

TABLE OF CONTENTS

A	Results 1 - Application of ball milling technology for production of co-crystals (Chapter 4)	3
A.1	Caffeine/oxalic acid	3
A.2	2,4,6-trinitrotoluene/naphthalene	11
A.3	2,4,6-trinitrotoluene/anthracene	19
A.4	2,4,6-trinitrotoluene/1,4-dimethoxybenzene	27
B	Results 2 – Manipulation of electrostatic potential and its impact on co-crystal formation (Chapter 5)	35
B.1	<i>N</i> -heterocyclic co-formers investigated in this study	35
B.2	2-naphthol/pyrrolidine	37
B.3	2-naphthol/3-pyrroline	38
B.4	2-naphthol/pyrrole	39
B.5	2-naphthol/2-nitropyrrole	40
B.6	2-naphthol/2-methylpyrrole	43
B.7	2-naphthol/3-methylpyrrole	44
B.8	2-naphthol/2,4-dimethylpyrrole	45
B.9	2-naphthol/2,5-dimethylpyrrole	46
B.10	2-naphthol/pyrazole	47
B.11	2-naphthol/3-nitropyrazole	50
B.12	2-naphthol/4-nitropyrazole	51
B.13	2-naphthol/5-methylpyrazole	52
B.14	2-naphthol/pyrazol-4-amine	53
B.15	2-naphthol/3-bromopyrazole	56
B.16	2-naphthol/4-bromopyrazole	57
B.17	2-naphthol/3,4-dimethylpyrazole	58
B.18	2-naphthol/3,5-dimethylpyrazole	61
B.19	2-naphthol/3,4,5-tribromopyrazole	62
B.20	2-naphthol/3-methyl-5-nitropyrazole	63
B.21	2-naphthol/5-methylpyrazol-3-amine	64
B.22	2-naphthol/4-bromopyrazol-3-amine	65
B.23	2-naphthol/3-bromopyrazol-5-amine	66
B.24	2-naphthol/3,5-dimethylpyrazol-4-amine	67
B.25	2-naphthol/3,4-dimethylpyrazol-5-amine	68
B.26	2-naphthol/3-methyl-4-bromopyrazole	71
B.27	2-naphthol/3-bromo-5-methylpyrazole	72
B.28	2-naphthol/4-bromo-3,5-dimethylpyrazole	73
B.29	2-naphthol/imidazole	74
B.30	2-naphthol/2-nitroimidazole	77
B.31	2-naphthol/2-methylimidazole	78

B.32	2-naphthol/4-methylimidazole.....	79
B.33	2-naphthol/imidazol-2-amine	82
B.34	2-naphthol/2-bromoimidazole	83
B.35	2-naphthol/4-bromoimidazole	84
B.36	2-naphthol/2,4-dimethylimidazole	85
B.37	2-naphthol/4,5-dinitroimidazole	86
B.38	2-naphthol/4,5-dichlororimidazole	87
B.39	2-naphthol/2,4,5-tribromoimidazole	88
B.40	2-naphthol/2-methyl-5-nitroimidazole	89
B.41	2-naphthol/4-methyl-5-nitroimidazole	90
B.42	2-naphthol/2-bromo-5-nitroimidazole.....	91
B.43	2-naphthol/4-bromo-2-methylimidazole	92
B.44	2-naphthol/5-bromo-4-methylimidazole	93
B.45	2-naphthol/4,5-dibromo-2-methylimidazole	94
B.46	2-naphthol/2,5-dibromo-4-methylimidazole	95
B.47	2-naphthol/1,2,3-triazole.....	96
B.48	2-naphthol/5-nitro-1,2,3-triazole	97
B.49	2-naphthol/1,2,4-triazole.....	98
B.50	2-naphthol/3-methyl-1,2,4-triazole	99
B.51	2-naphthol/1,2,4-triazol-3-amine.....	100
B.52	2-naphthol/5-bromo-1,2,4-triazole	101
B.53	2-naphthol/1,2,4-triazol-3,5-diamine	102
B.54	2-naphthol/3,5-dimethyl-1,2,4-triazole	103
B.55	2-naphthol/3,5-dibromo-1,2,4-triazole.....	106
B.56	2-naphthol/1,2,3,4-tetrazole.....	107
B.57	2-naphthol/1,2,3,4-tetrazol-5-amine.....	108
B.58	2-naphthol/5-methyl-1,2,3,4-tetrazole.....	109
B.59	2-naphthol/3-nitro-1,2,4-triazol-5-one	110
B.60	Molecular Electrostatic Potentials.....	111

