2,4-triazole

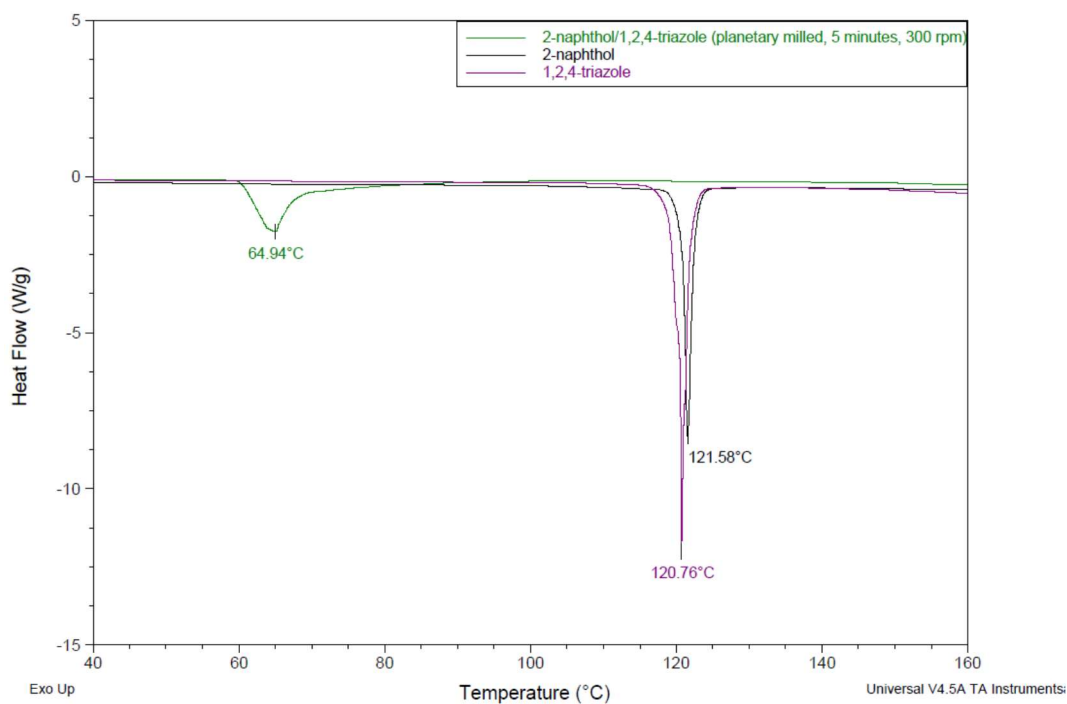


Figure C.80 - Thermal analysis of 2-naphthol/1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

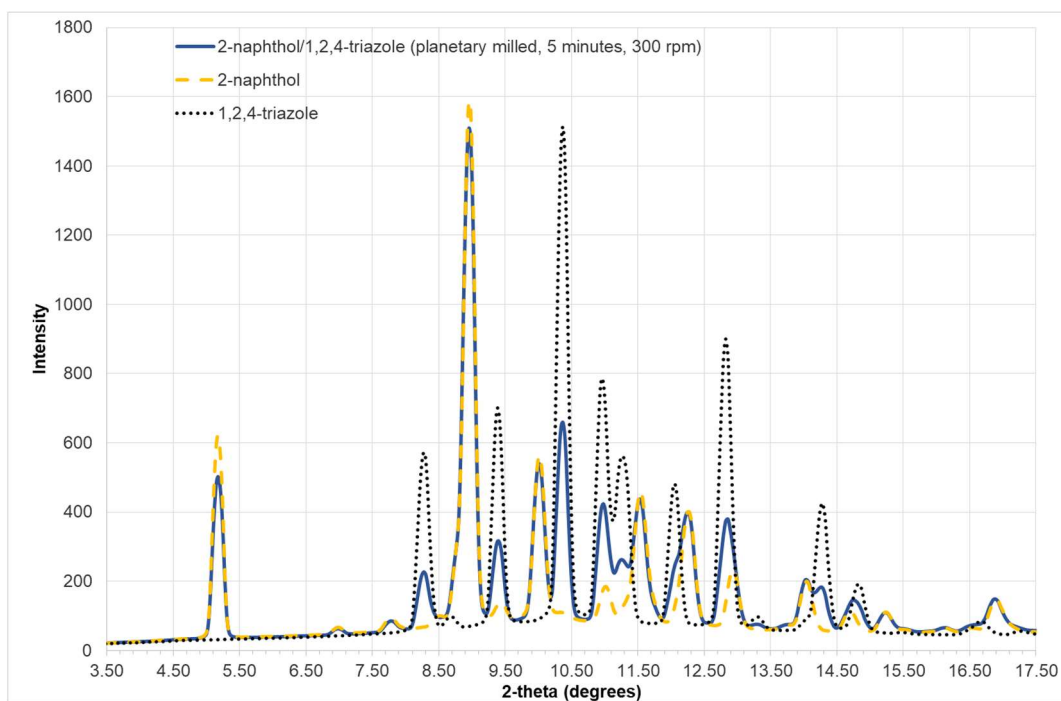


Figure C.81 – Powder x-ray pattern of 2-naphthol/1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

C.49 2-naphthol/3-methyl-1,2,4-triazole

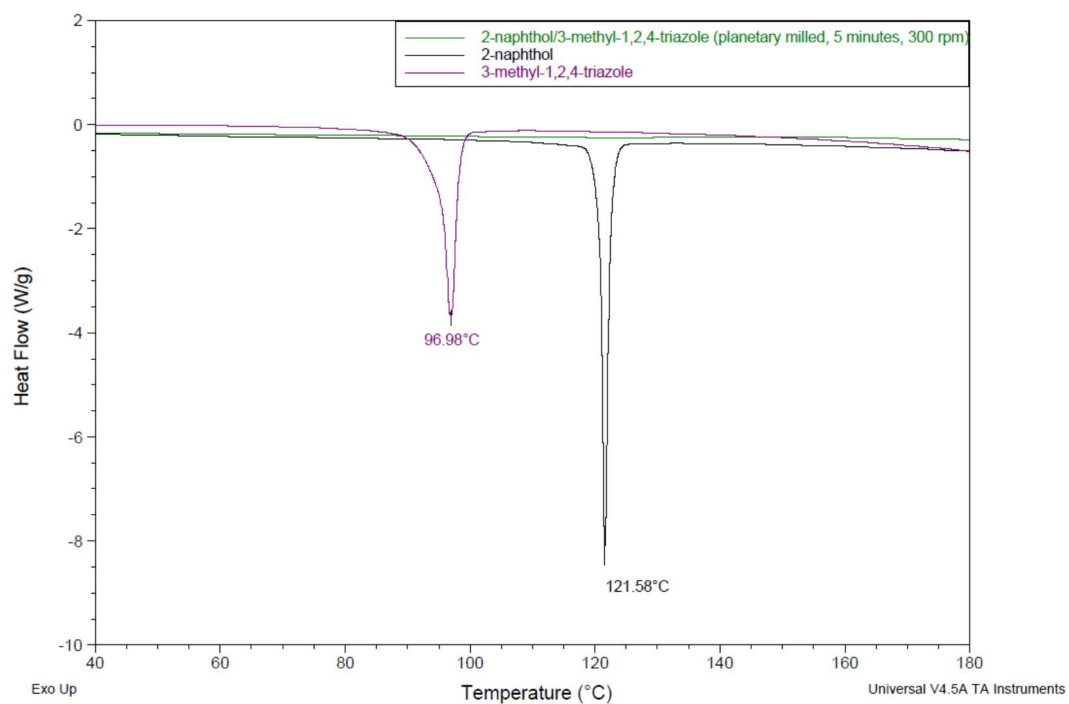


Figure C.82 - Thermal analysis of 2-naphthol/3-methyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

C.50 2-naphthol/1,2,4-triazol-3-amine

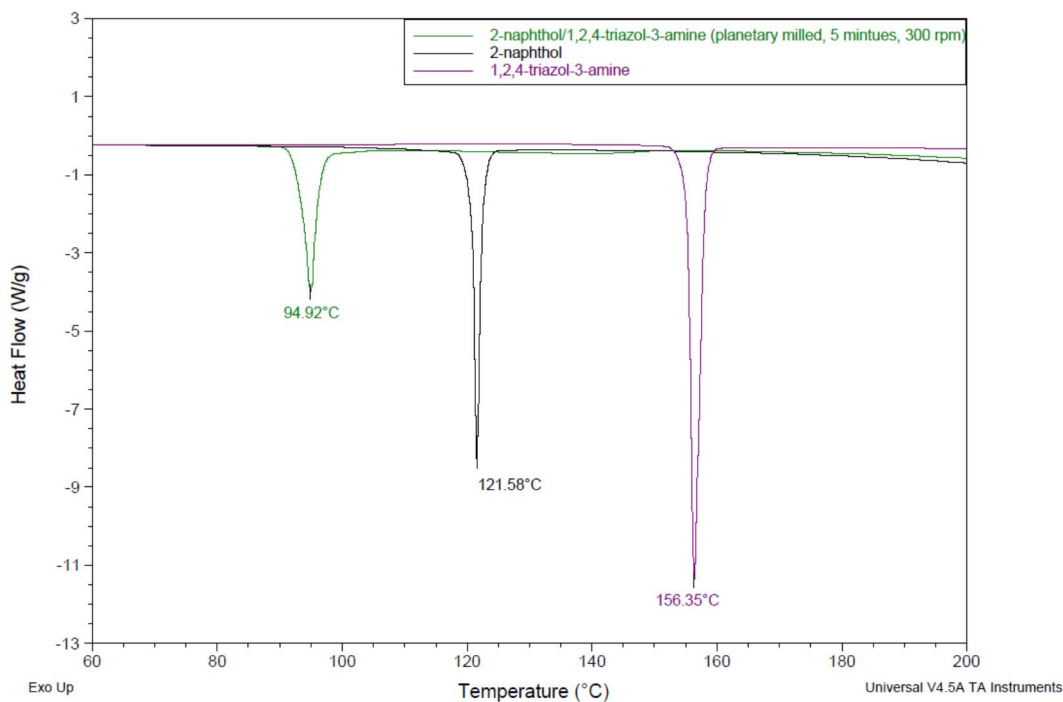


Figure C.83 - Thermal analysis of 2-naphthol/1,2,4-triazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

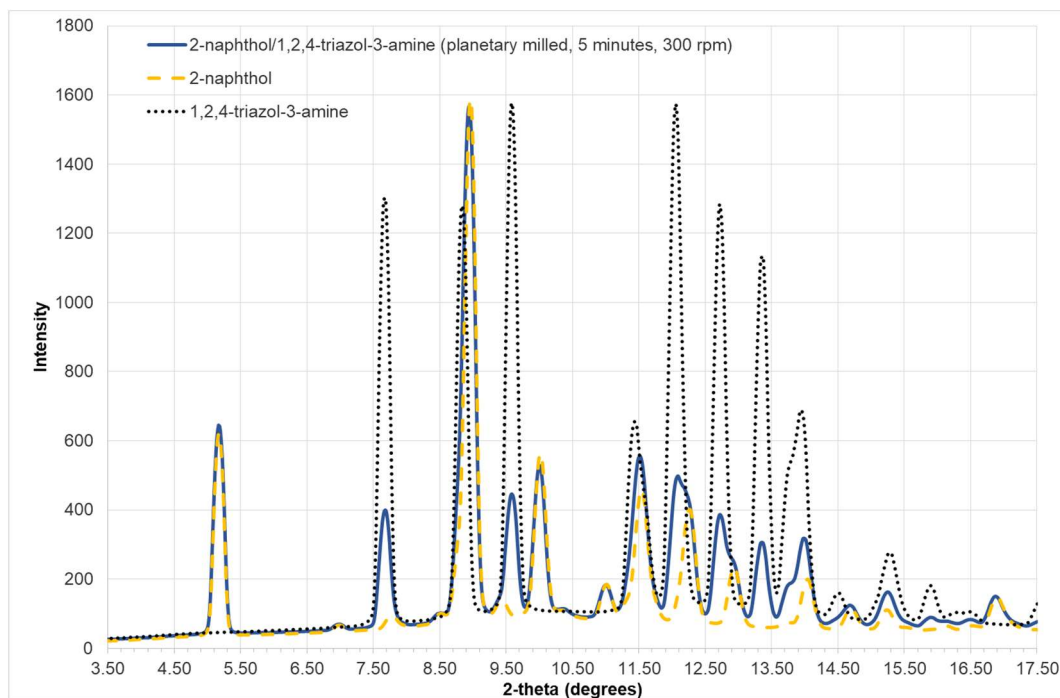


Figure C.84 – Powder x-ray pattern of 2-naphthol/1,2,4-triazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

C.51 2-naphthol/5-bromo-1,2,4-triazole

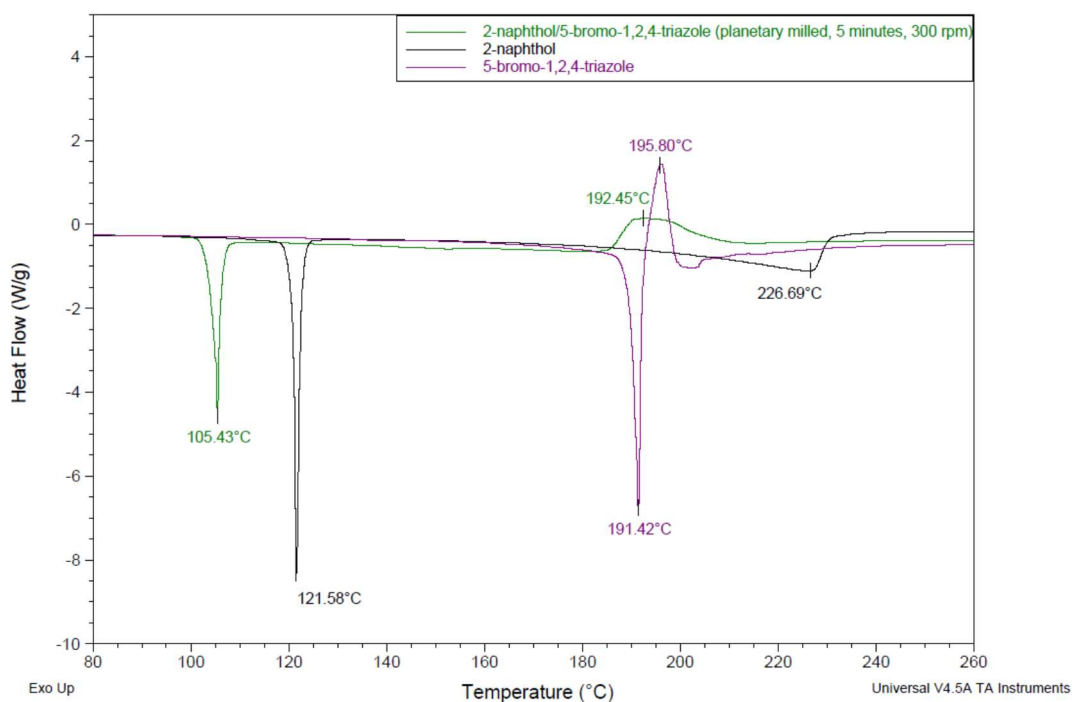


Figure C.85 - Thermal analysis of 2-naphthol/5-bromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

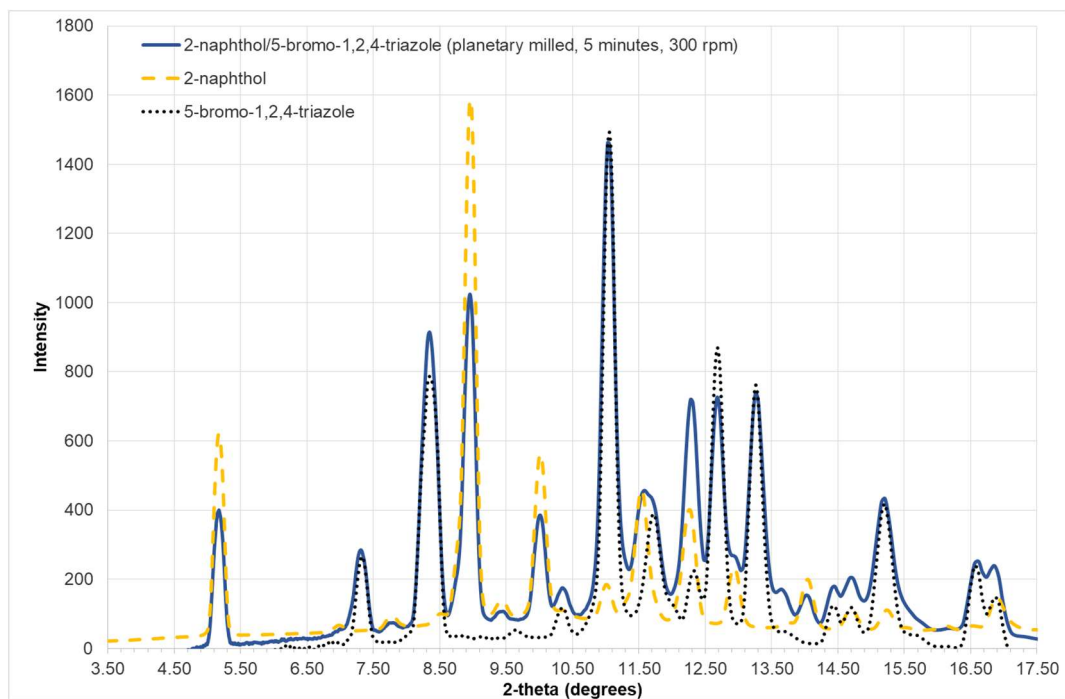


Figure C.86 – Powder x-ray pattern of 2-naphthol/5-bromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

C.52 2-naphthol/1,2,4-triazol-3,5-diamine

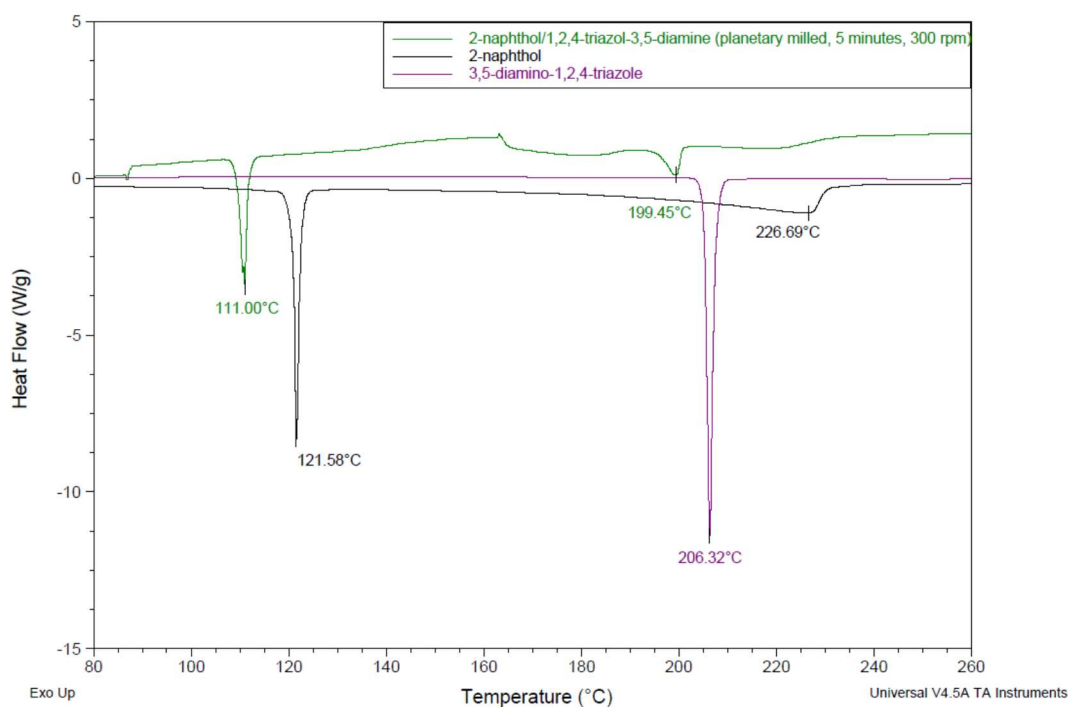


Figure C.87 - Thermal analysis of 2-naphthol/1,2,4-triazol-3,5-diamine produced by planetary milling for 5 minutes at 300 rpm.

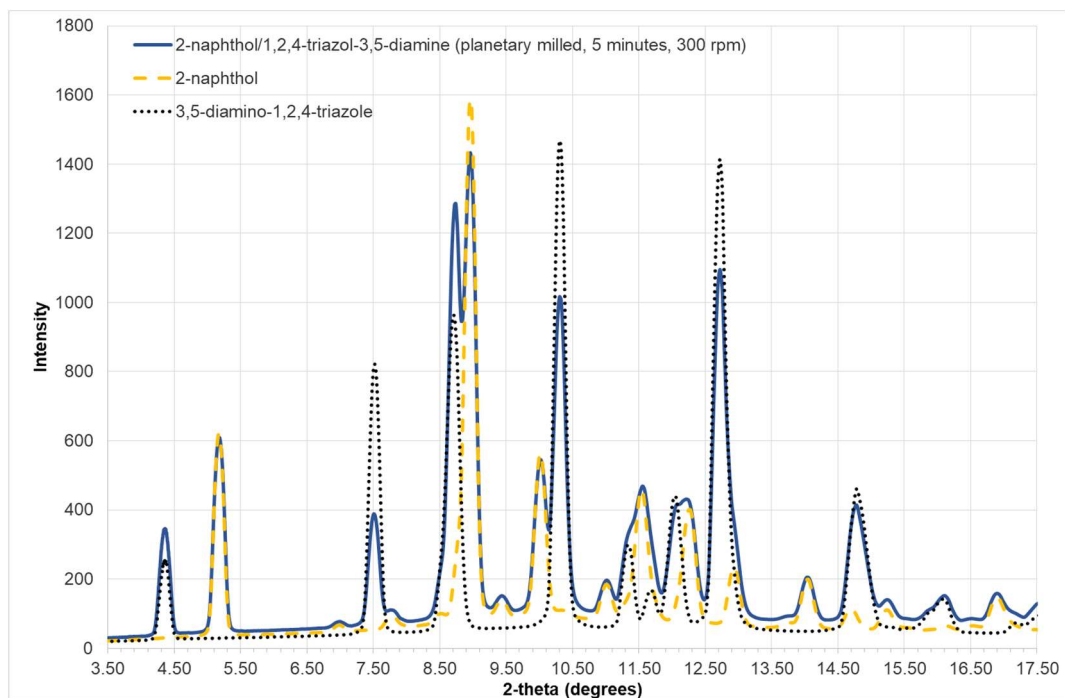


Figure C.88 – Powder x-ray pattern of 2-naphthol/1,2,4-triazol-3,5-diamine produced by planetary milling for 5 minutes at 300 rpm.