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

A.1 Caffeine/oxalic acid

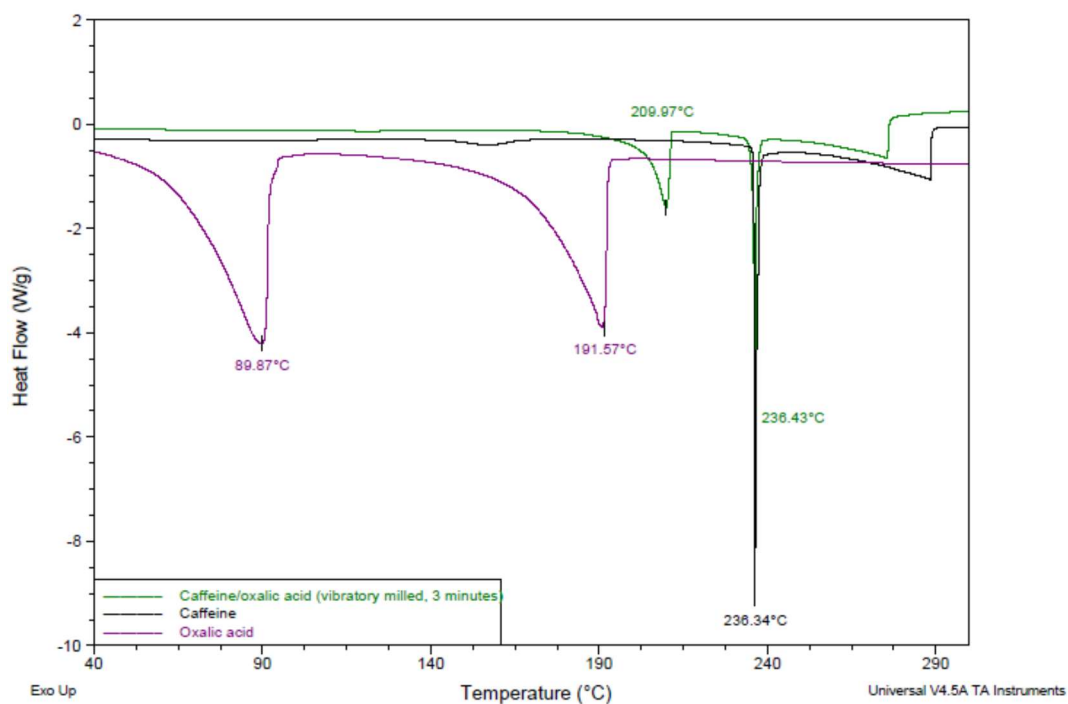


Figure A.1 - Thermal analysis of caffeine/oxalic acid produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

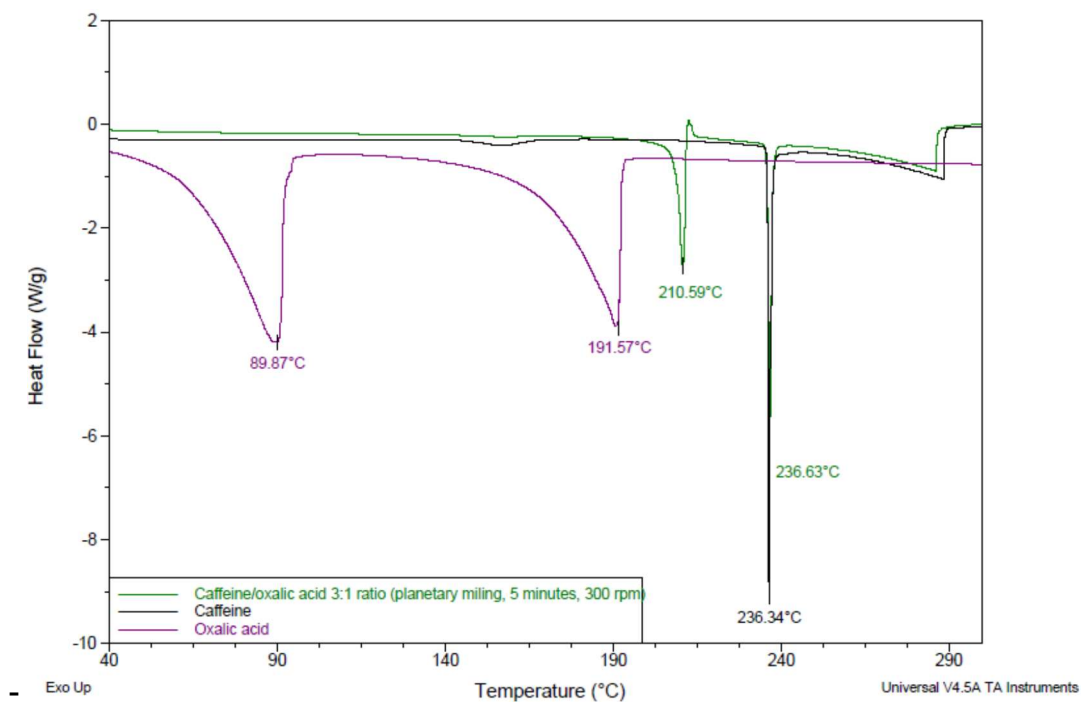


Figure A.2 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

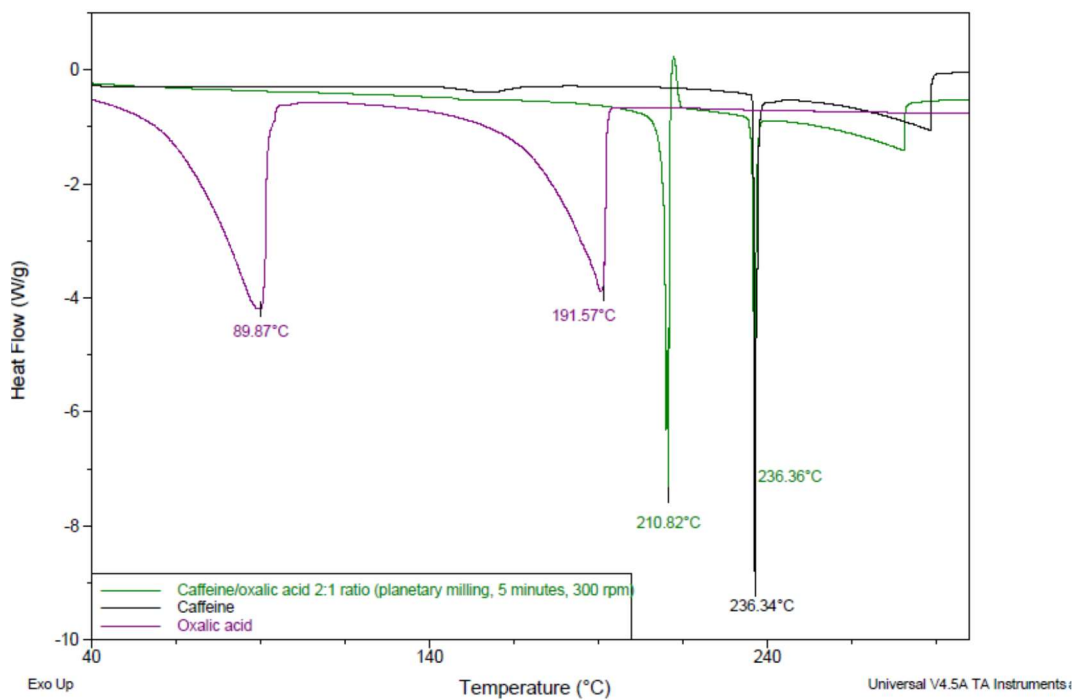


Figure A.3 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

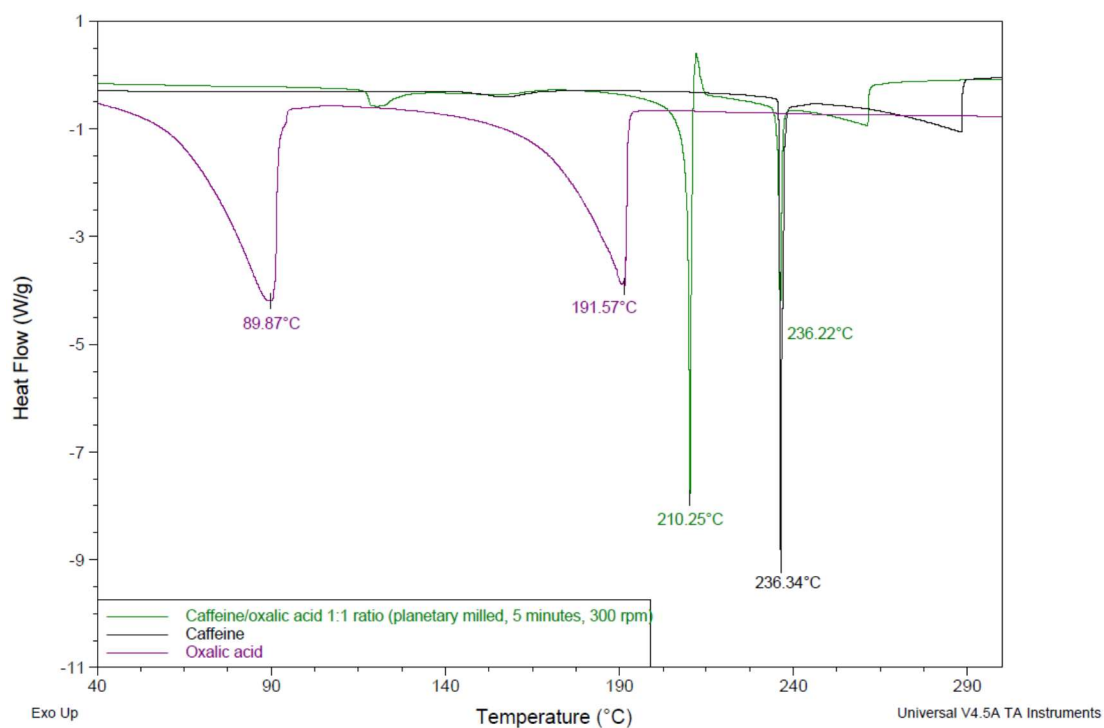