C.53 2-naphthol/3,5-dimethyl-1,2,4-triazole

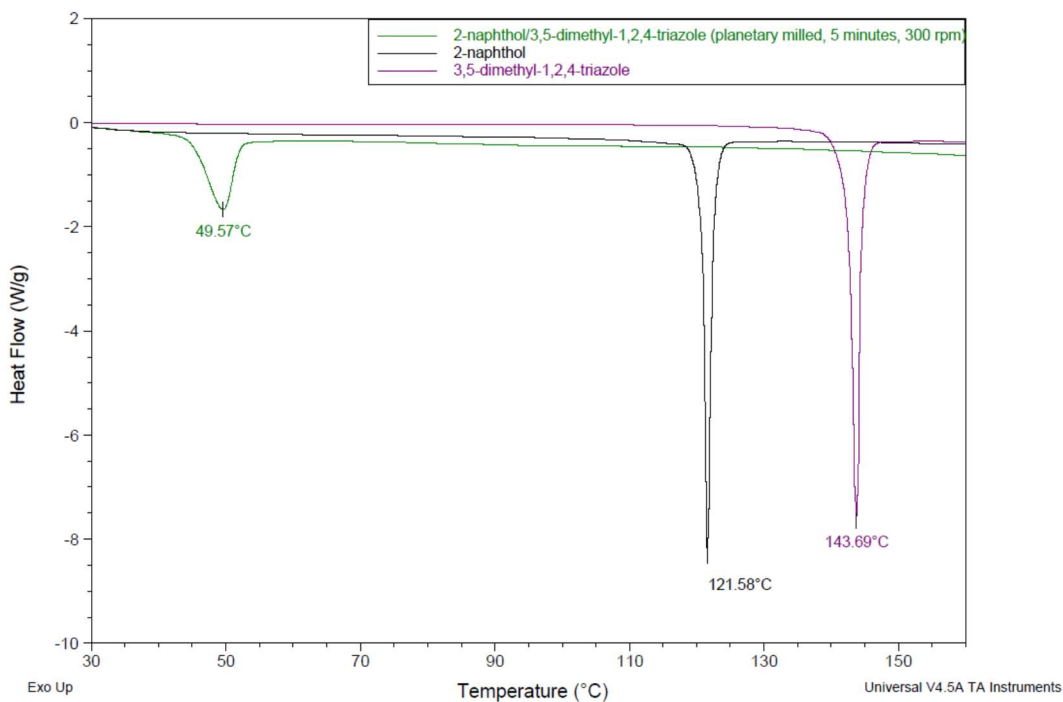


Figure C.89 - Thermal analysis of 2-naphthol/3,5-dimethyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

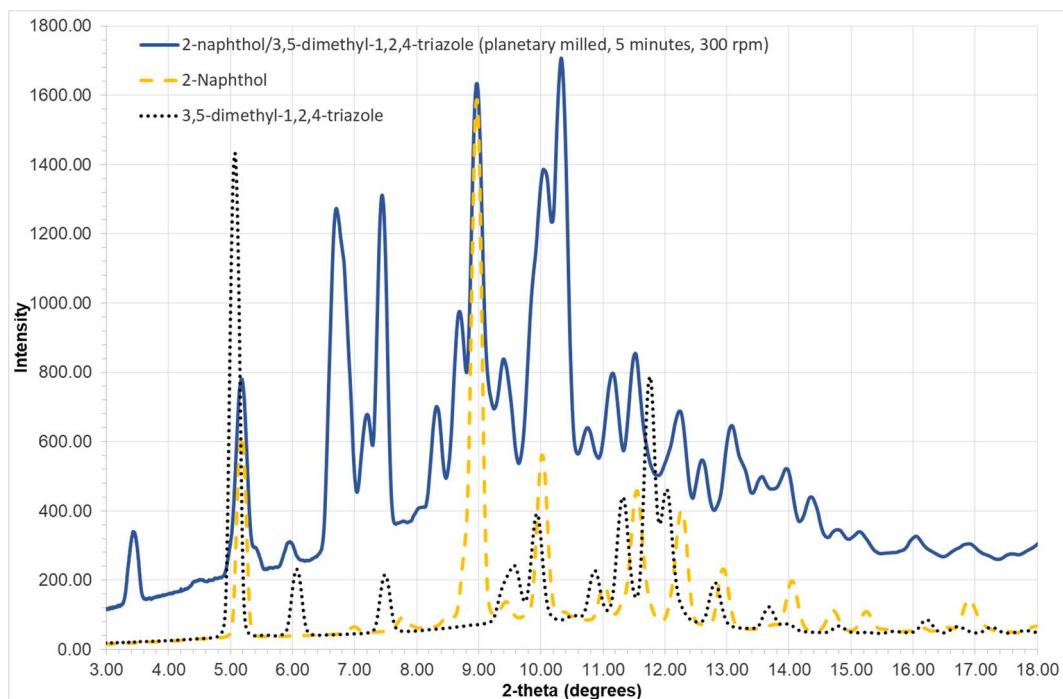


Figure C.90 – Powder x-ray pattern of 2-naphthol/3,5-dimethyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

C.54 2-naphthol/3,5-dibromo-1,2,4-triazole

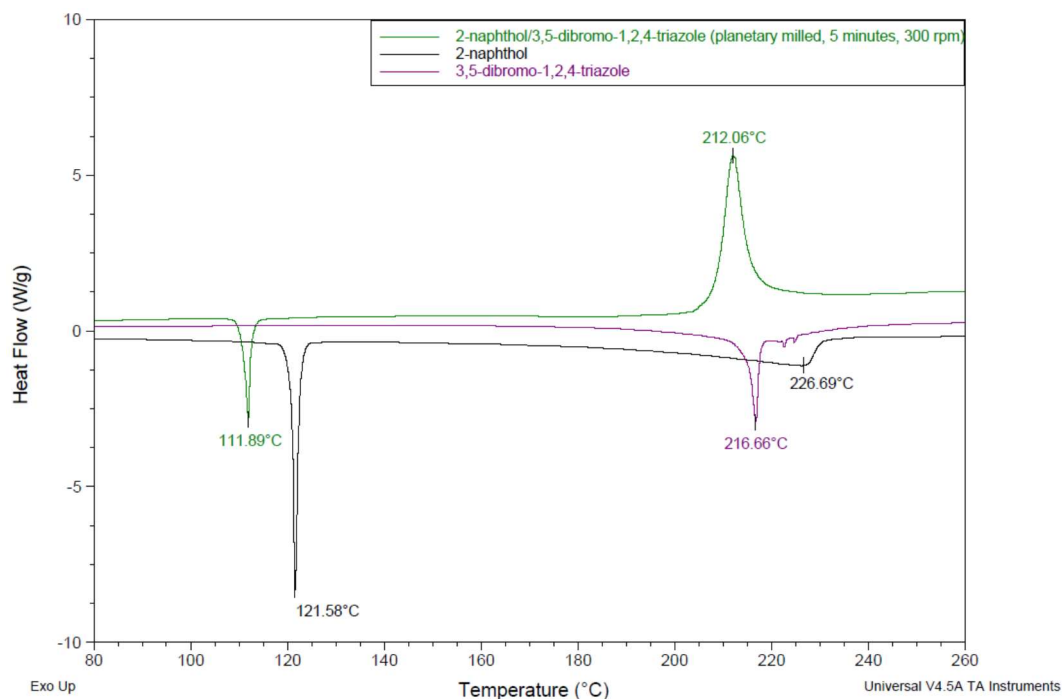


Figure C.91 - Thermal analysis of 2-naphthol/3,5-dibromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

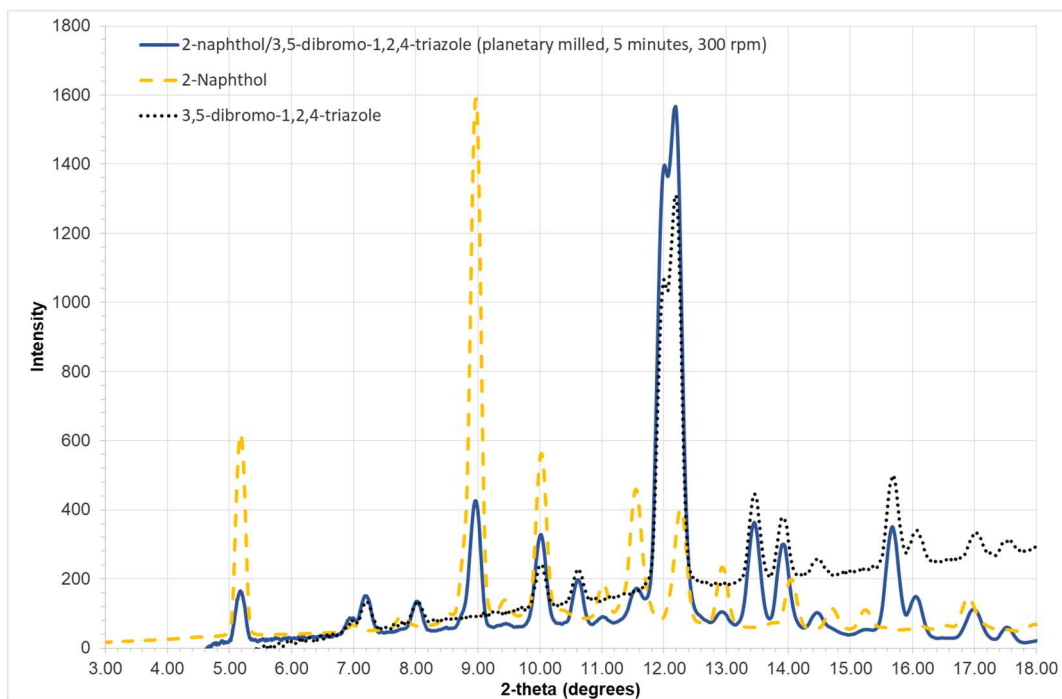


Figure C.92 – Powder x-ray analysis of 2-naphthol/3,5-dibromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

C.55 2-naphthol/1,2,3,4-tetrazole

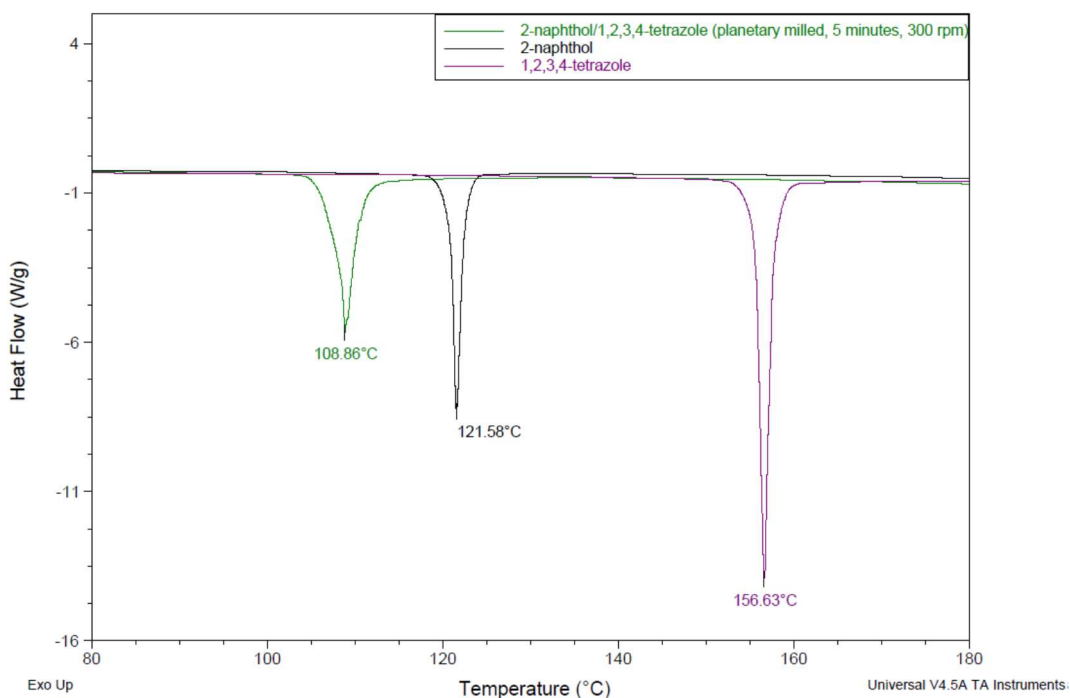


Figure C.93 - Thermal analysis of 2-naphthol/1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

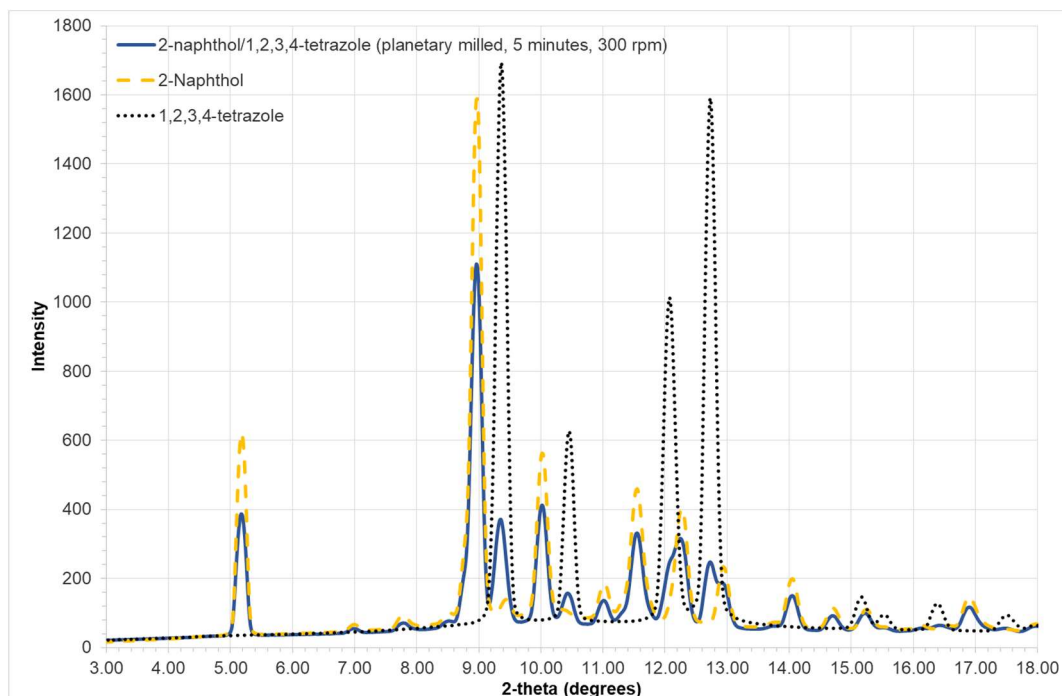


Figure C.94 – Powder x-ray pattern of 2-naphthol/1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

C.56 2-naphthol/1,2,3,4-tetrazol-5-amine

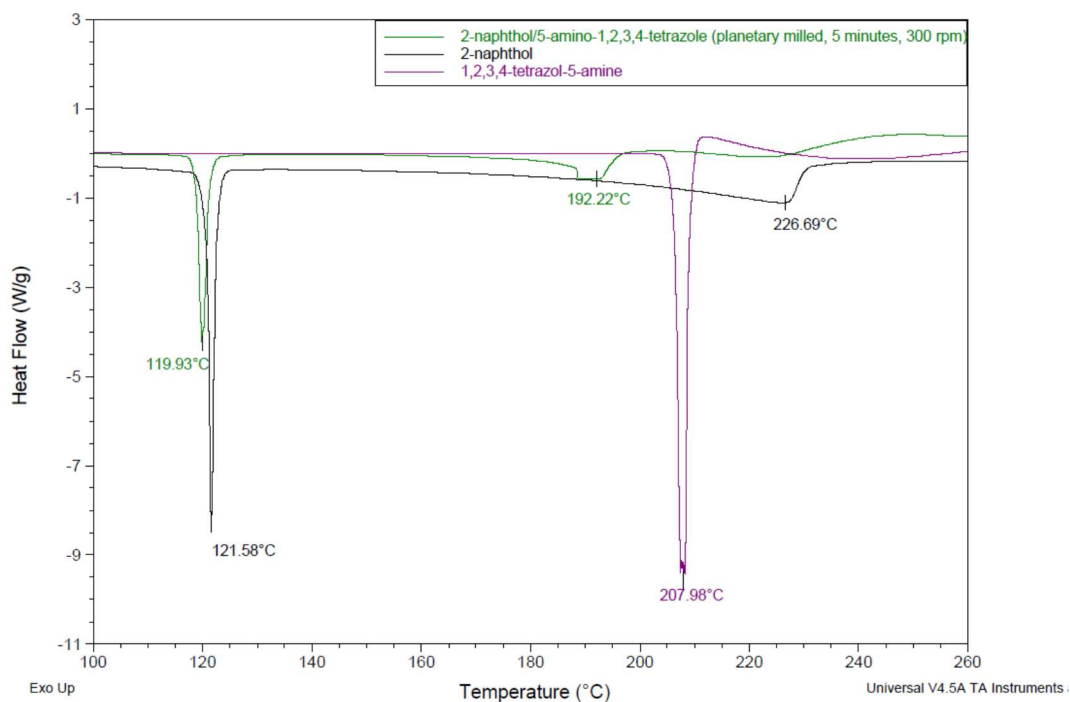


Figure C.95 - Thermal analysis of 2-naphthol/1,2,3,4-tetrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

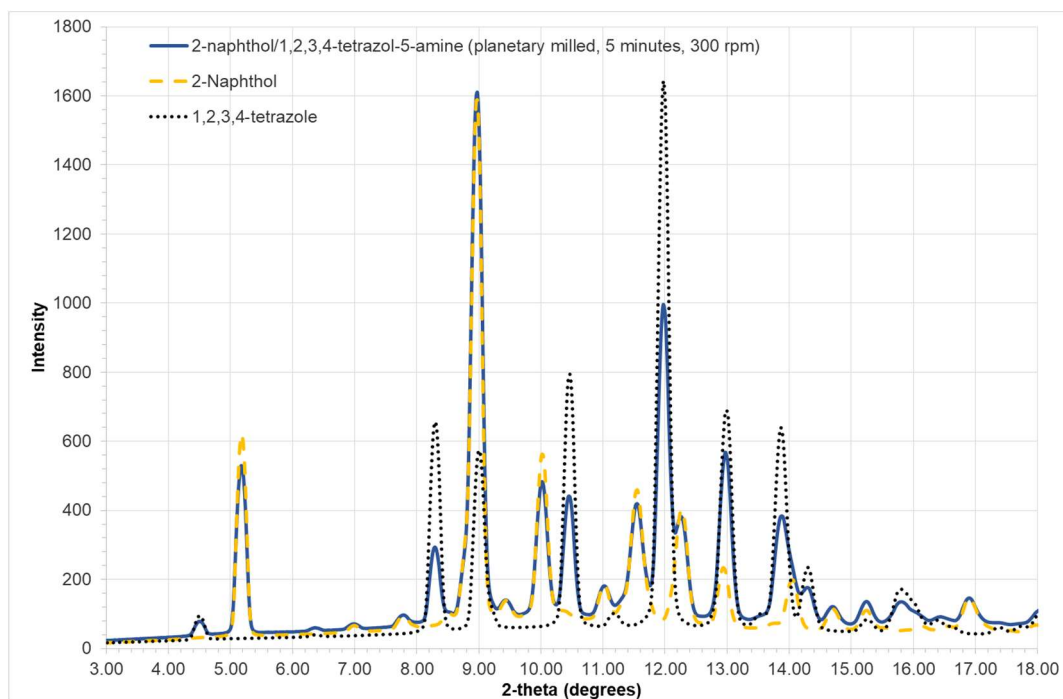


Figure C.96 – Powder x-ray pattern of 2-naphthol/1,2,3,4-tetrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