Figure A.4 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

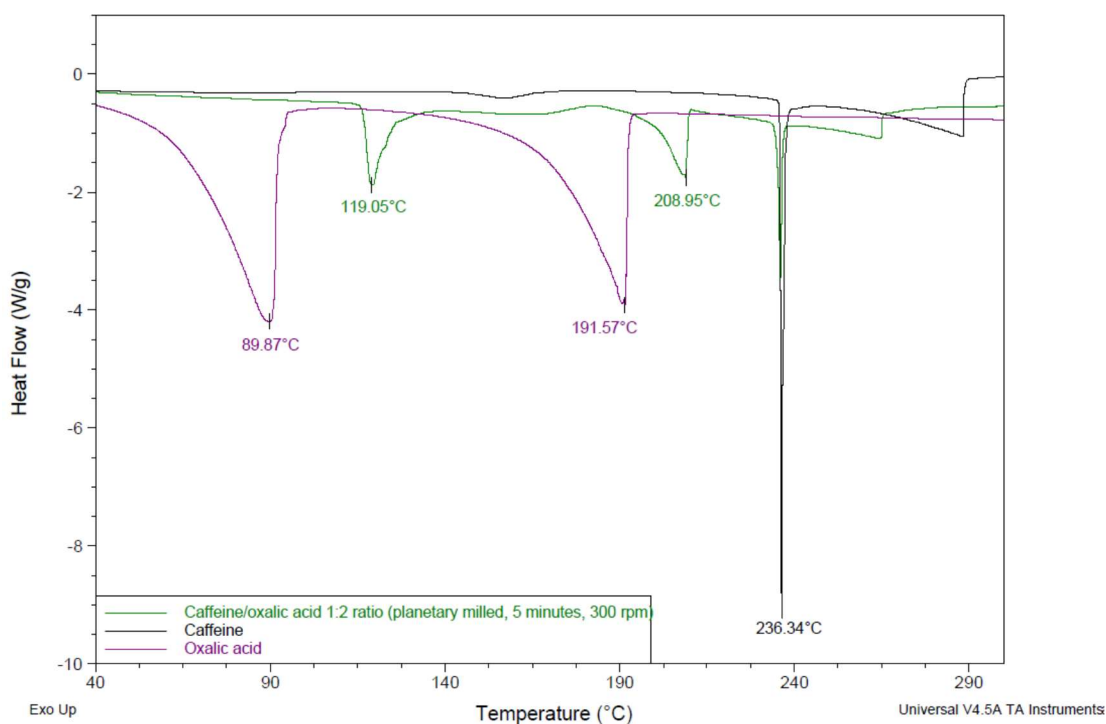


Figure A.5 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

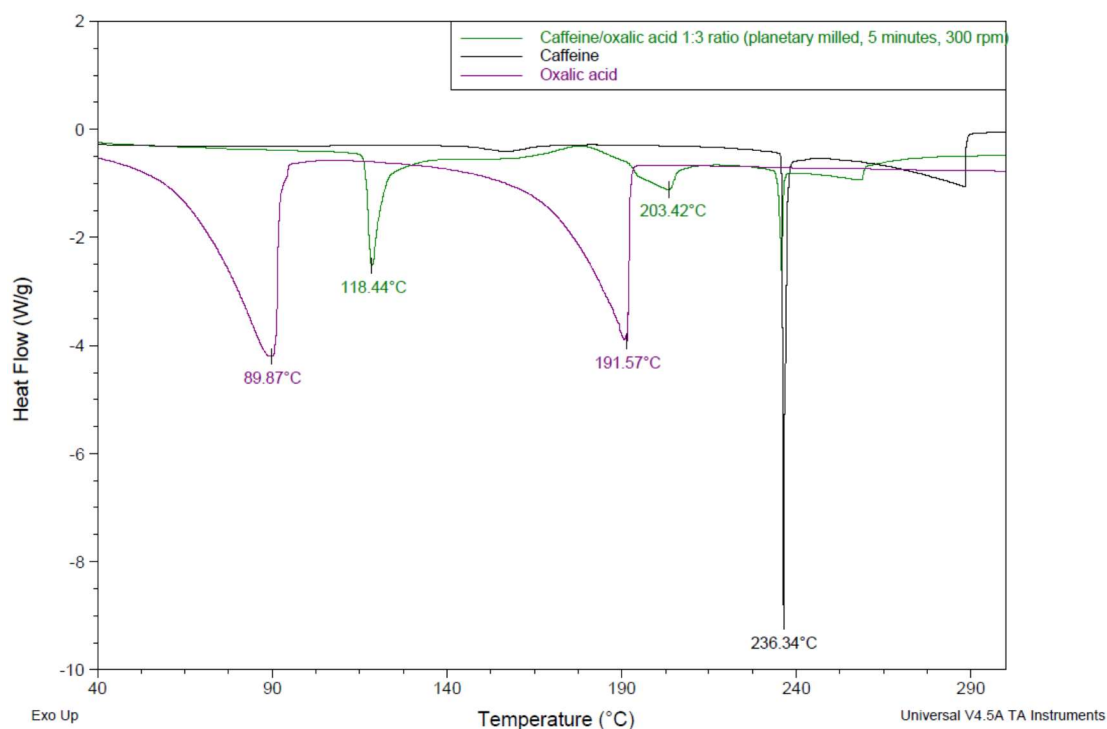


Figure A.6 - Thermal analysis of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