C.57 2-naphthol/5-methyl-1,2,3,4-tetrazole

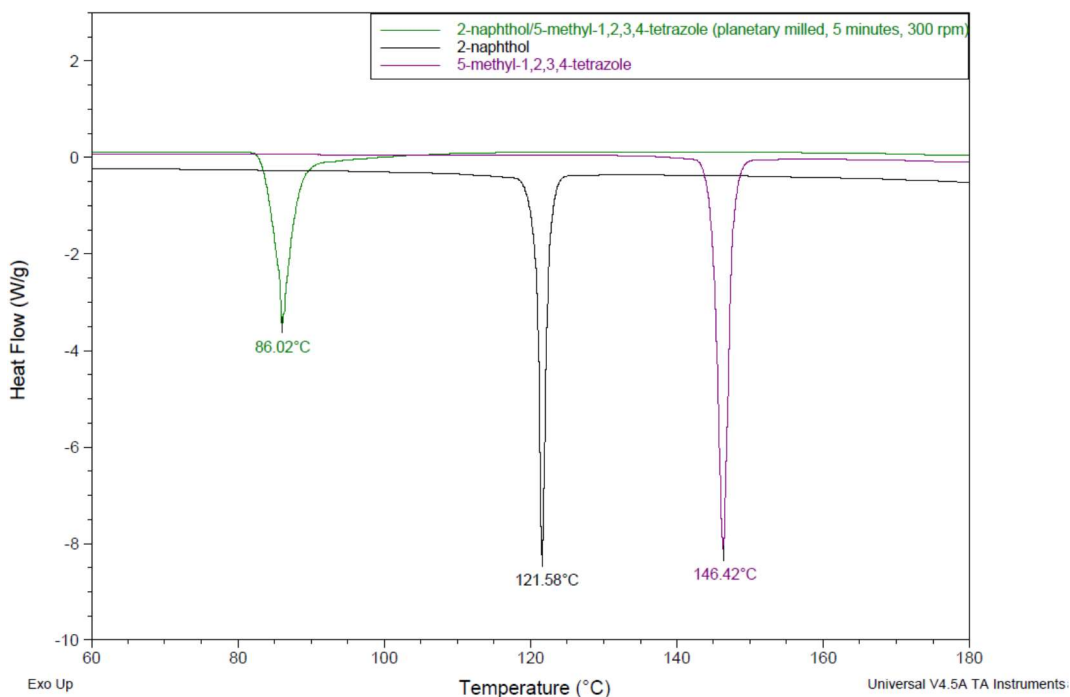


Figure C.97 - Thermal analysis of 2-naphthol/5-methyl-1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

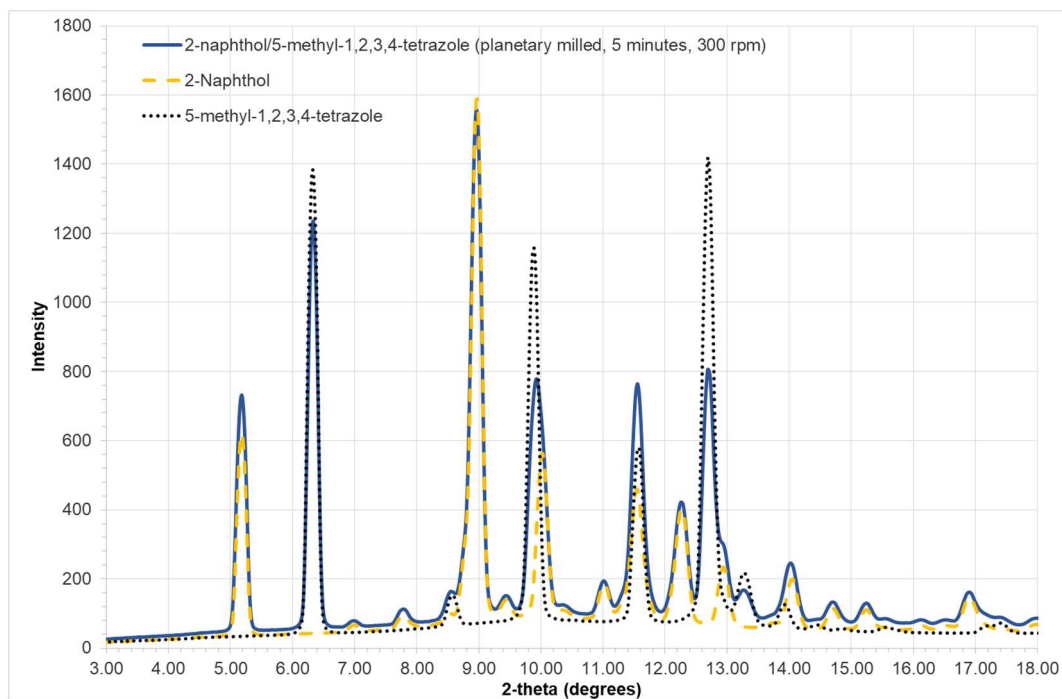


Figure C.98 – Powder x-ray pattern of 2-naphthol/5-methyl-1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

C.58 2-naphthol/3-nitro-1,2,4-triazol-5-one

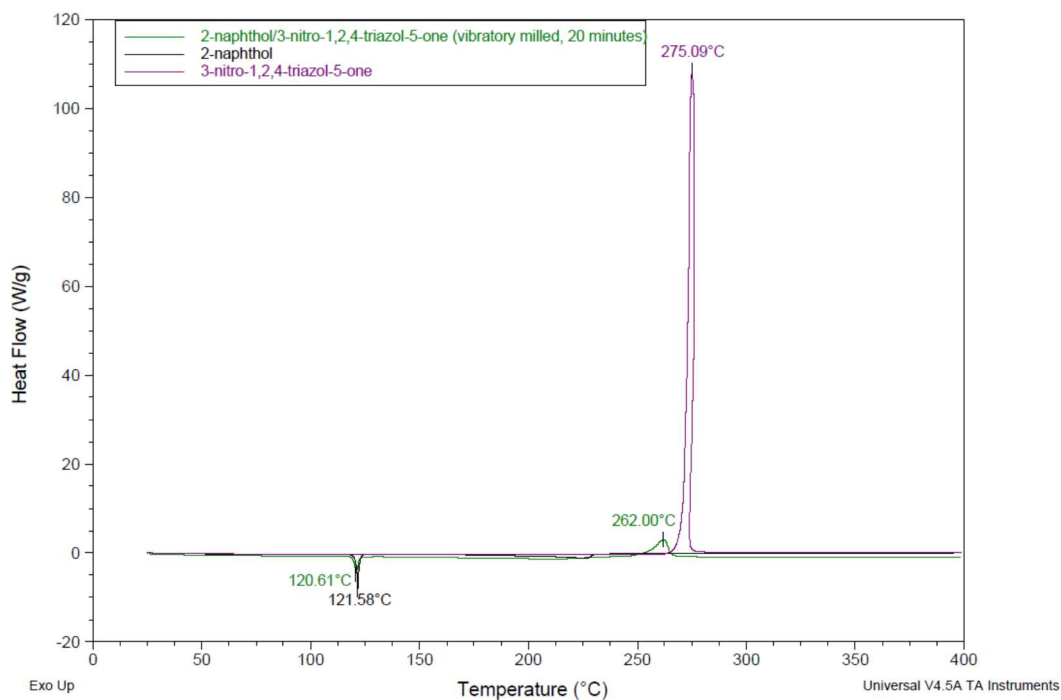


Figure C.99 - Thermal analysis of 2-naphthol/3-nitro-1,2,4-triazol-5-one produced by planetary milling for 5 minutes at 300 rpm.

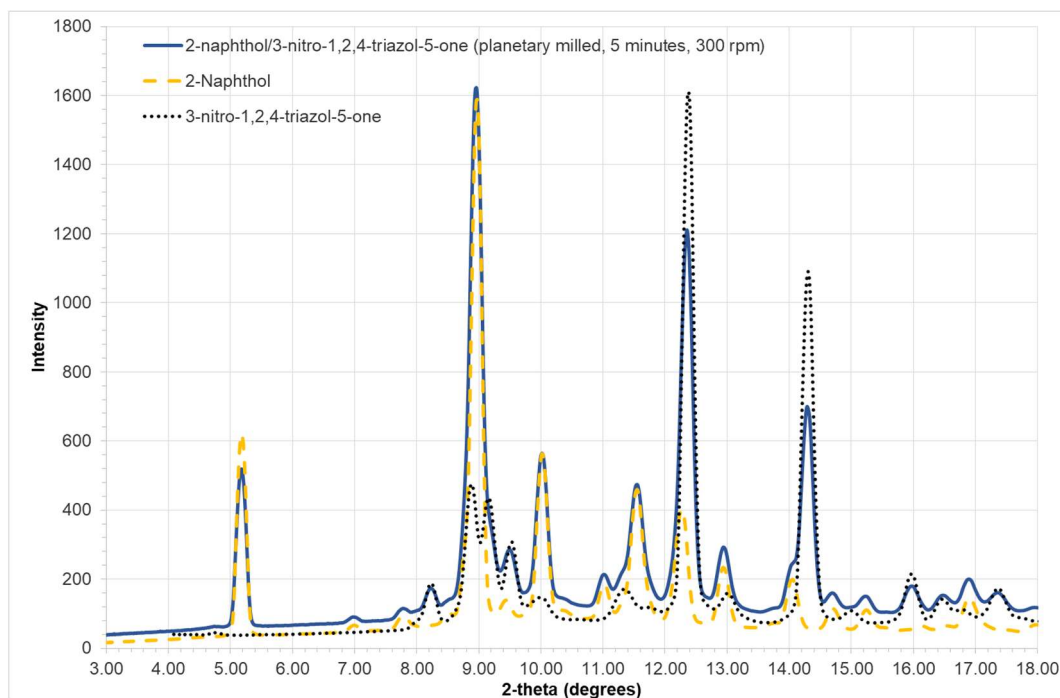


Figure C.100 – Powder x-ray analysis of 2-naphthol/3-nitro-1,2,4-triazol-5-one produced by planetary milling for 5 minutes at 300 rpm.

C.59 Molecular Electrostatic Potentials

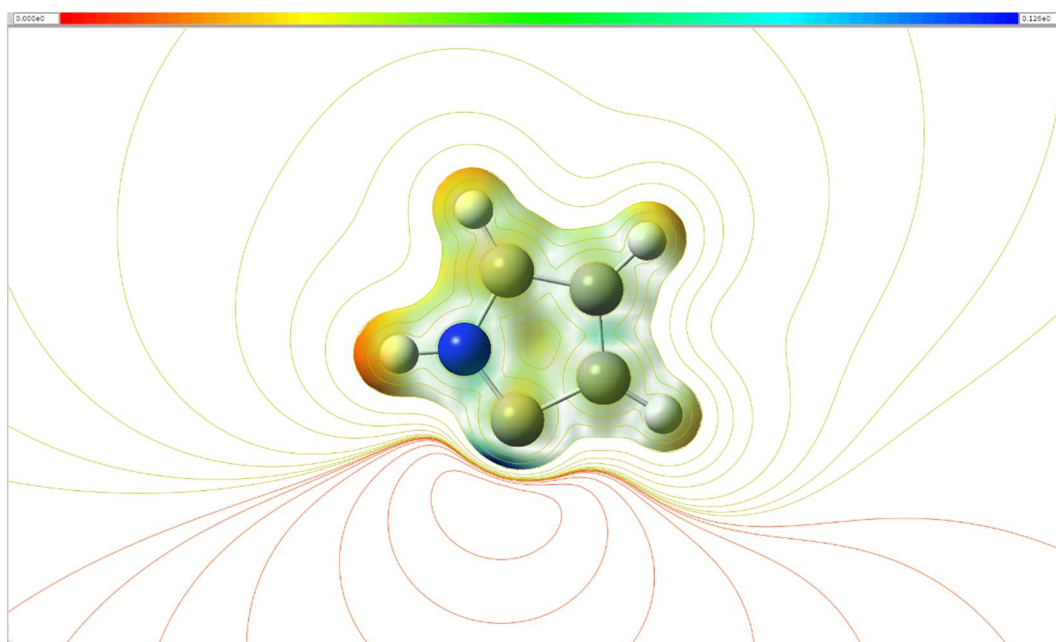


Figure C.101 - Molecular electrostatic potential map of pyrrolidine.

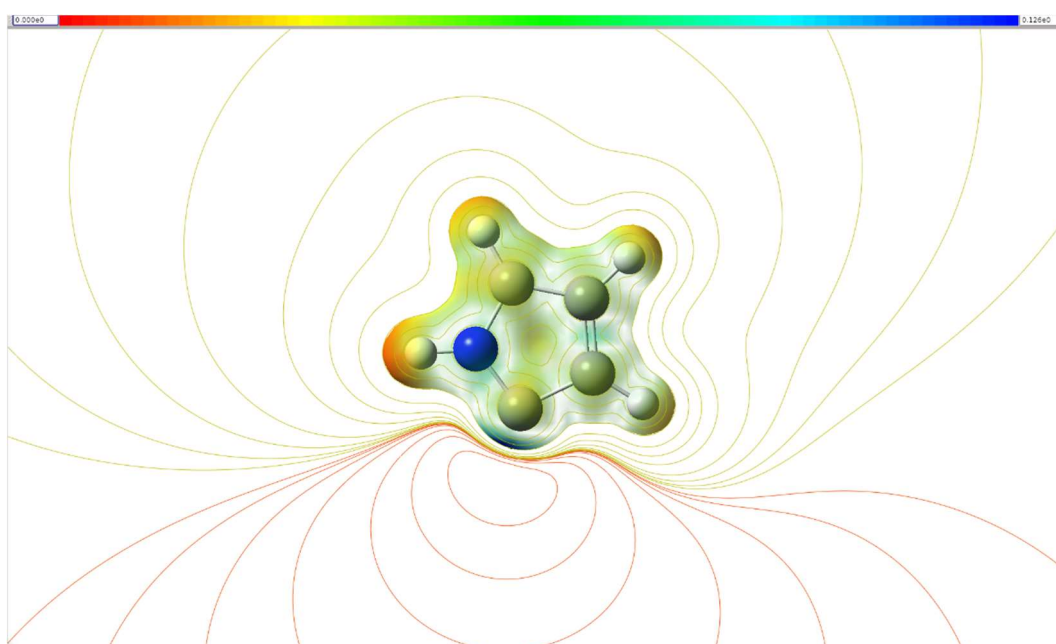


Figure C.102 - Molecular electrostatic potential map of 3-pyrroline.

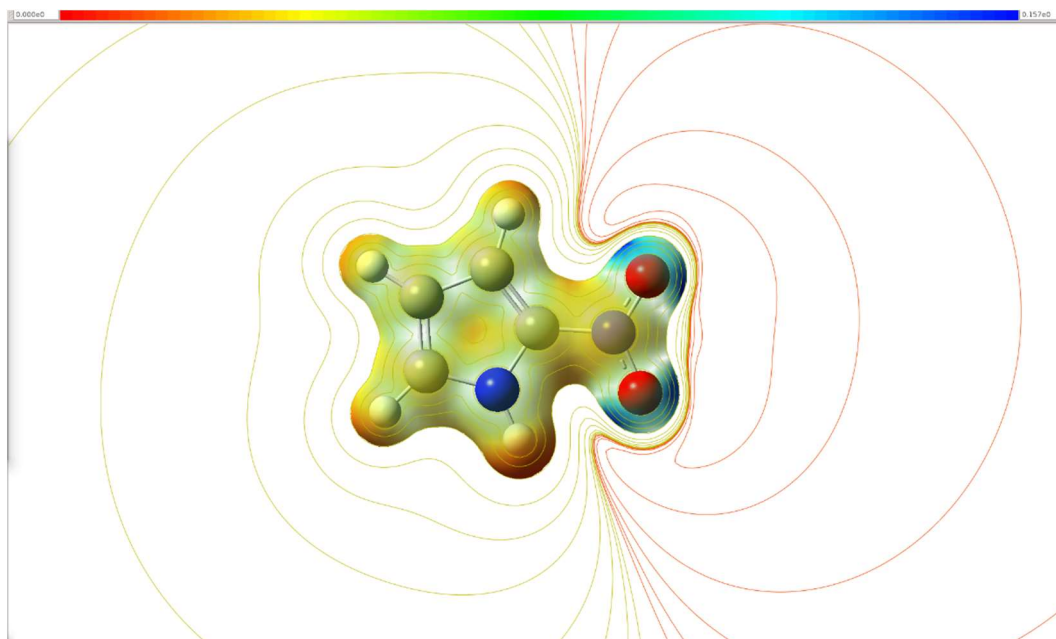


Figure C.103 - Molecular electrostatic potential map of 2-nitropyrrole.

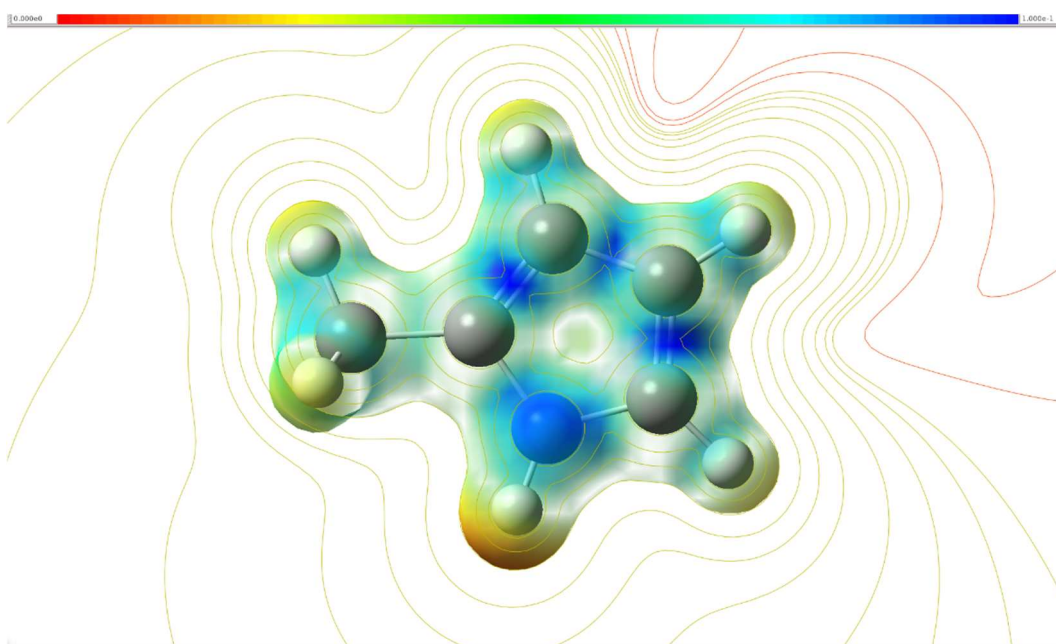


Figure C.104 - Molecular electrostatic potential map of 2-methylpyrrole.

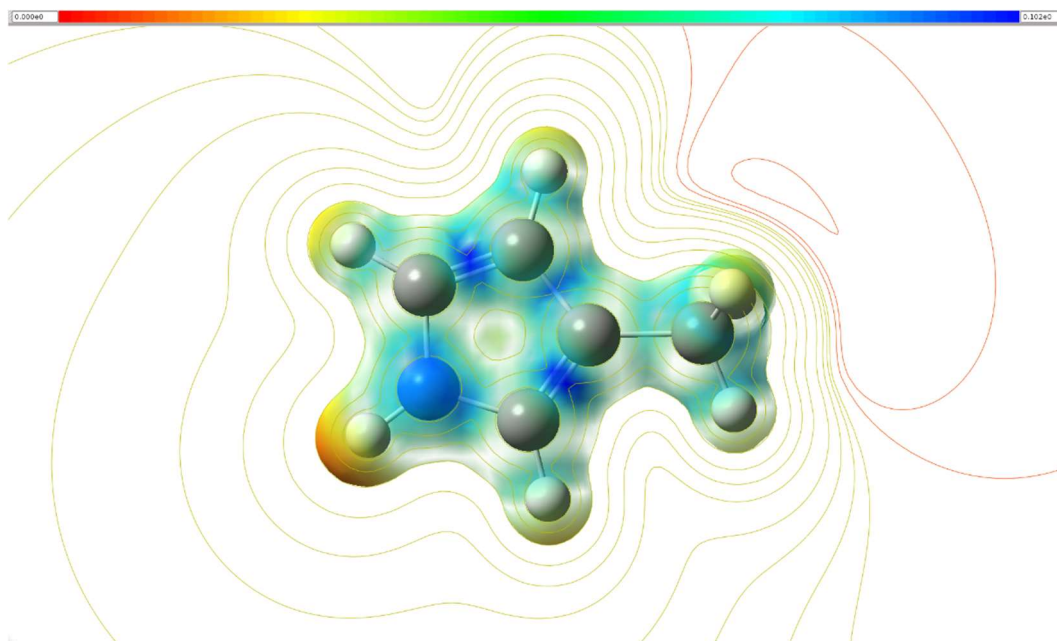


Figure C.105 - Molecular electrostatic potential map of 3-methylpyrrole.

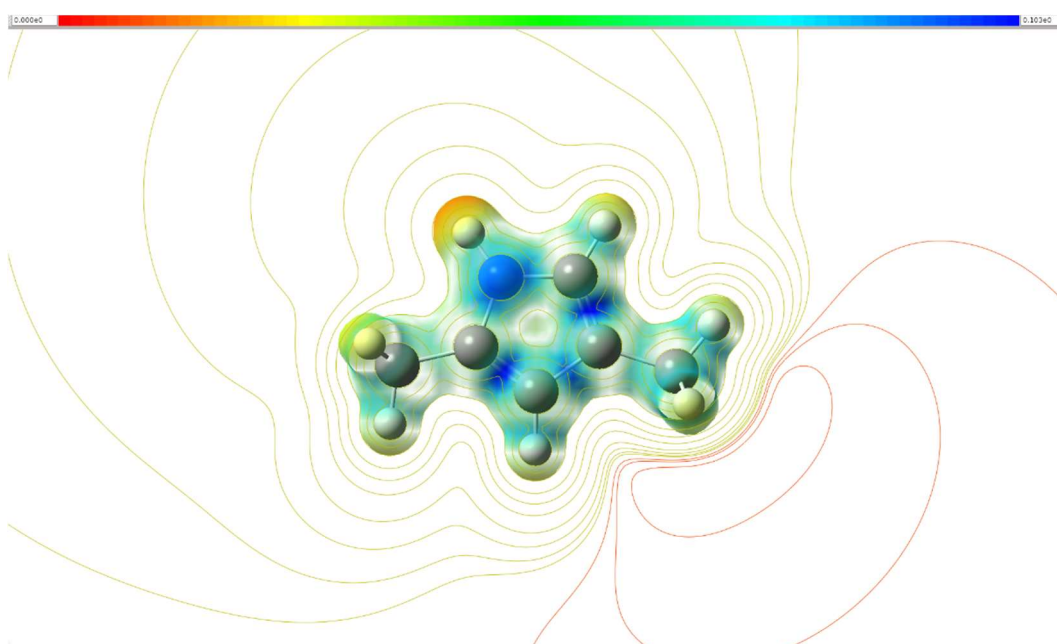


Figure C.106 - Molecular electrostatic potential map of 2,4-dimethylpyrrole.