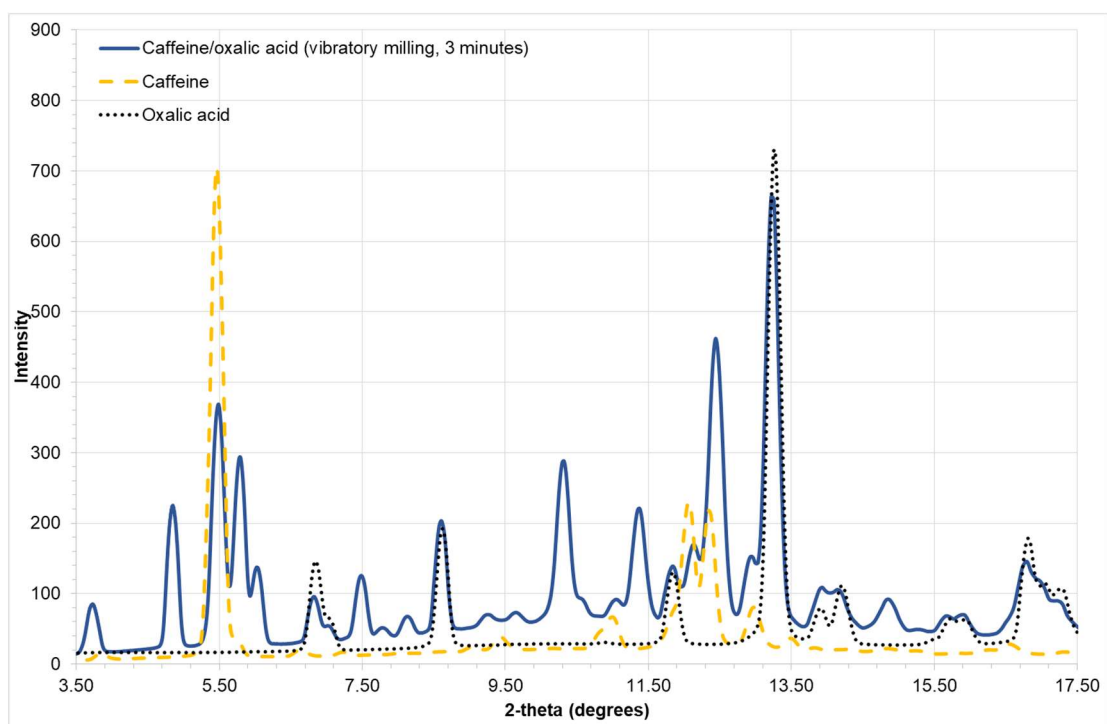


Figure A.7 - Powder x-ray pattern of caffeine/oxalic acid produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

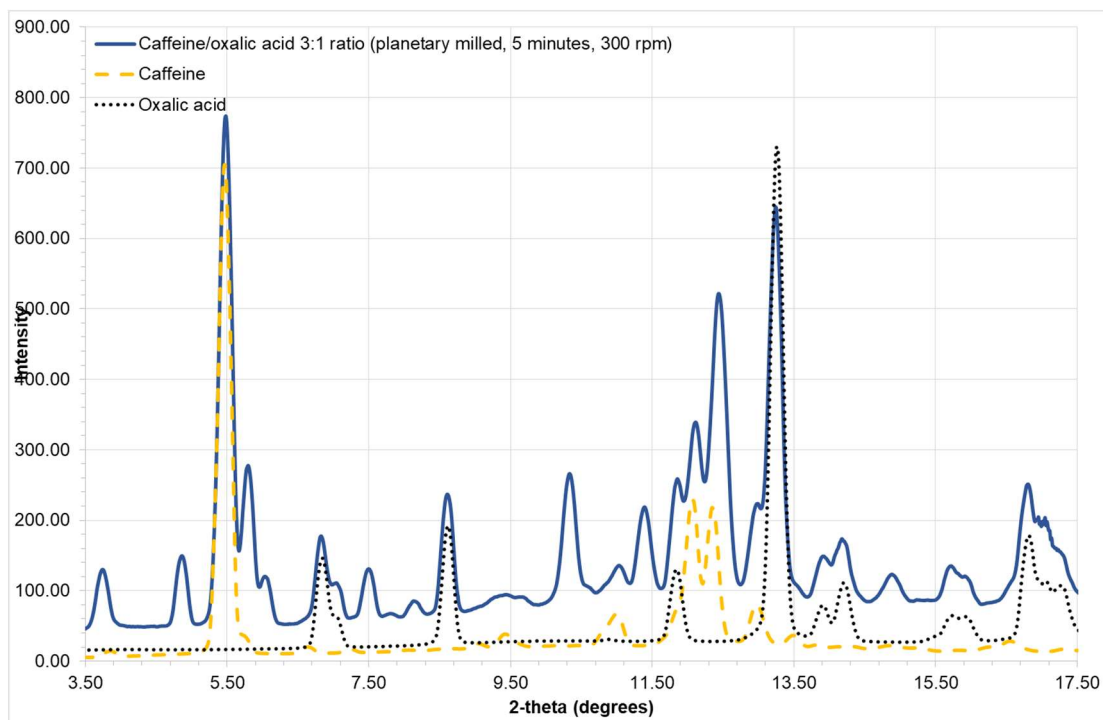


Figure A.8 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 3:1 stoichiometry.