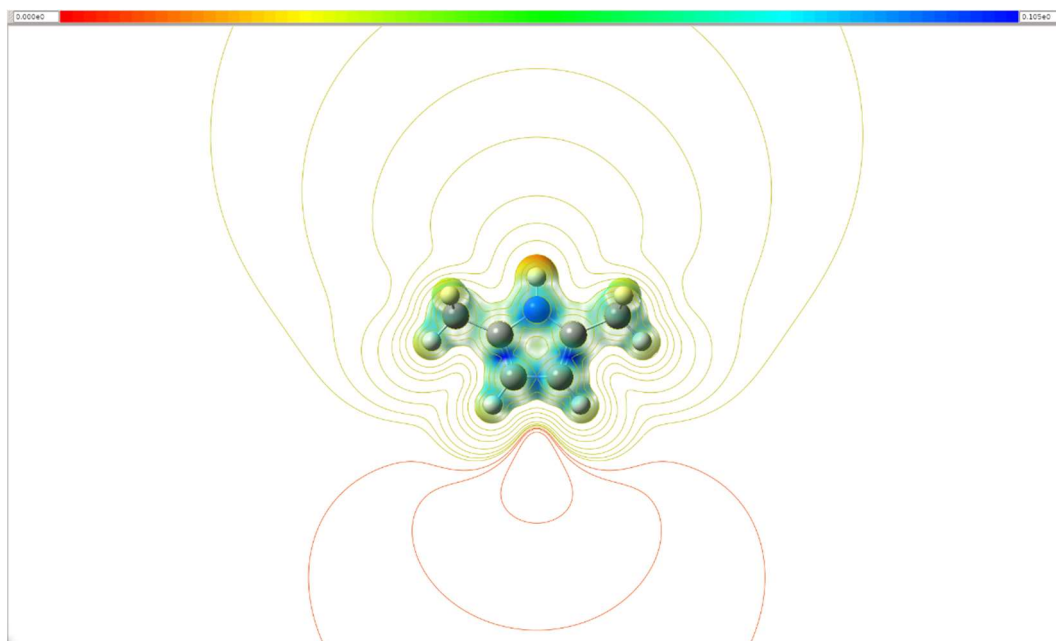


Figure C.107 - Molecular electrostatic potential map of 2,5-dimethylpyrrole.

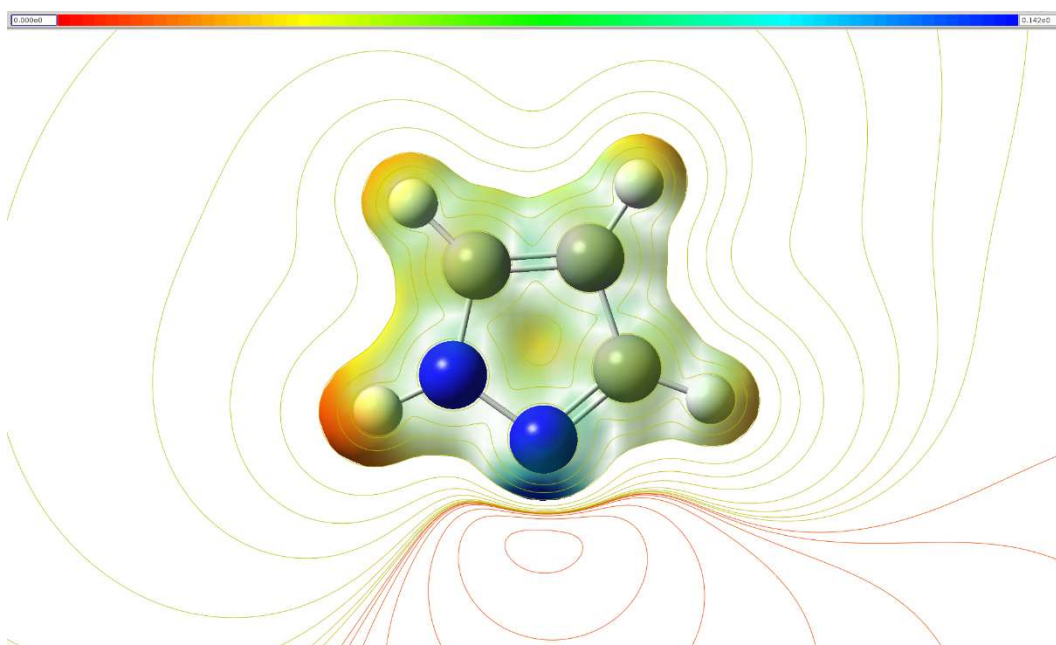


Figure C.108 - Molecular electrostatic potential map of pyrazole.

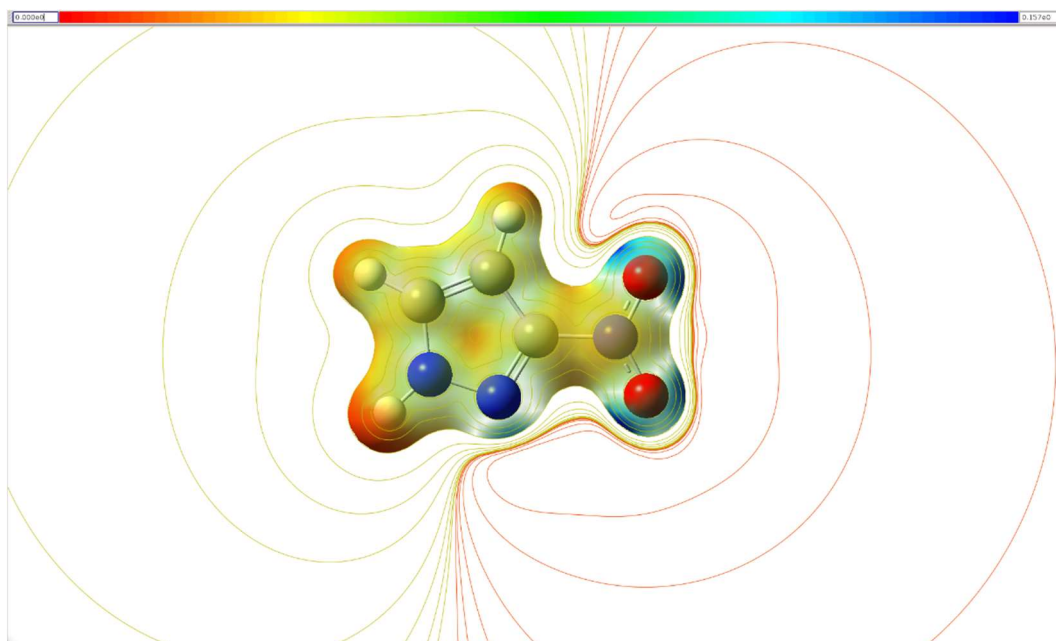


Figure C.109 - Molecular electrostatic potential map of 3-nitropyrazole.

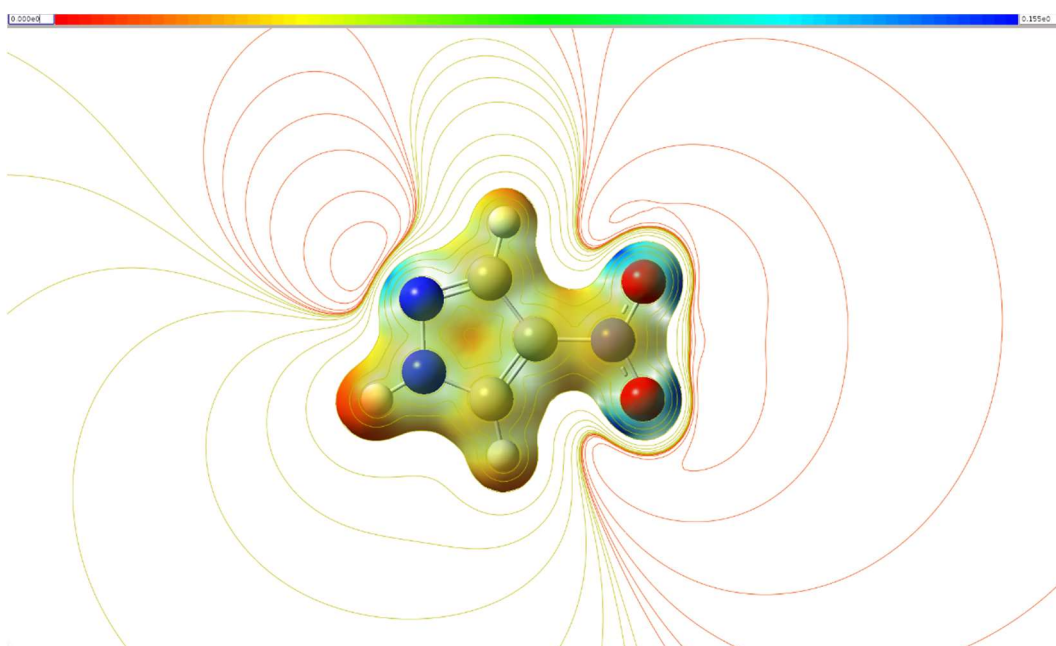


Figure C.110 - Molecular electrostatic potential map of 4-nitropyrazole.

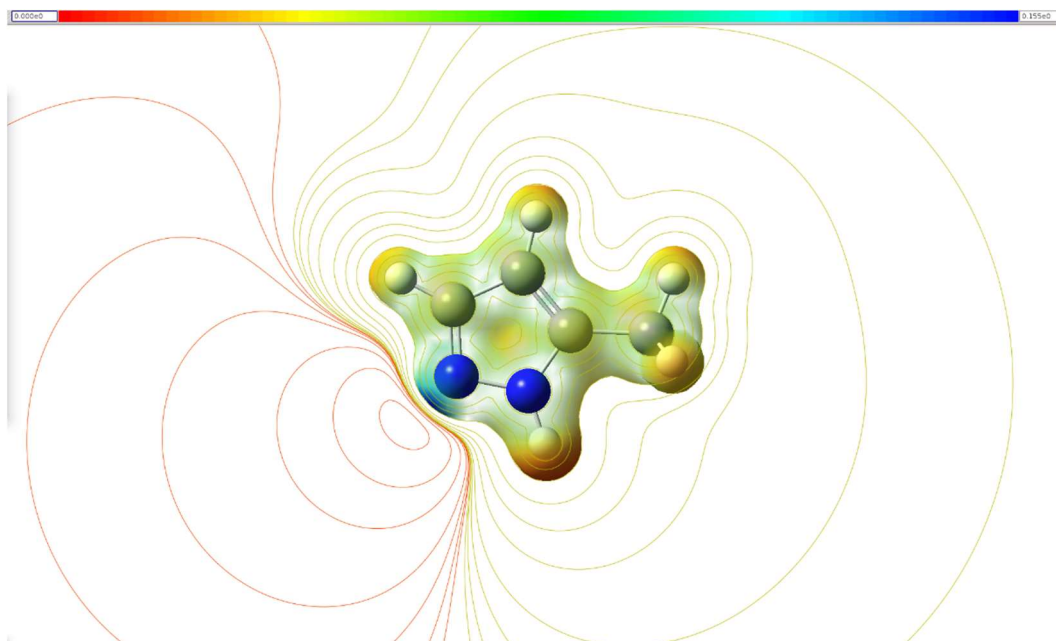


Figure C.111 - Molecular electrostatic potential map of 5-methylpyrazole.

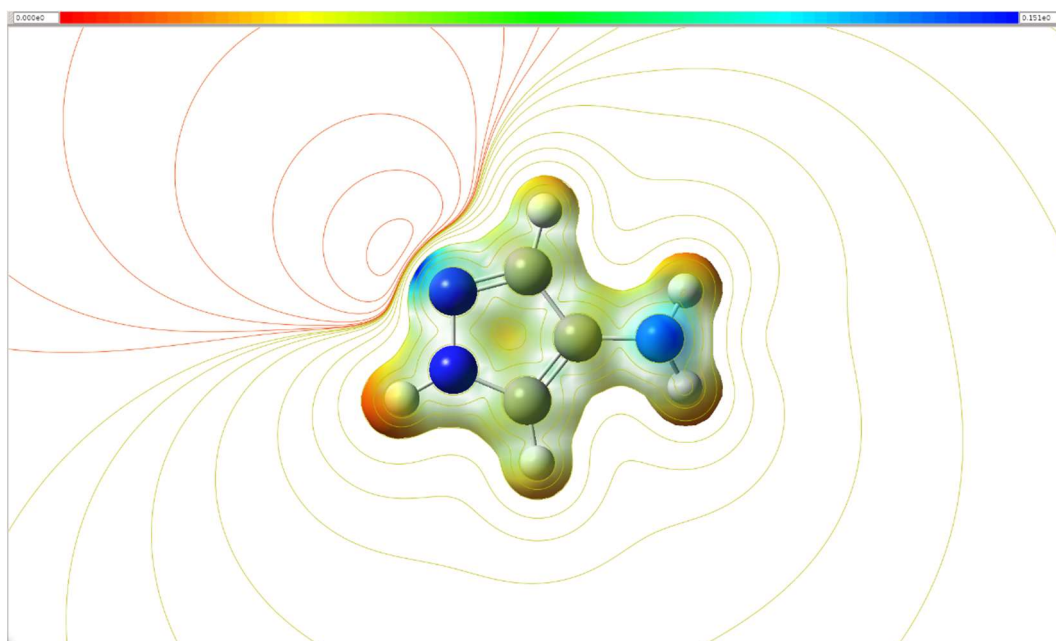


Figure C.112 - Molecular electrostatic potential map of pyrazol-4-amine.

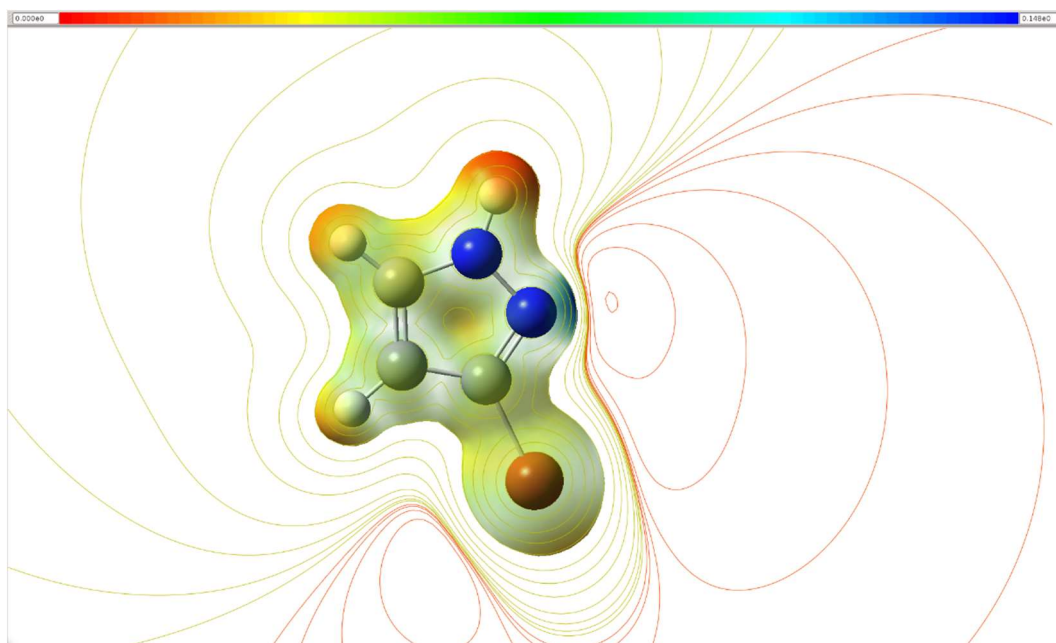


Figure C.113 - Molecular electrostatic potential map of 3-bromopyrazole.

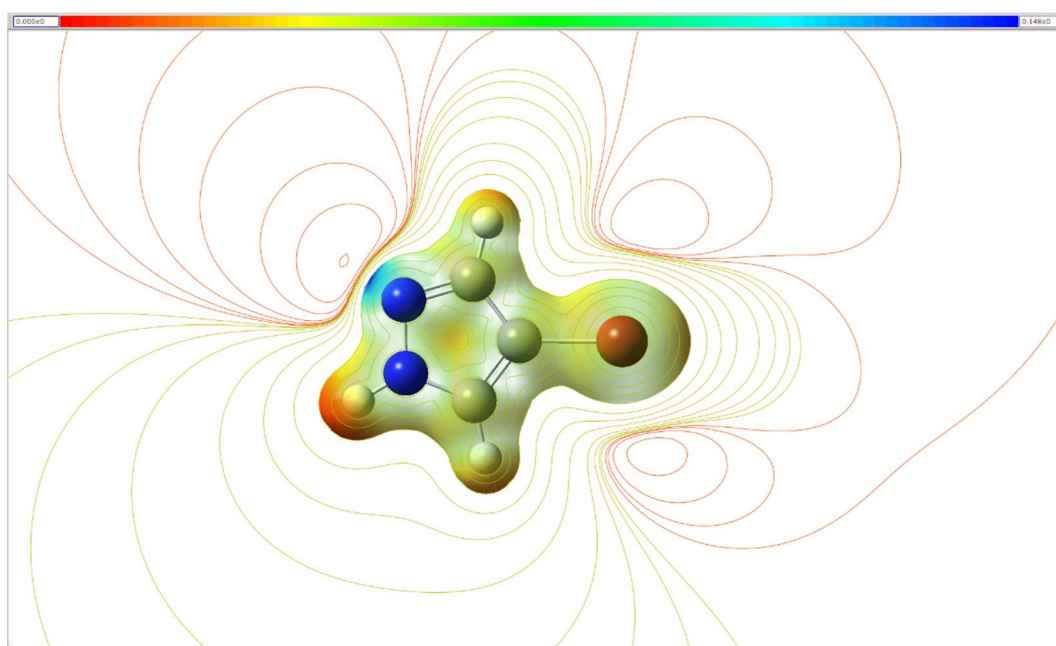


Figure C.114 - Molecular electrostatic potential map of 4-bromopyrazole.

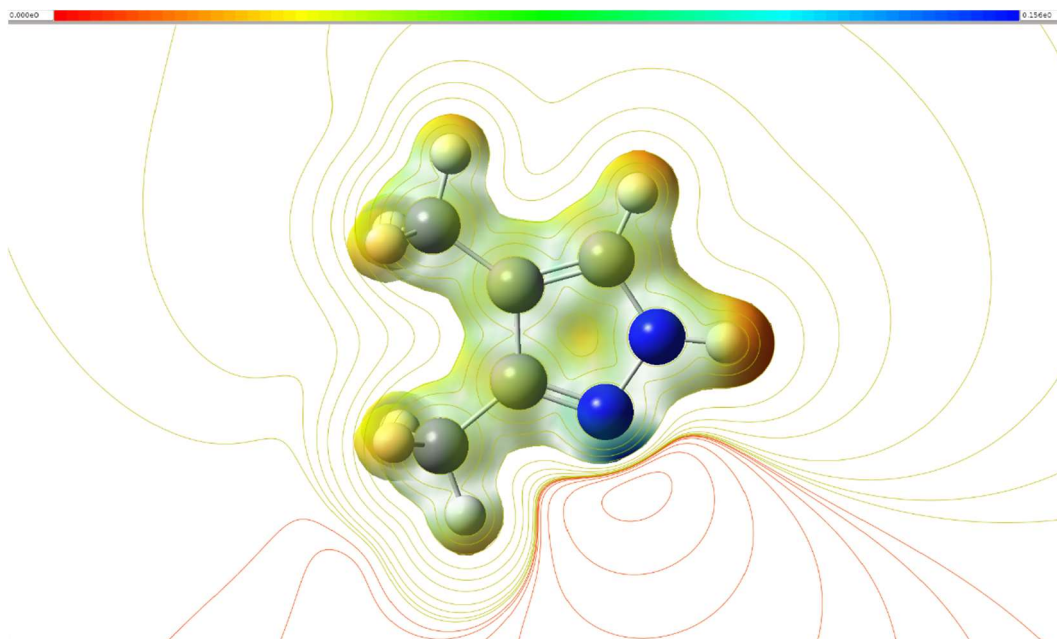


Figure C.115 - Molecular electrostatic potential map of 3,4-dimethylpyrazole.