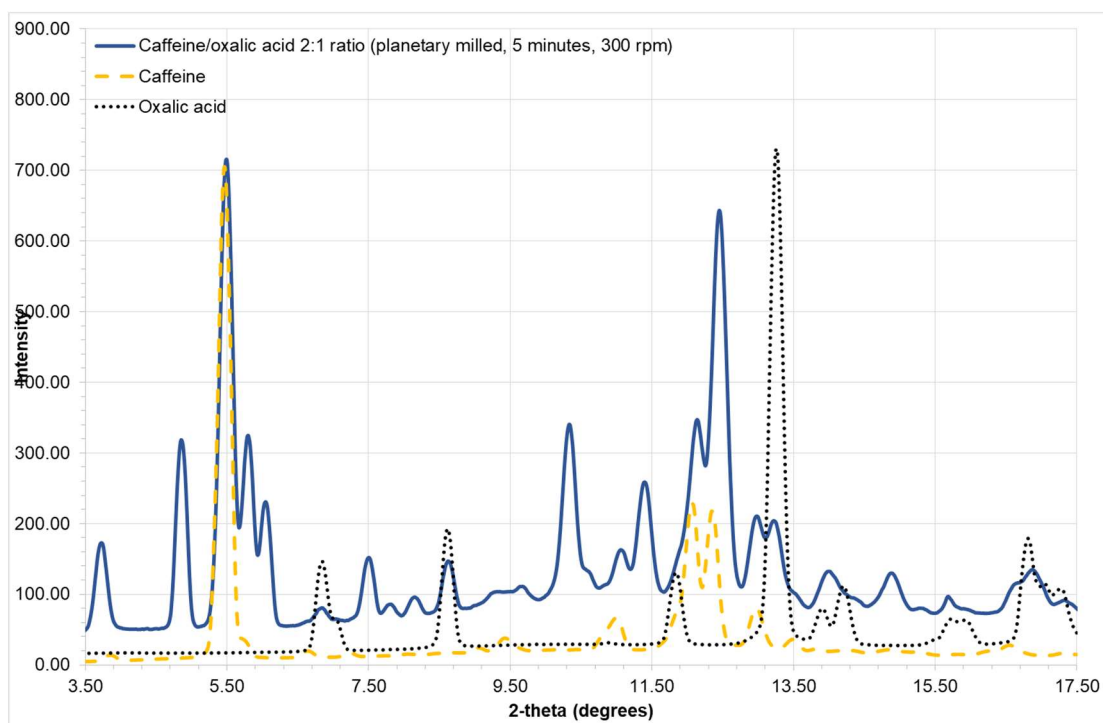


Figure A.9 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 2:1 stoichiometry.

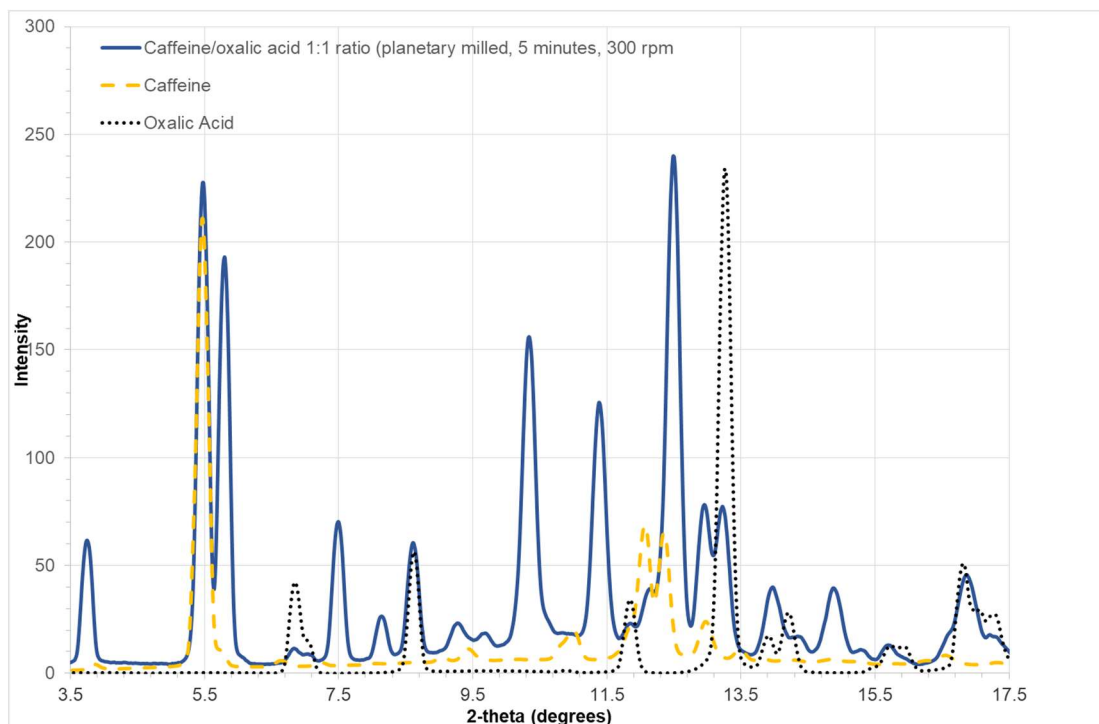


Figure A.10 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

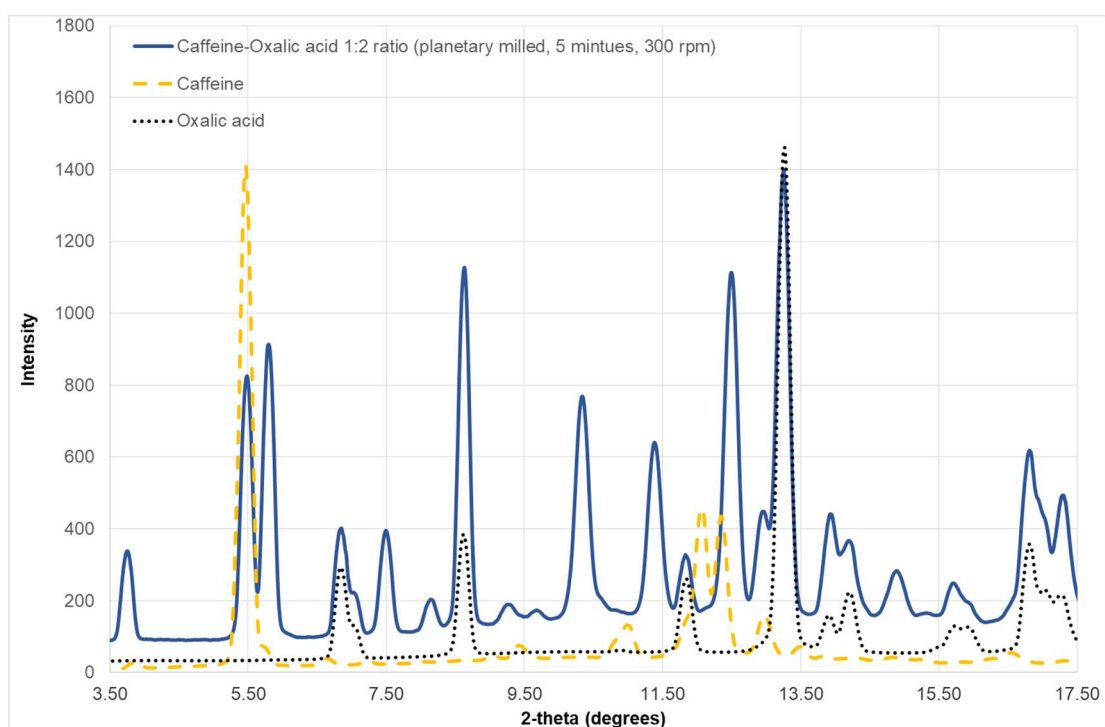


Figure A.11 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:2 stoichiometry.

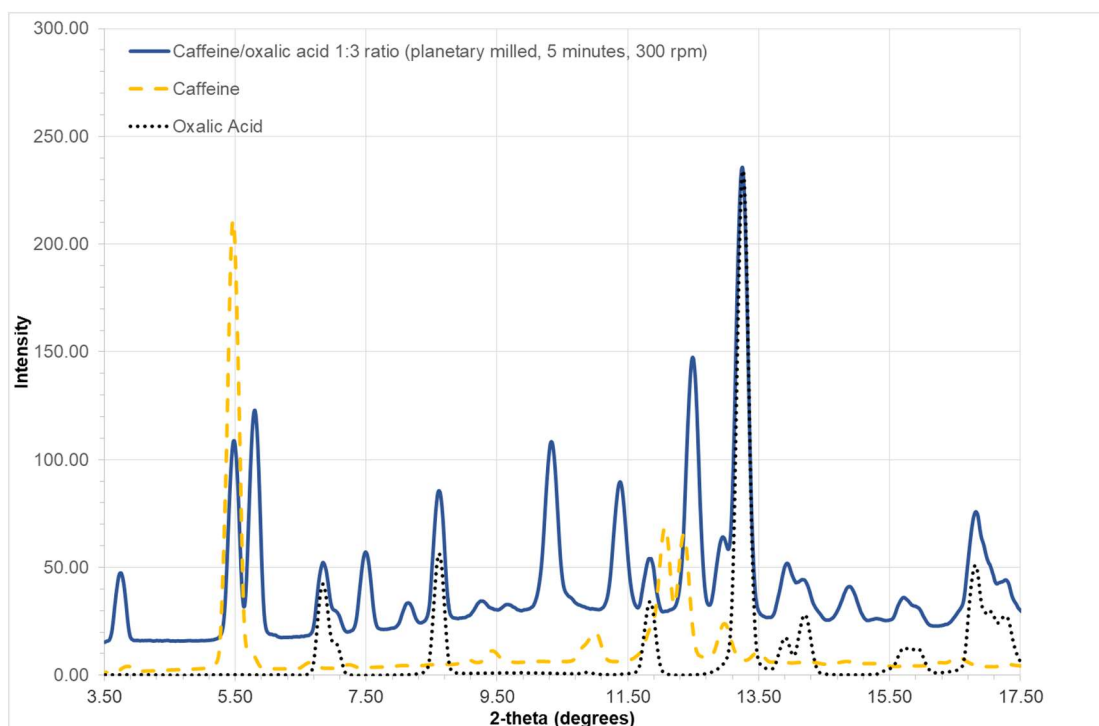


Figure A.12 - Powder x-ray pattern of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:3 stoichiometry.