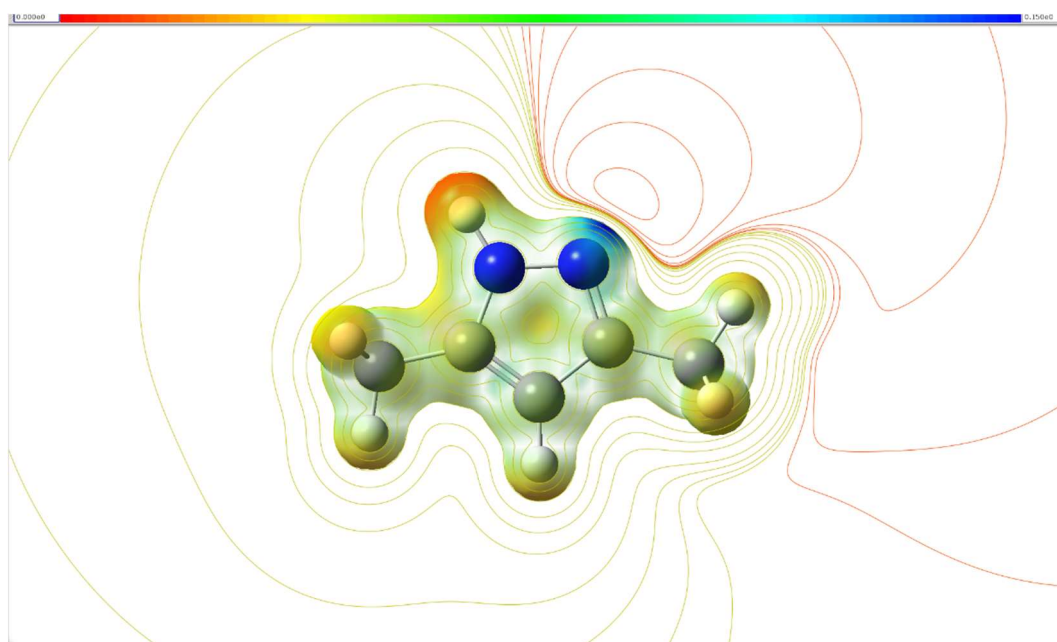


Figure C.116 - Molecular electrostatic potential map of 3,4-dimethylpyrazole.

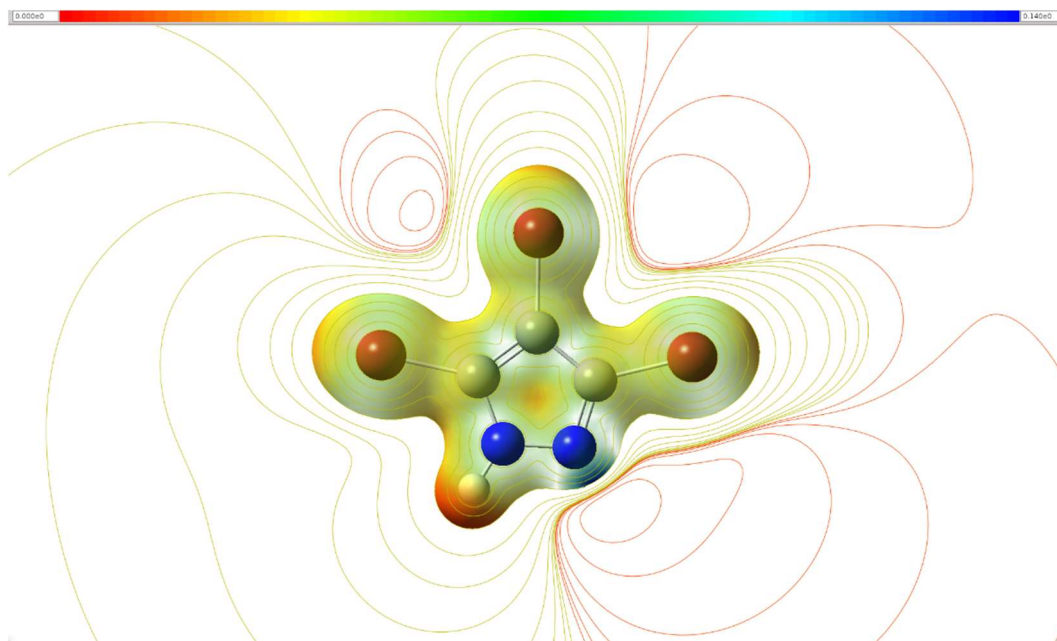


Figure C.117 - Molecular electrostatic potential map of 3,4,5-tribromopyrazole.

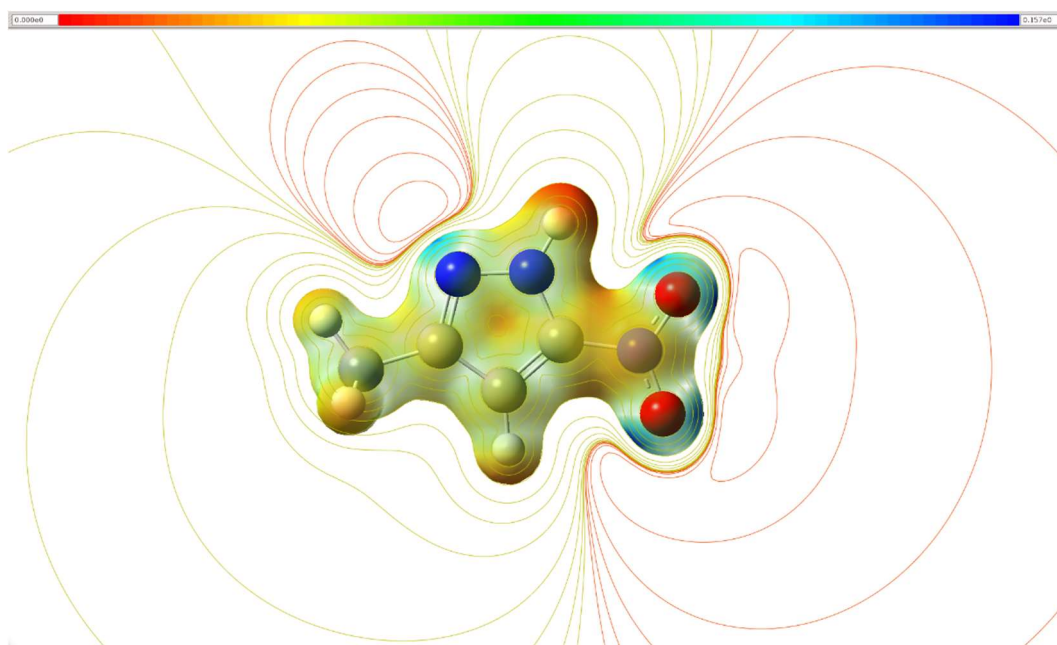


Figure C.118 - Molecular electrostatic potential map of 3-methyl-5-nitropyrazole.

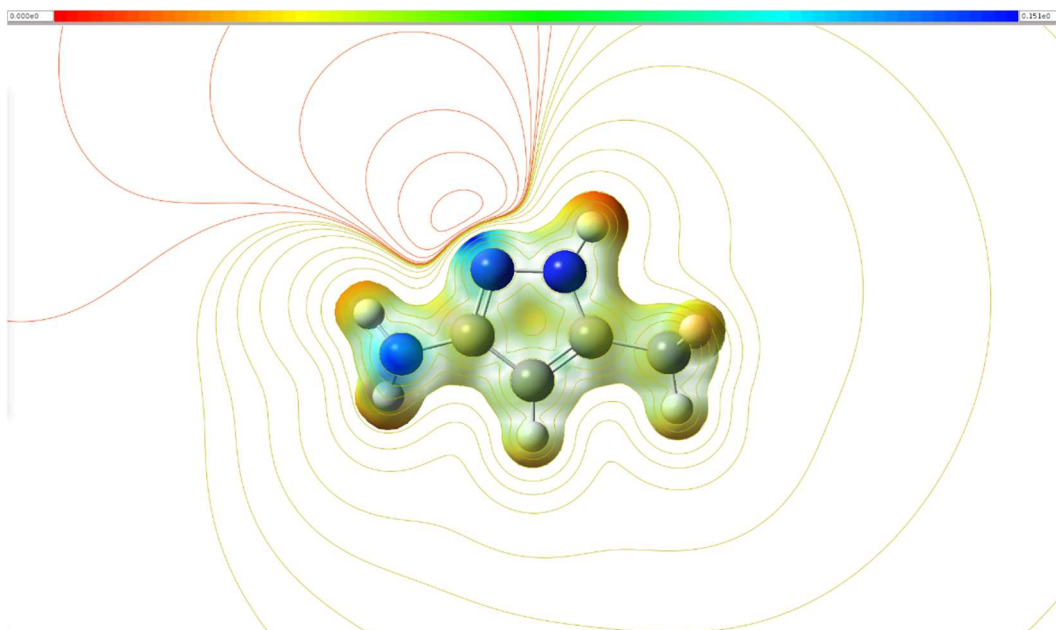


Figure C.119 - Molecular electrostatic potential map of 5-methylpyrazol-3-amine.

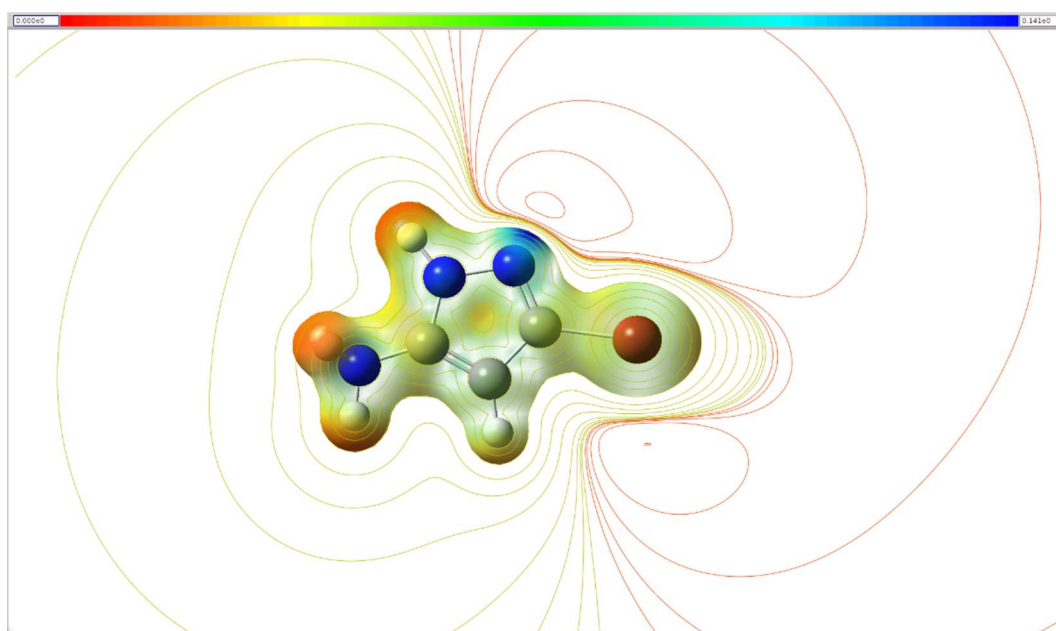


Figure C.120 - Molecular electrostatic potential map of 3-bromopyrazol-5-amine.

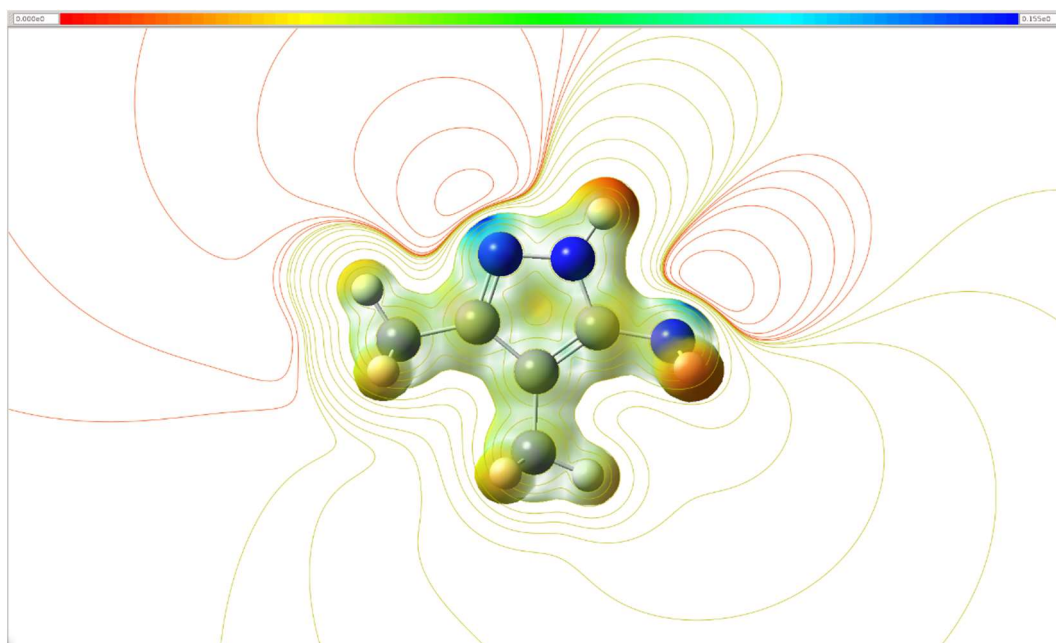


Figure C.121 - Molecular electrostatic potential map of 3,4-dimethylpyrazol-5-amine.

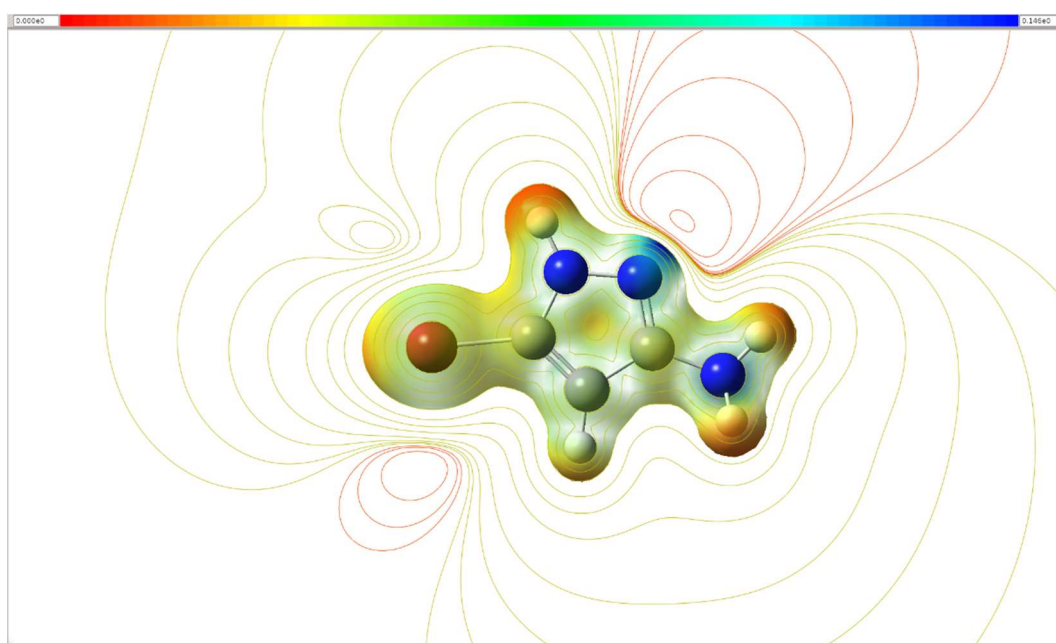


Figure C.122 - Molecular electrostatic potential map of 3-methyl-4-bromopyrazole.

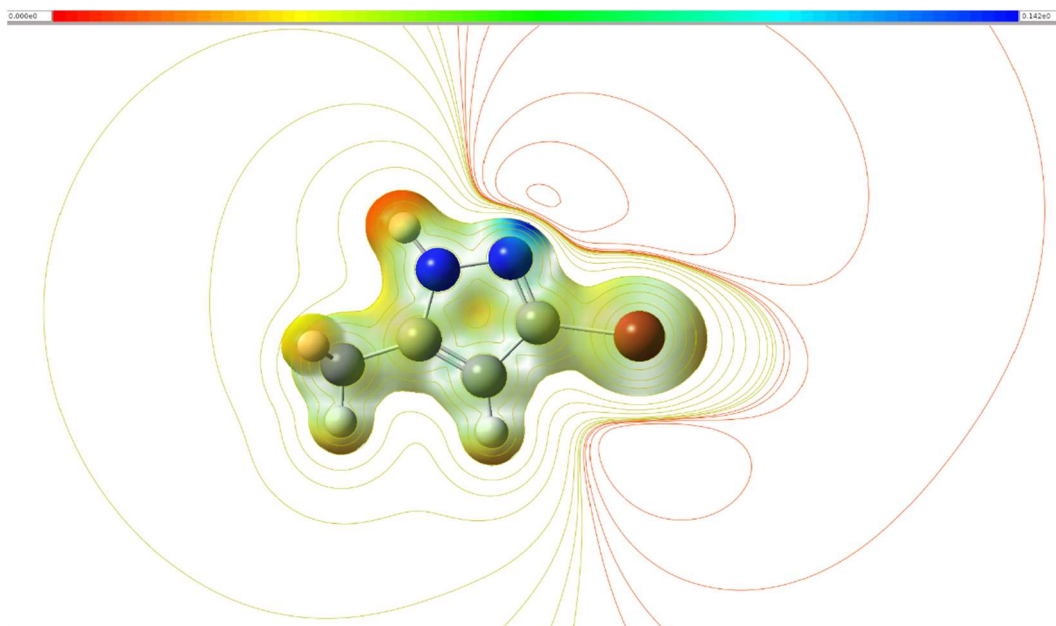


Figure C.123 - Molecular electrostatic potential map of 3-bromo-5-methylpyrazole.

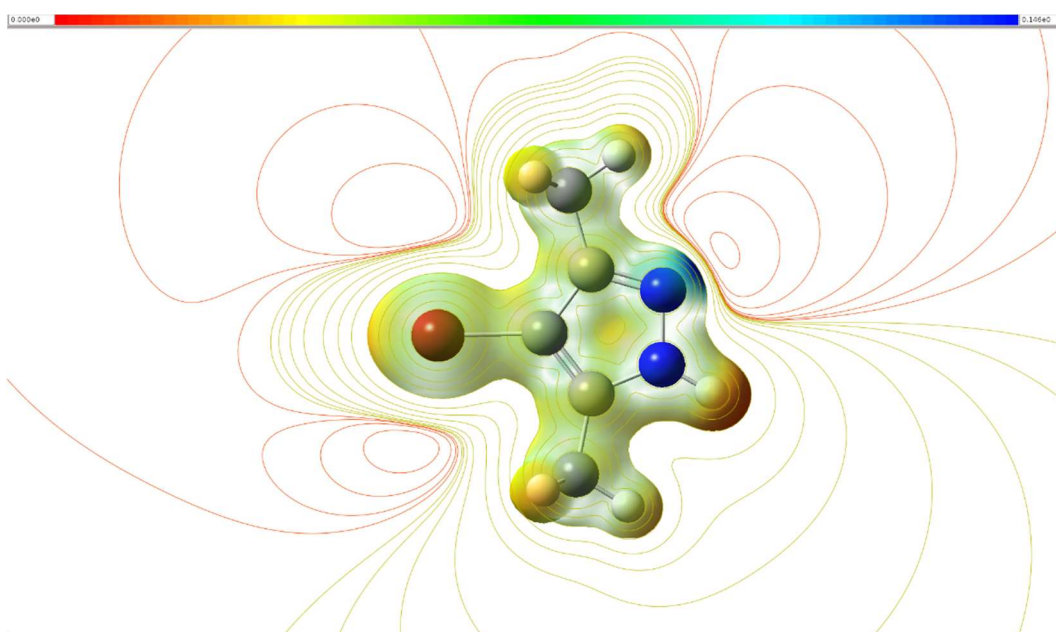


Figure C.124 - Molecular electrostatic potential map of 4-bromo-3,5-dimethylpyrazole.

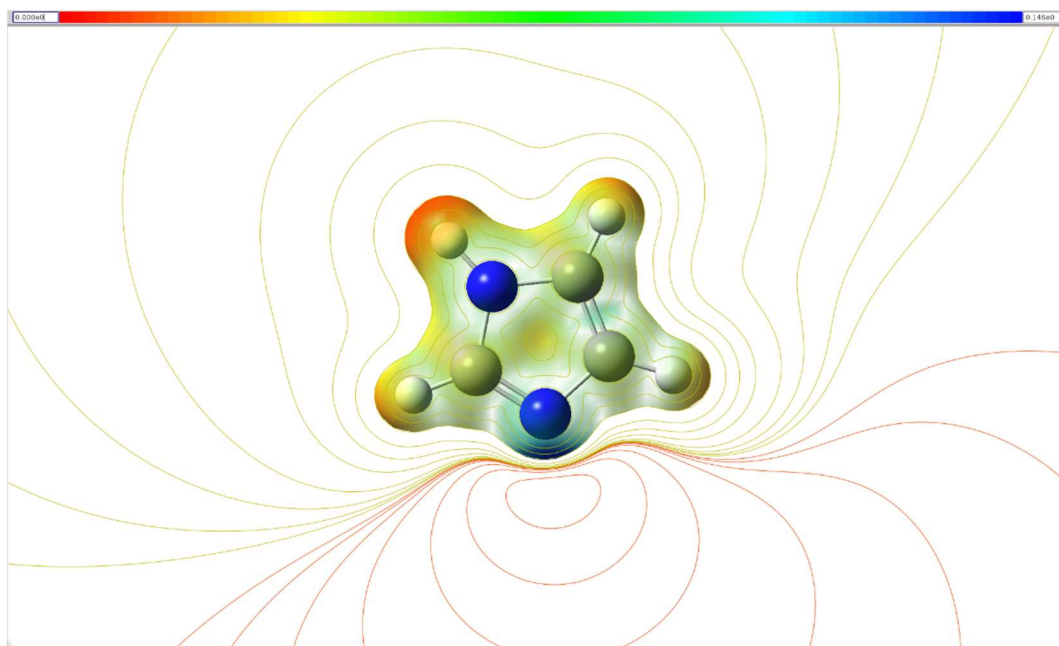


Figure C.125 - Molecular electrostatic potential map of imidazole.

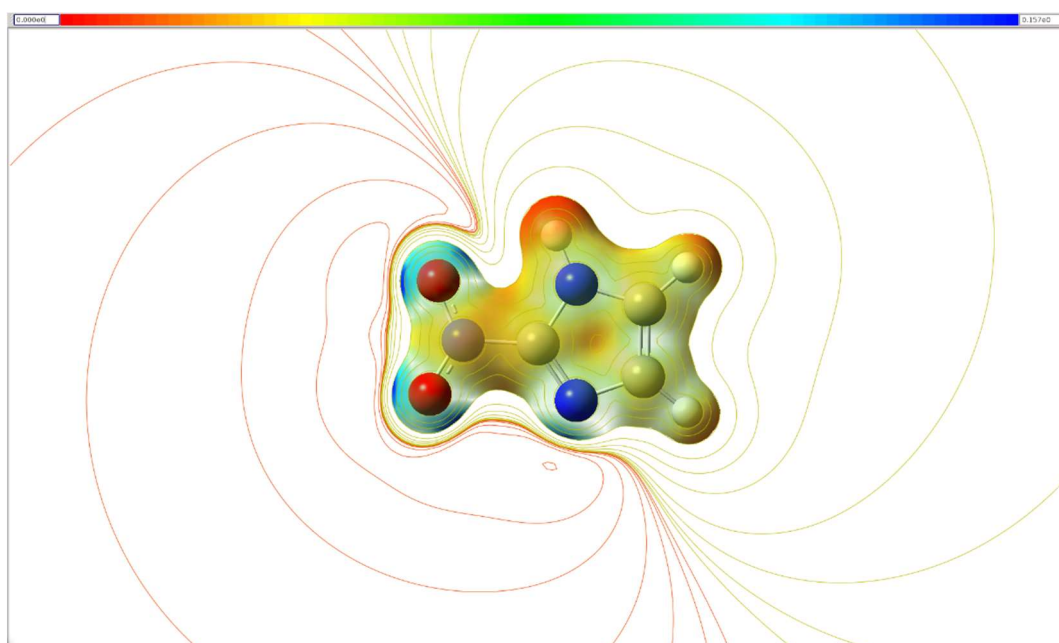


Figure C.126 - Molecular electrostatic potential map of 2-nitroimidazole.

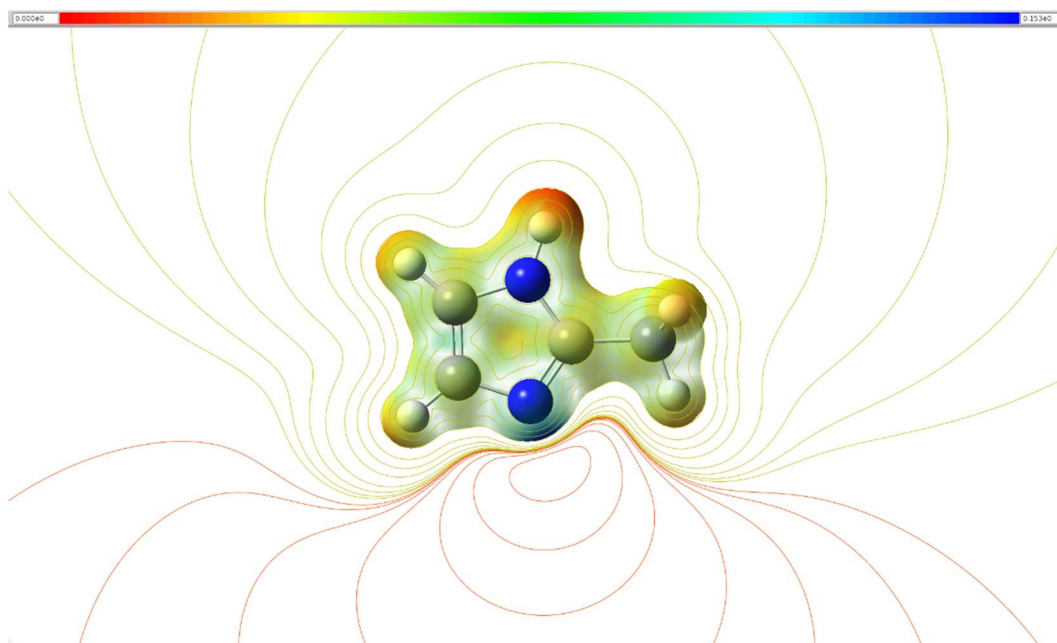


Figure C.127 - Molecular electrostatic potential map of 2-methylimidazole.

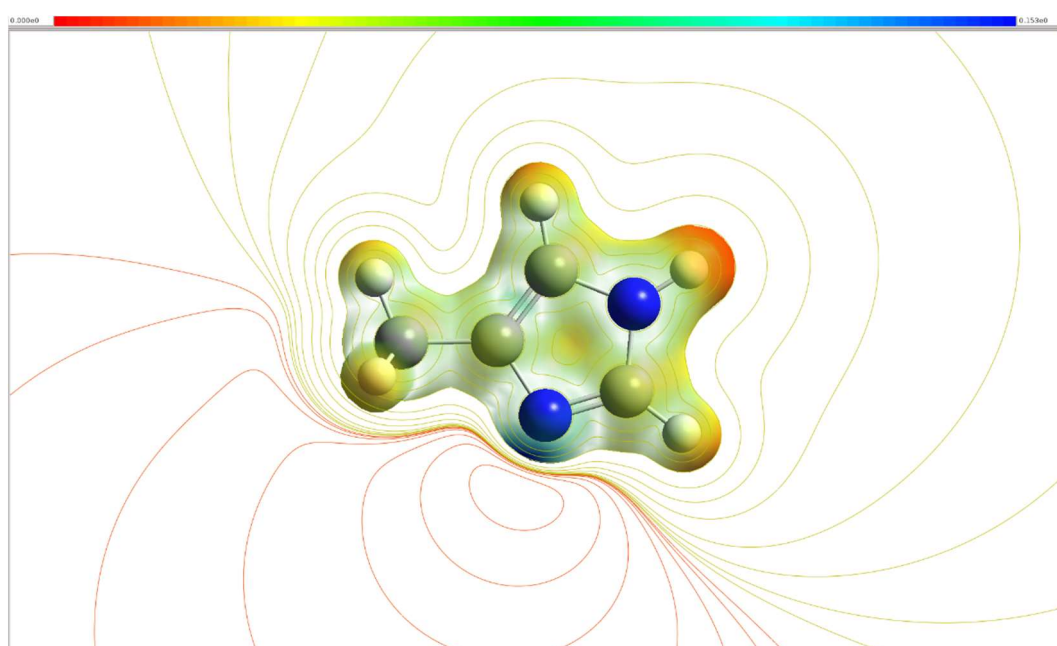


Figure C.128 - Molecular electrostatic potential map of 4-methylimidazole.

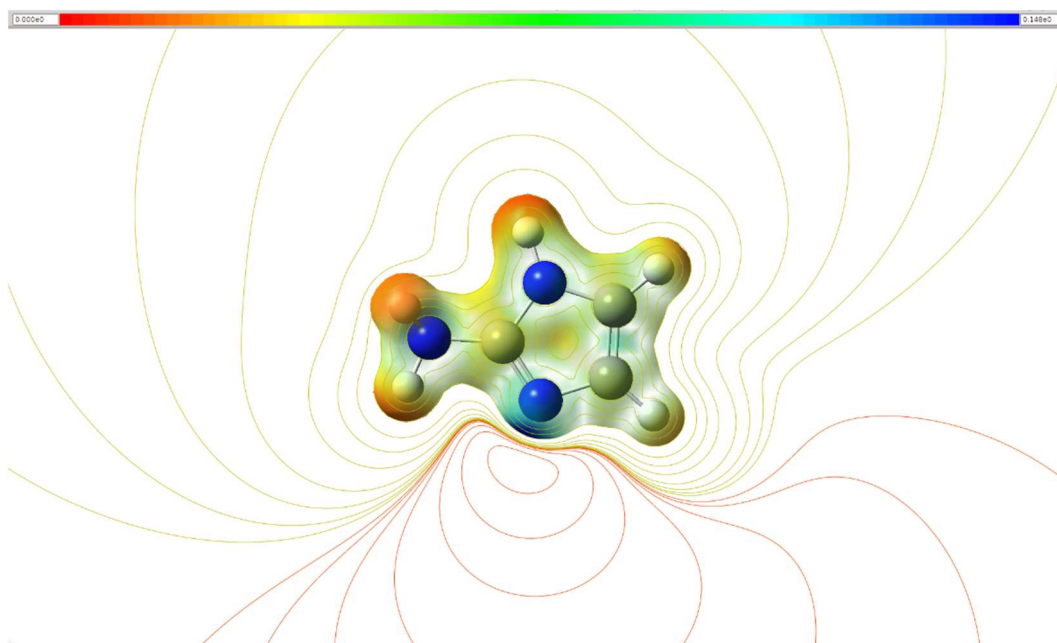


Figure C.129 - Molecular electrostatic potential map of imidazol-2-amine.

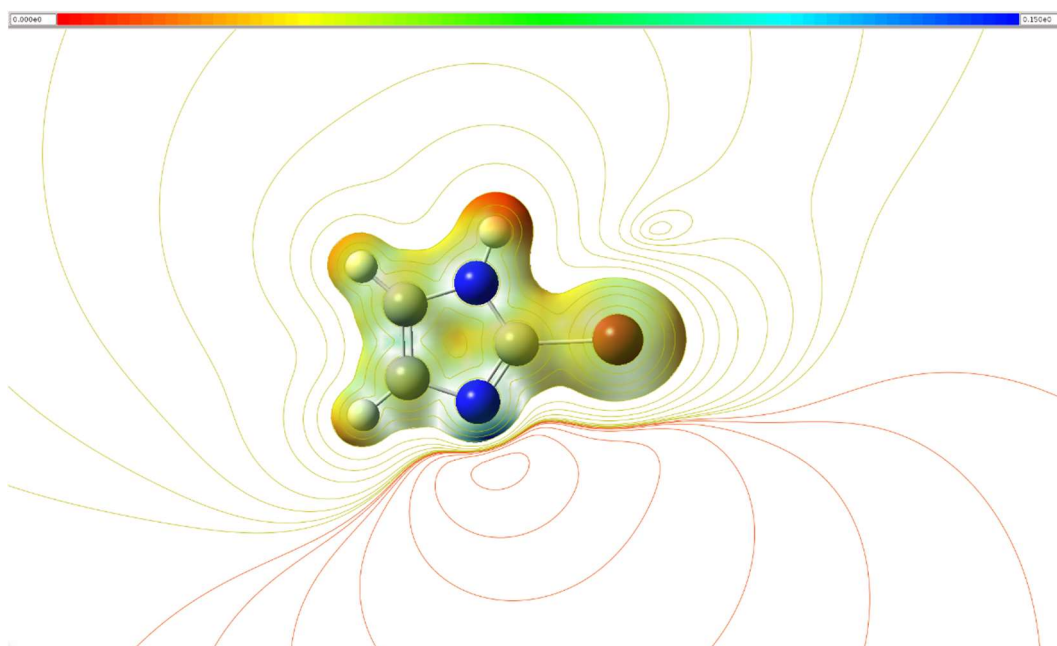


Figure C.130 - Molecular electrostatic potential map of 2-bromoimidazole.

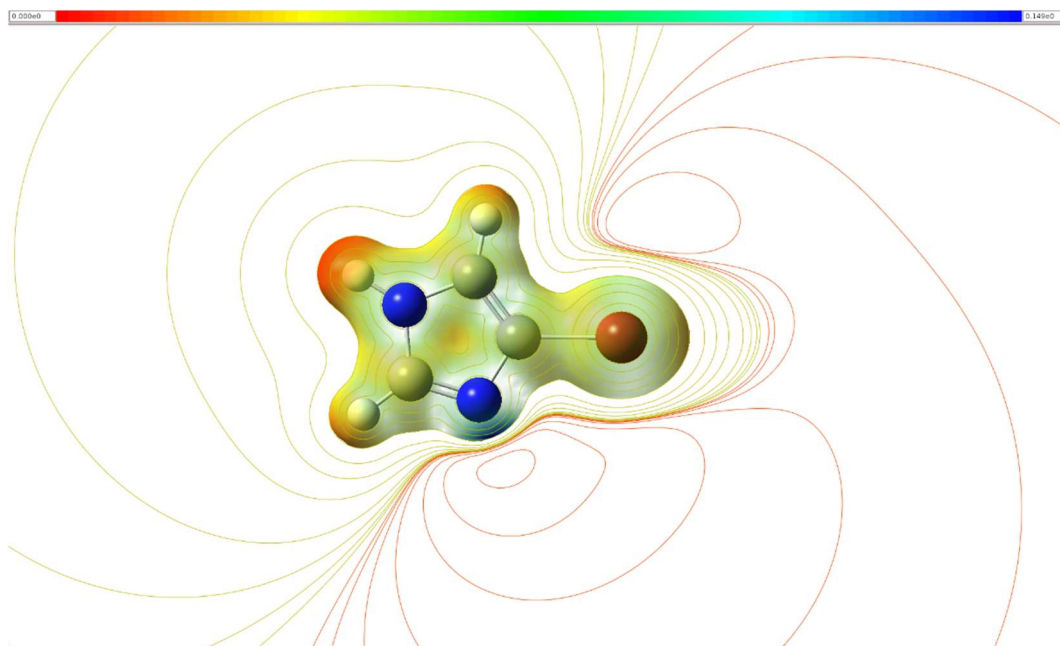


Figure C.131 - Molecular electrostatic potential map of 4-bromoimidazole.

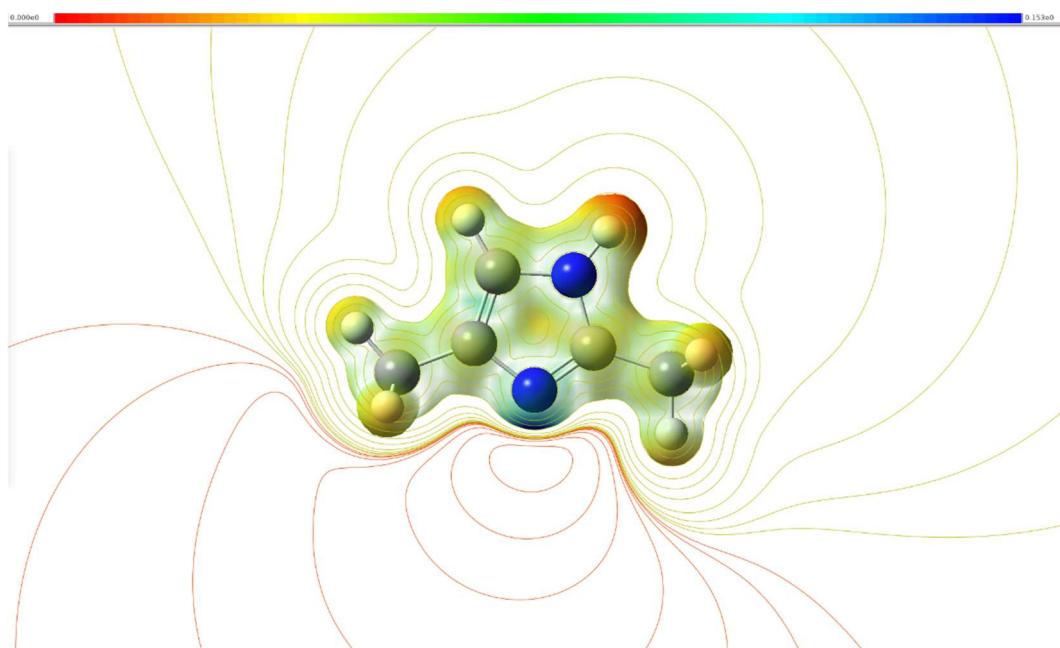


Figure C.132 - Molecular electrostatic potential map of 2,4-dimethylimidazole.

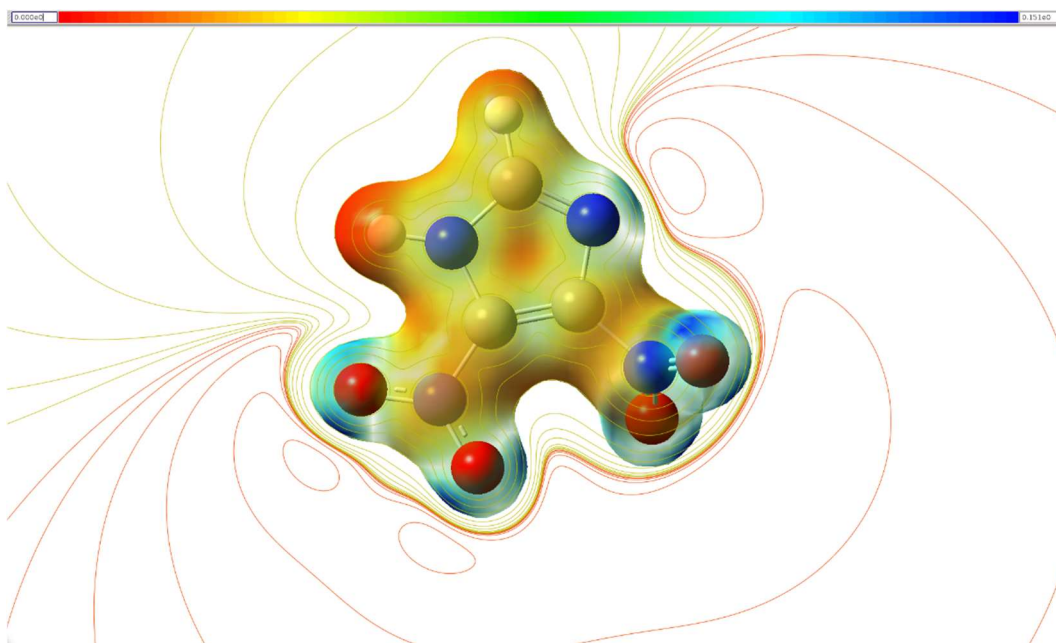


Figure C.133 - Molecular electrostatic potential map of 4,5-dinitroimidazole.

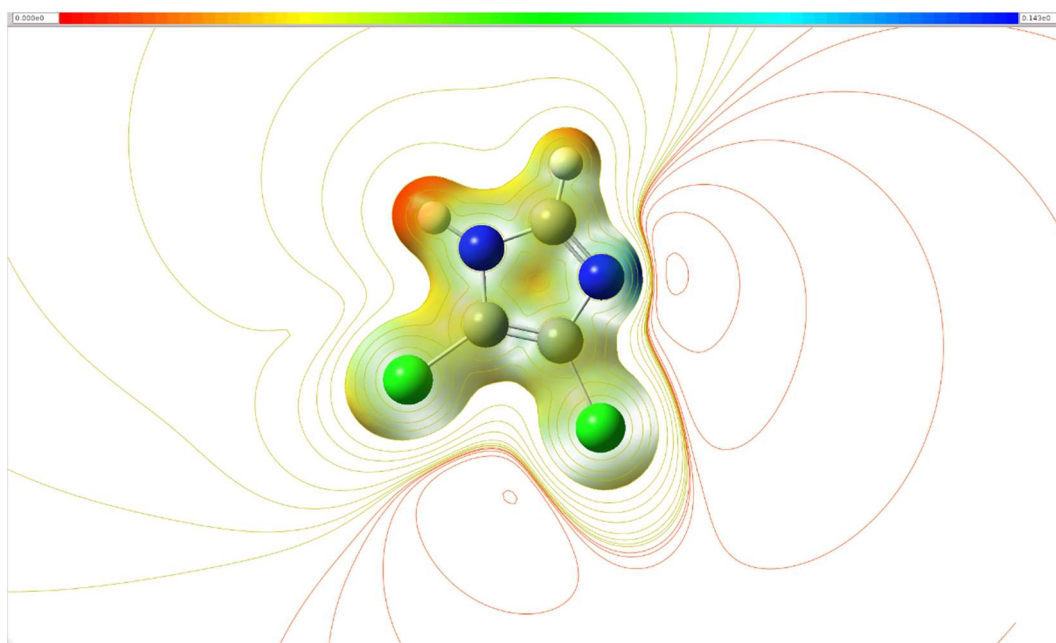


Figure C.134 - Molecular electrostatic potential map of 4,5-dichloroimidazole.

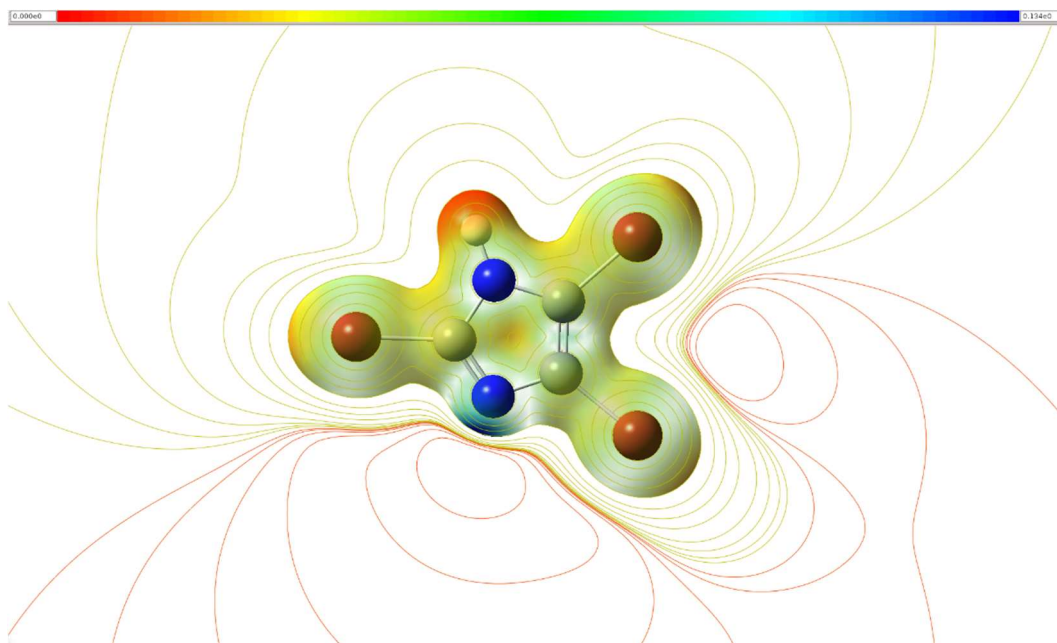


Figure C.135 - Molecular electrostatic potential map of 2,4,5-tribromoimidazole.

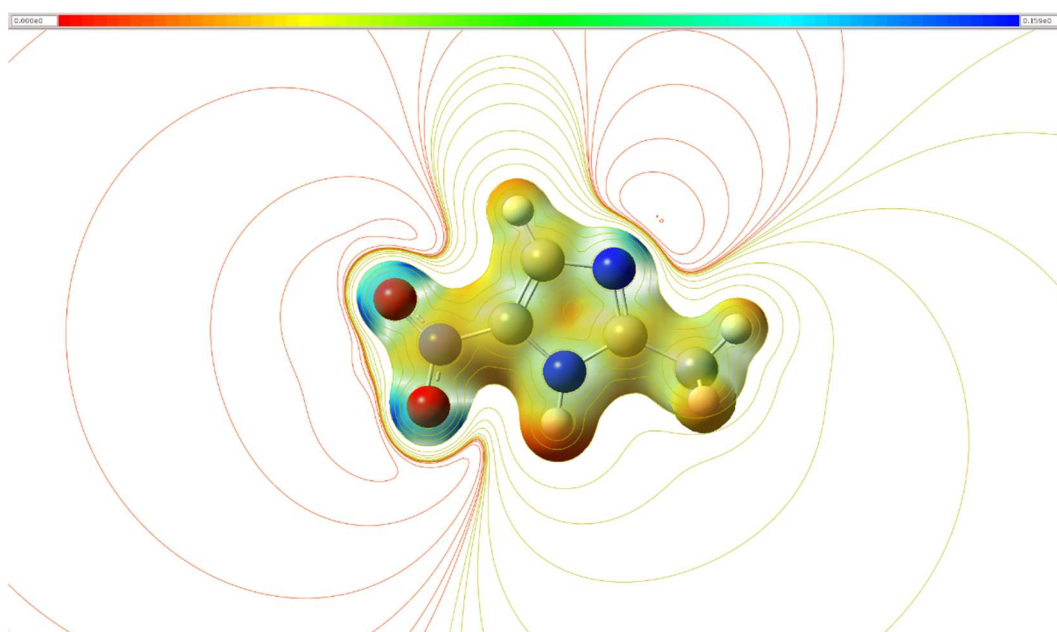


Figure C.136 - Molecular electrostatic potential map of 2-methyl-5-nitroimidazole.

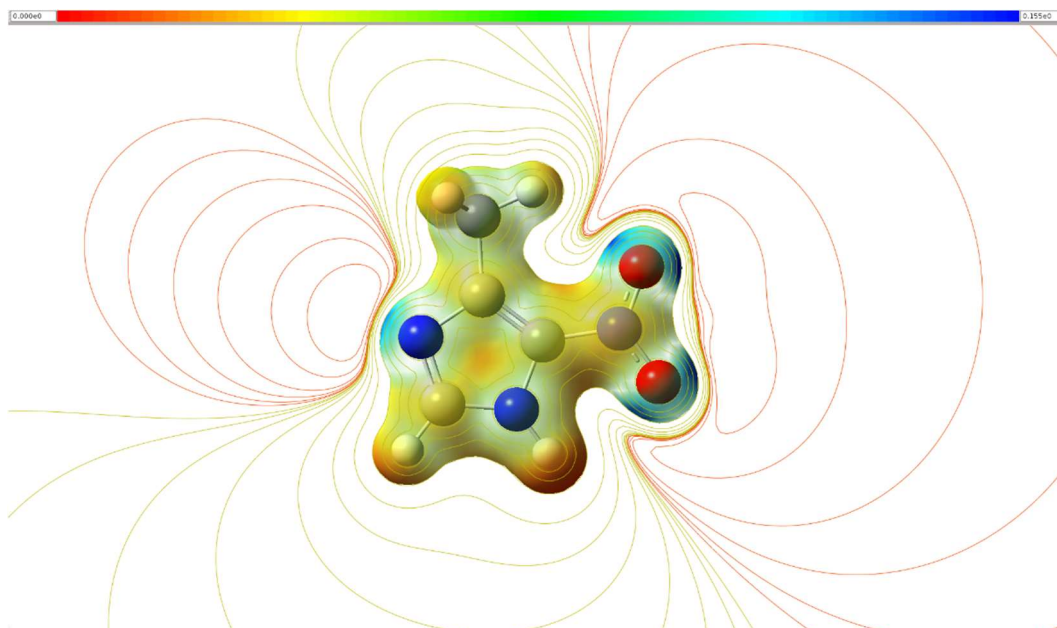


Figure C.137 - Molecular electrostatic potential map of 4-methyl-5-nitroimidazole.

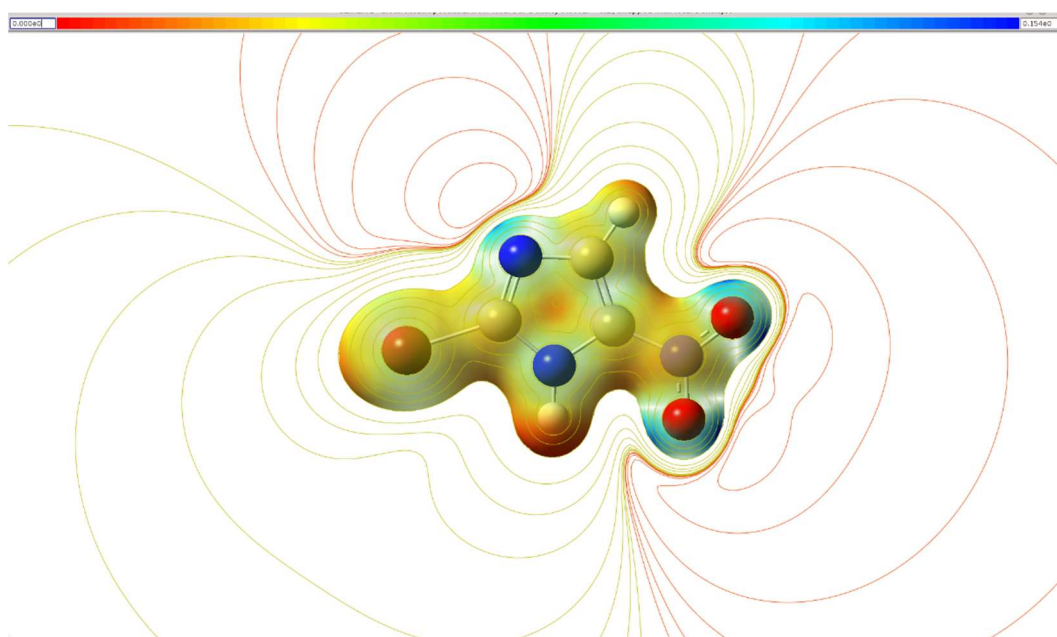


Figure C.138 - Molecular electrostatic potential map of 2-bromo-5-nitroimidazole.

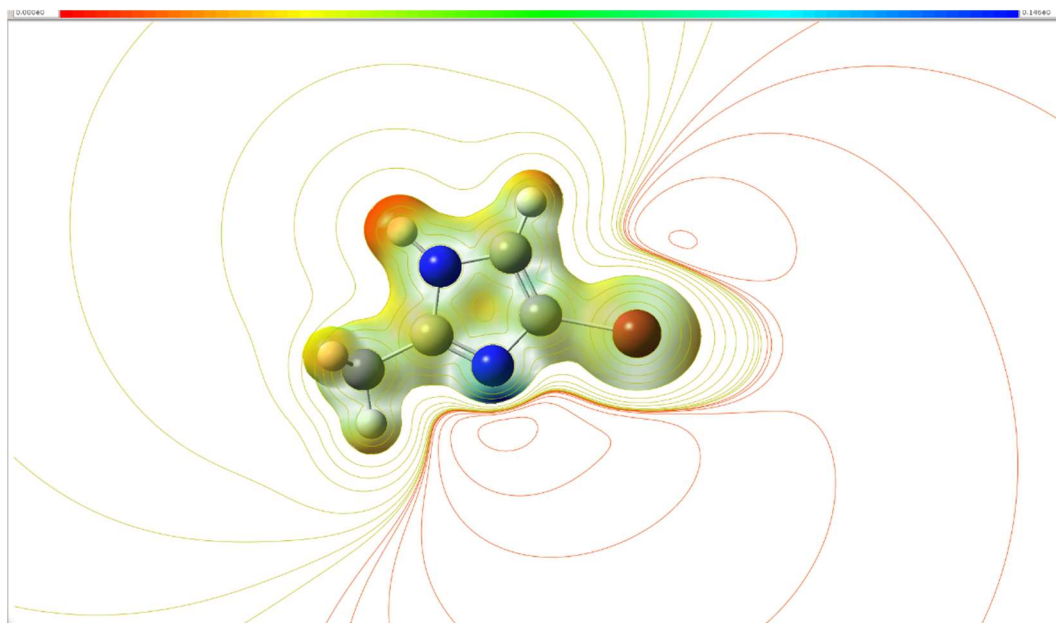


Figure C.139 - Molecular electrostatic potential map of 4-bromo-2-methylimidazole.

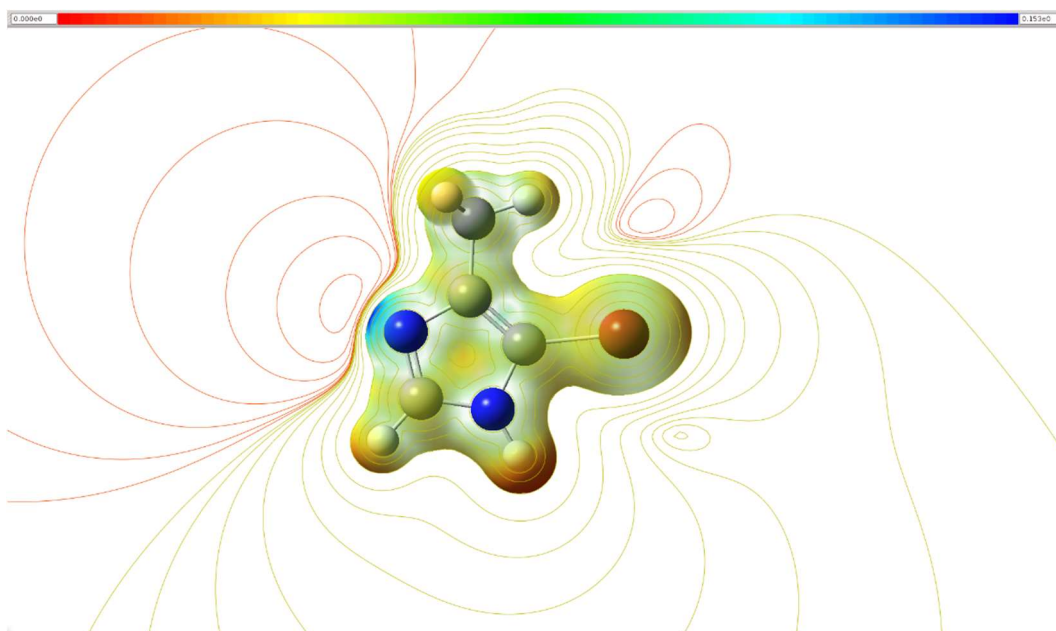


Figure C.140 - Molecular electrostatic potential map of 5-bromo-4-methylimidazole.

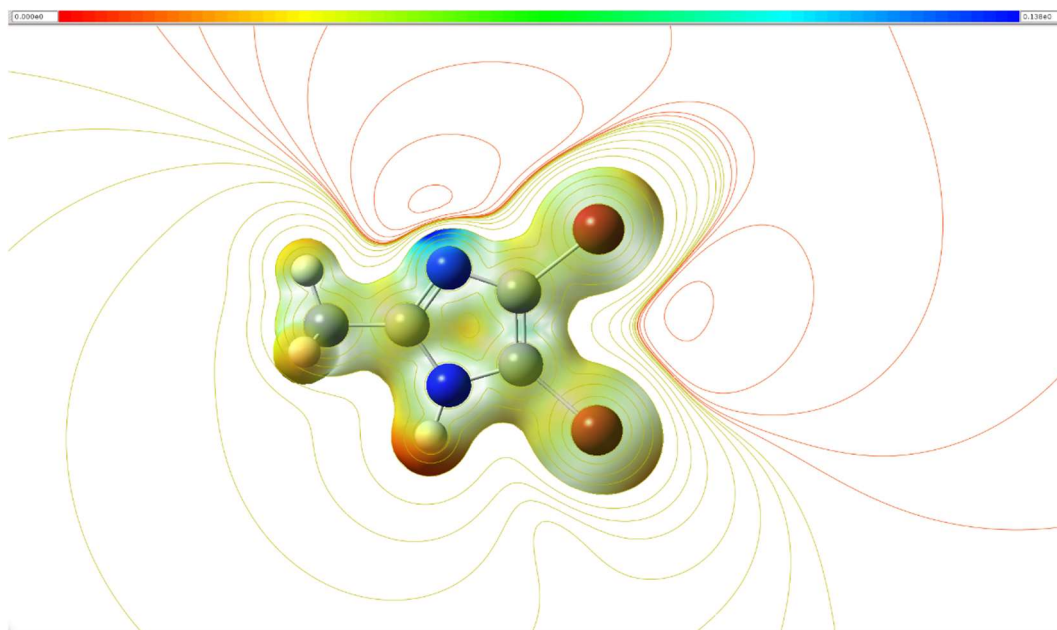


Figure C.141 - Molecular electrostatic potential map of 4,5-dibromo-2-methylimidazole.

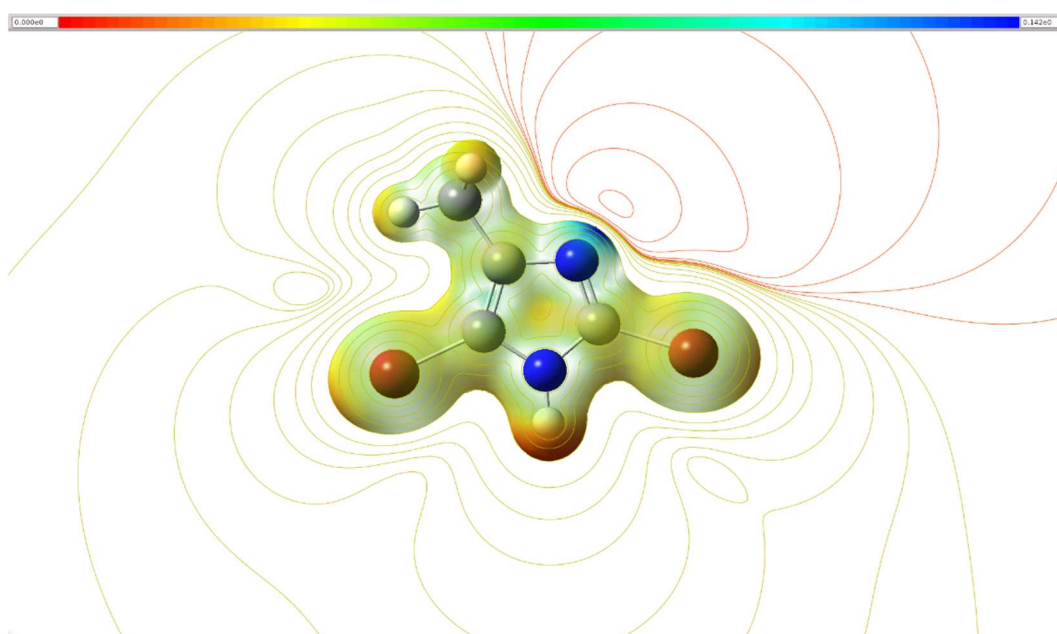


Figure C.142 - Molecular electrostatic potential map of 2,5-dibromo-4-methylimidazole.

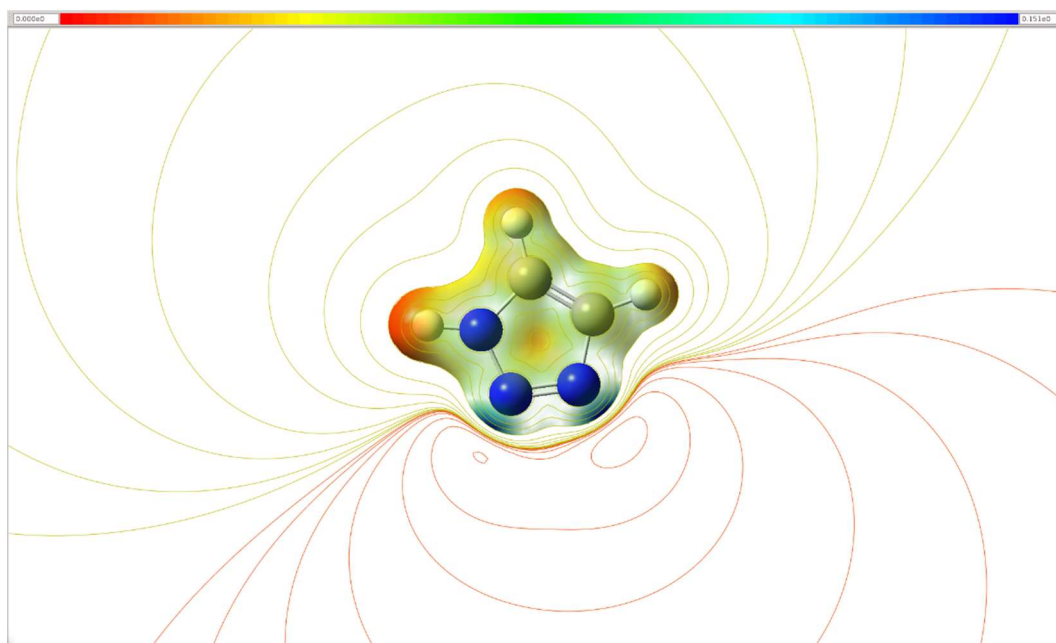


Figure C.143 - Molecular electrostatic potential map of 1,2,3-triazole.

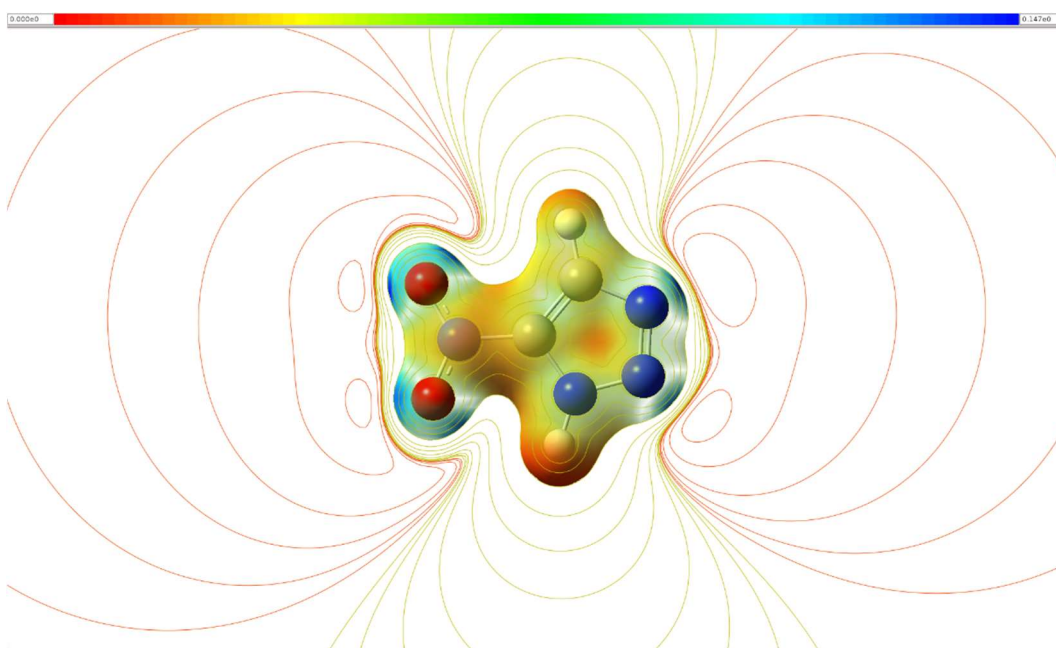


Figure C.144 - Molecular electrostatic potential map of 5-nitro-1,2,3-triazole.

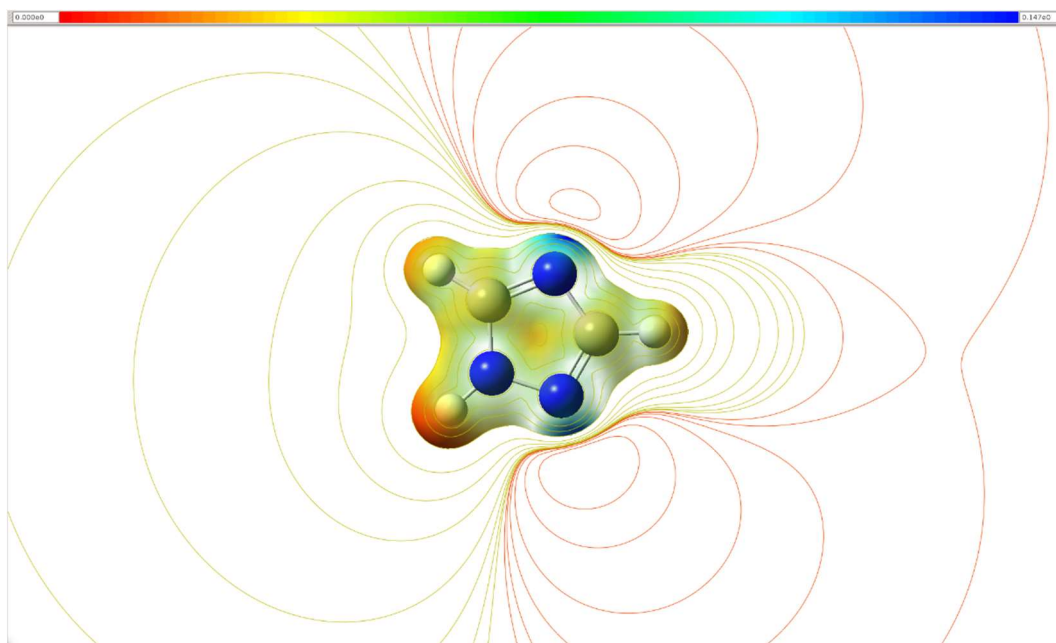


Figure C.145 - Molecular electrostatic potential map of 1,2,4-triazole.

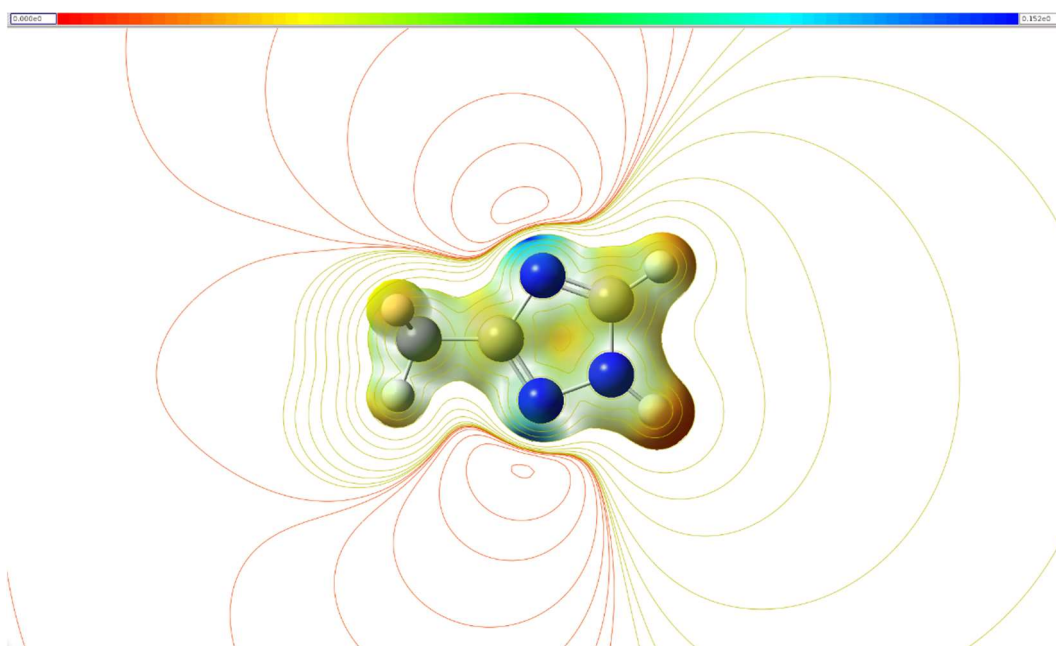


Figure C.146 - Molecular electrostatic potential map of 3-methyl-1,2,4-triazole.

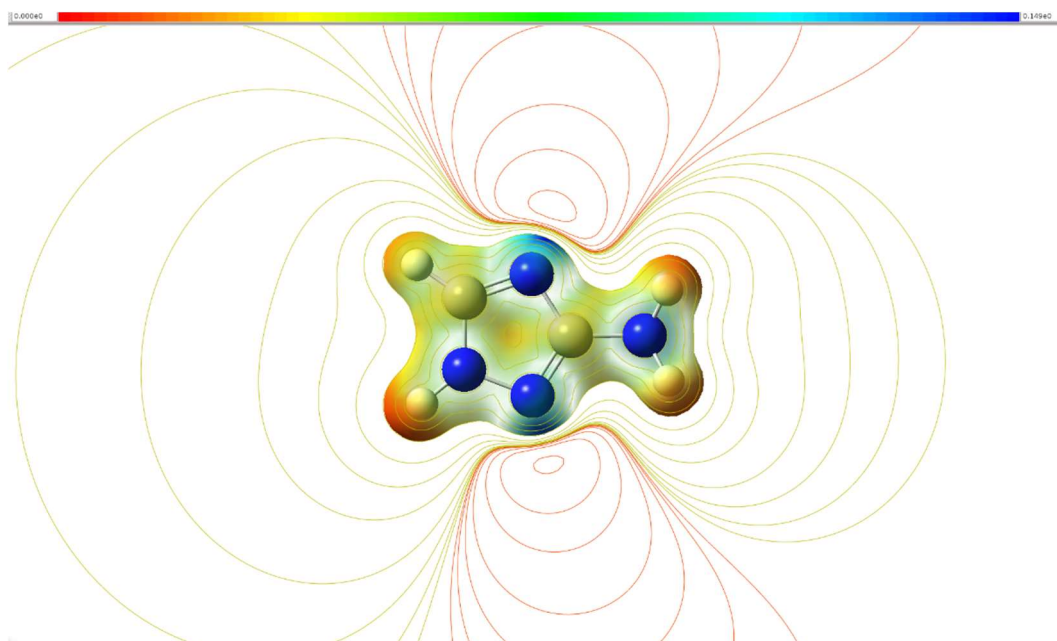


Figure C.147 - Molecular electrostatic potential map of 1,2,4-triazol-3-amine.

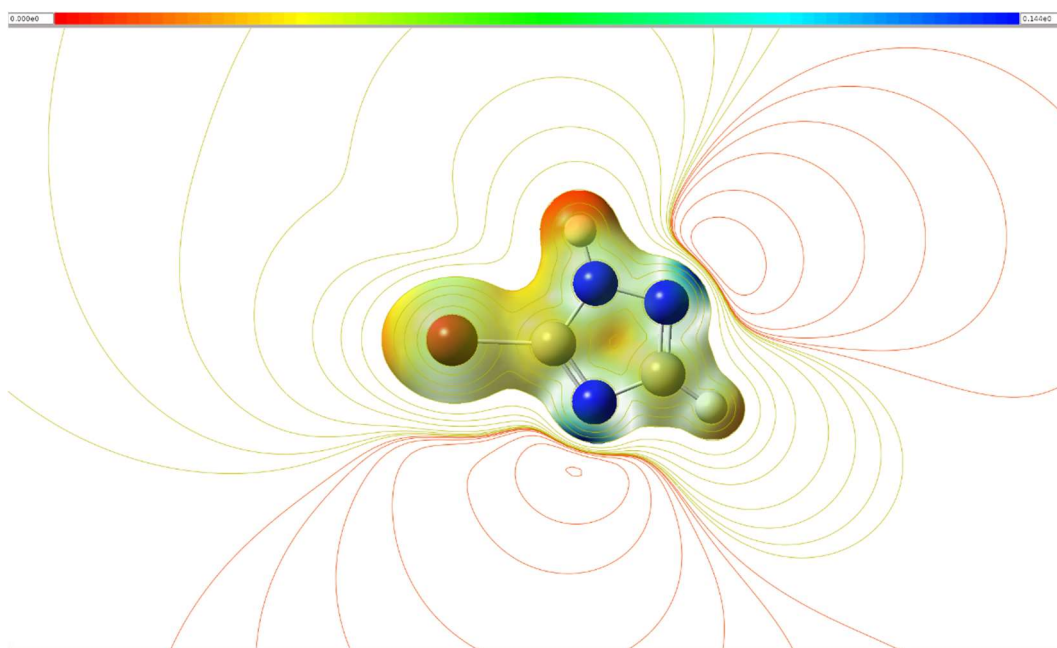


Figure C.148 - Molecular electrostatic potential map of 5-bromo-1,2,4-triazole.

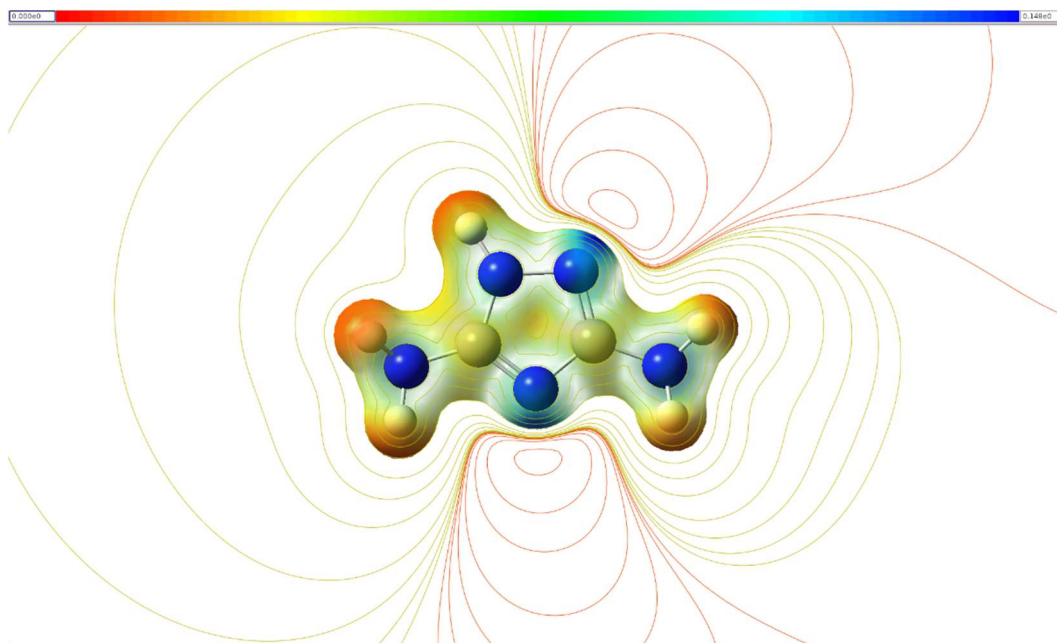


Figure C.149 - Molecular electrostatic potential map of 1,2,4-triazol-3,5-diamine.

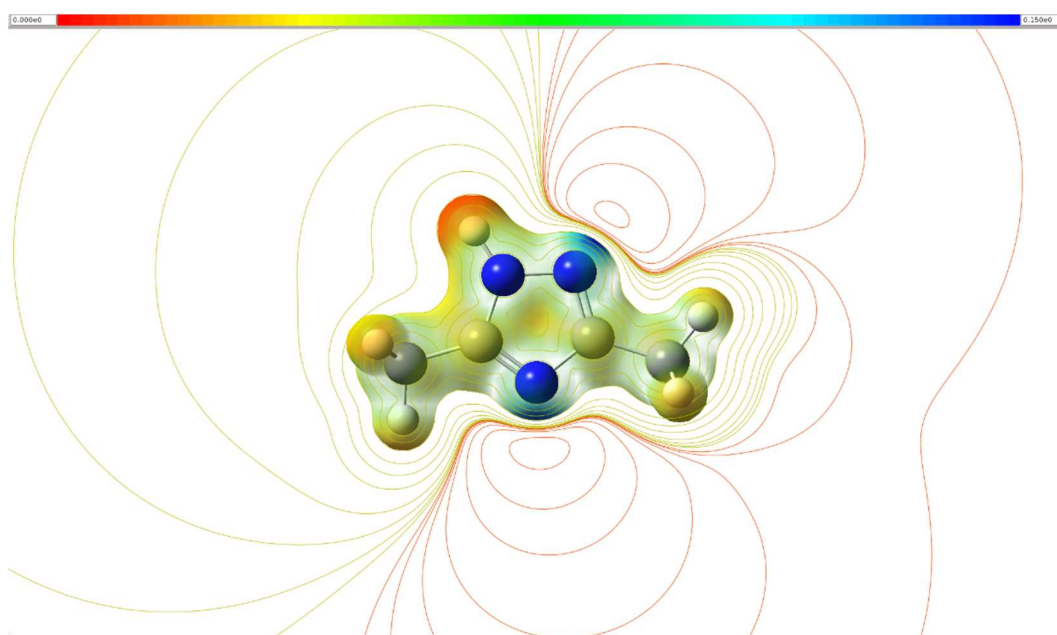


Figure C.150 - Molecular electrostatic potential map of 3,5-dimethyl-1,2,4-triazole.

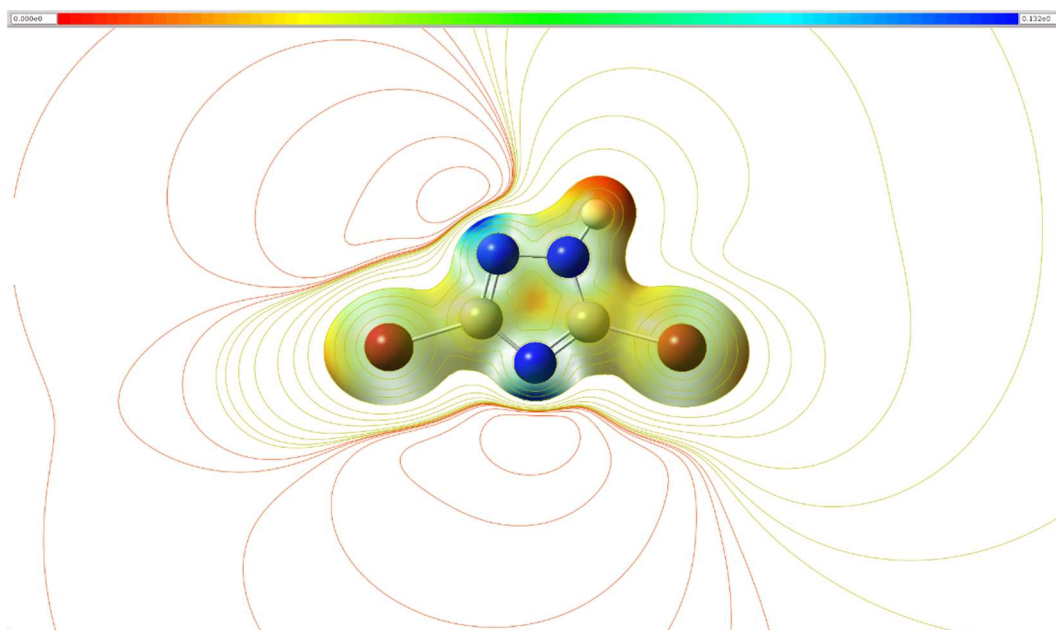


Figure C.151 - Molecular electrostatic potential map of 3,5-dibromo-1,2,4-triazole.

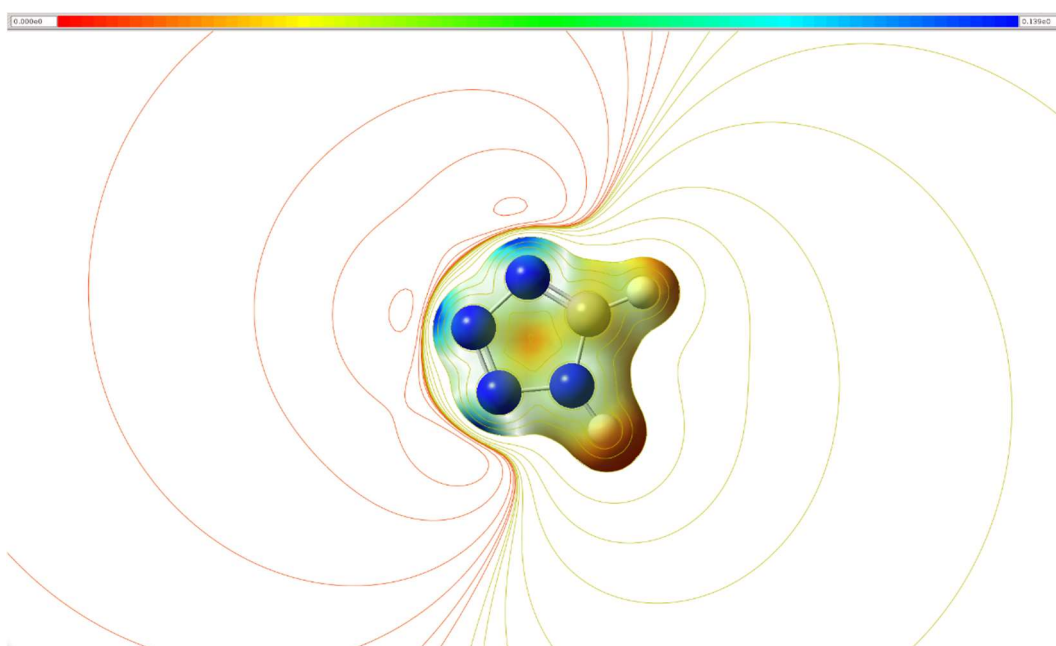


Figure C.152 - Molecular electrostatic potential map of 1,2,3,4-tetrazole.

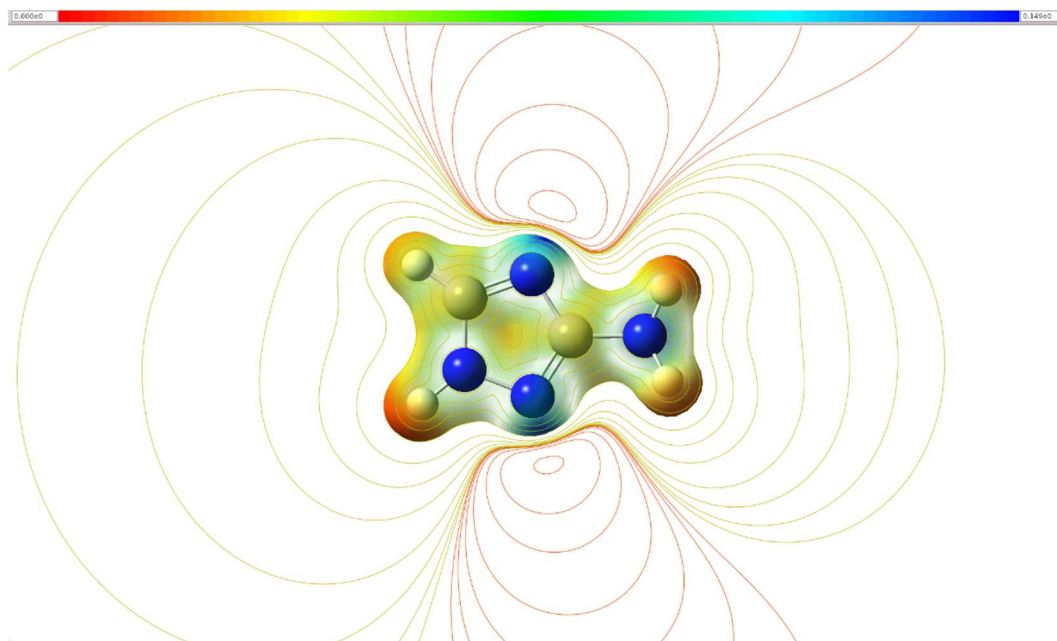


Figure C.153 - Molecular electrostatic potential map of 1,2,3,4-tetrazol-5-amine.

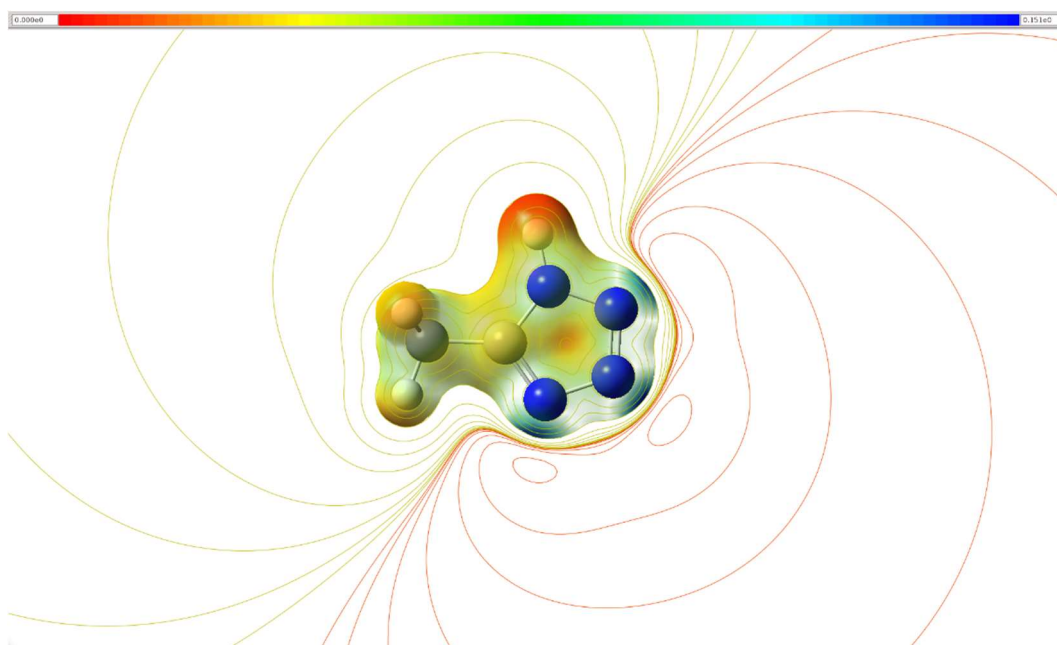


Figure C.154 - Molecular electrostatic potential map of 5-methyl-1,2,3,4-tetrazole.