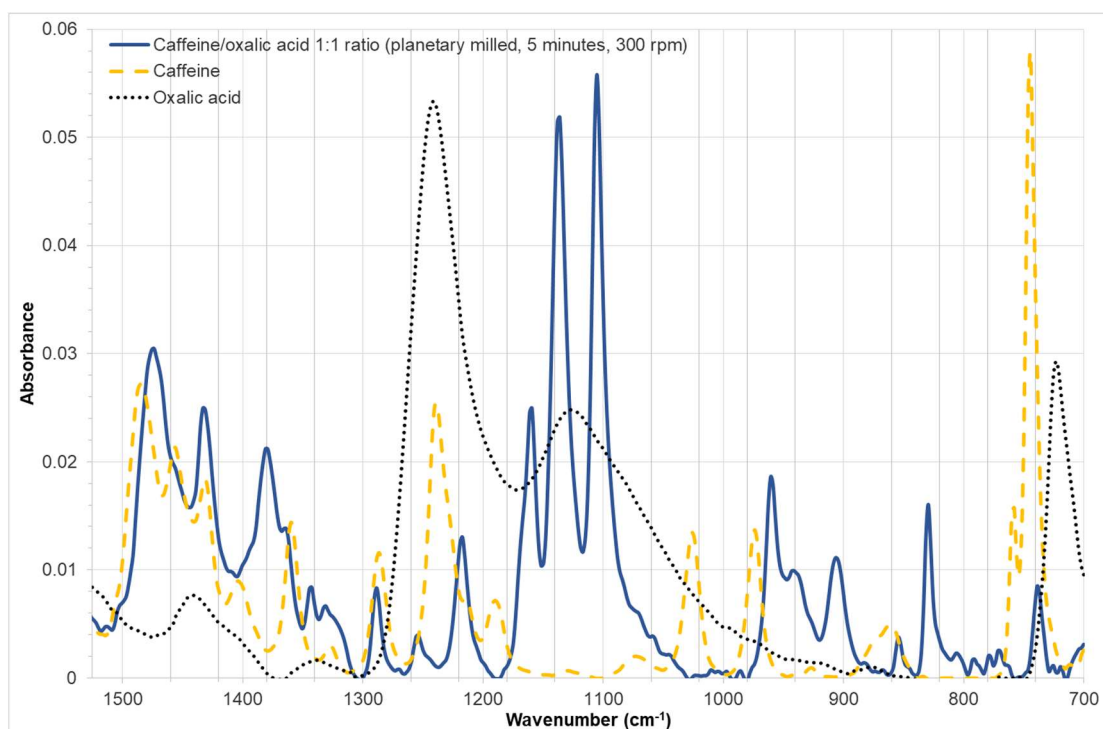


Figure A.13 - Infra-red spectra of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Table A.1 - Infrared spectra peak positions and heights of caffeine/oxalic acid produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)
1701.86	0.03
1661.04	0.05
1543.58	0.02
1501.83	0.01
1449.3	0.01
1433.87	0.01
1286.89	0.01
1229.26	0.02
1206.15	0.03
1174.59	0.03
1029.58	0.02
1010.87	0.01
975.57	0.01
923.61	0.01
898.93	0.02
875.31	0.01
848.11	0.01
839.83	0.01
807.88	0.01
794.96	0.01
761.94	0.02
748.36	0.04
723.25	0.01
707.15	0.03

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

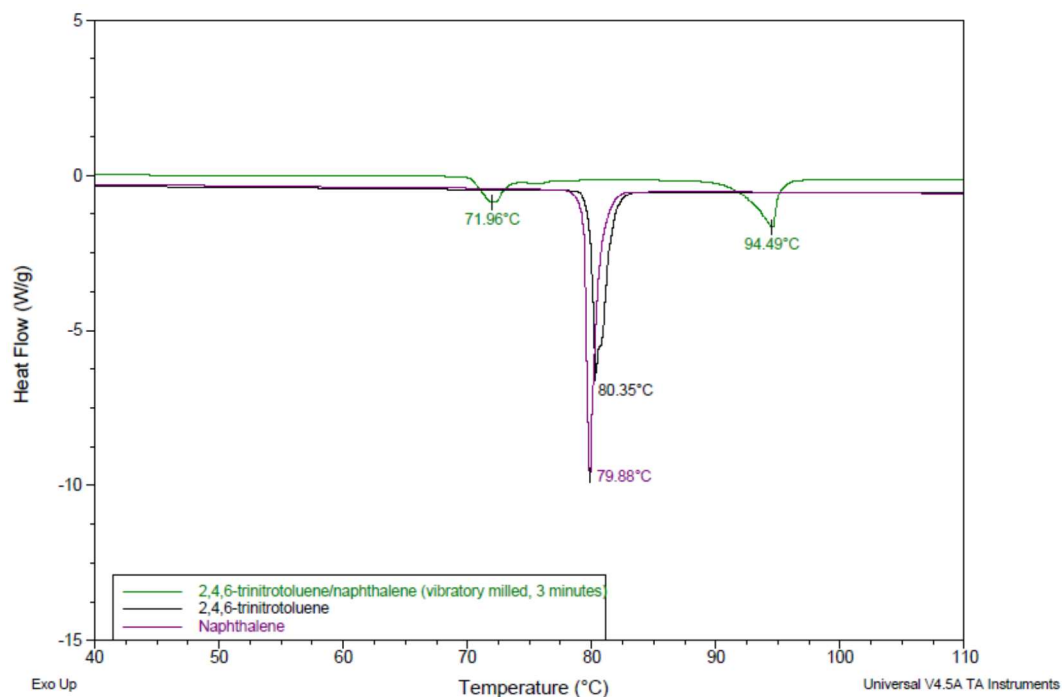


Figure A.14 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

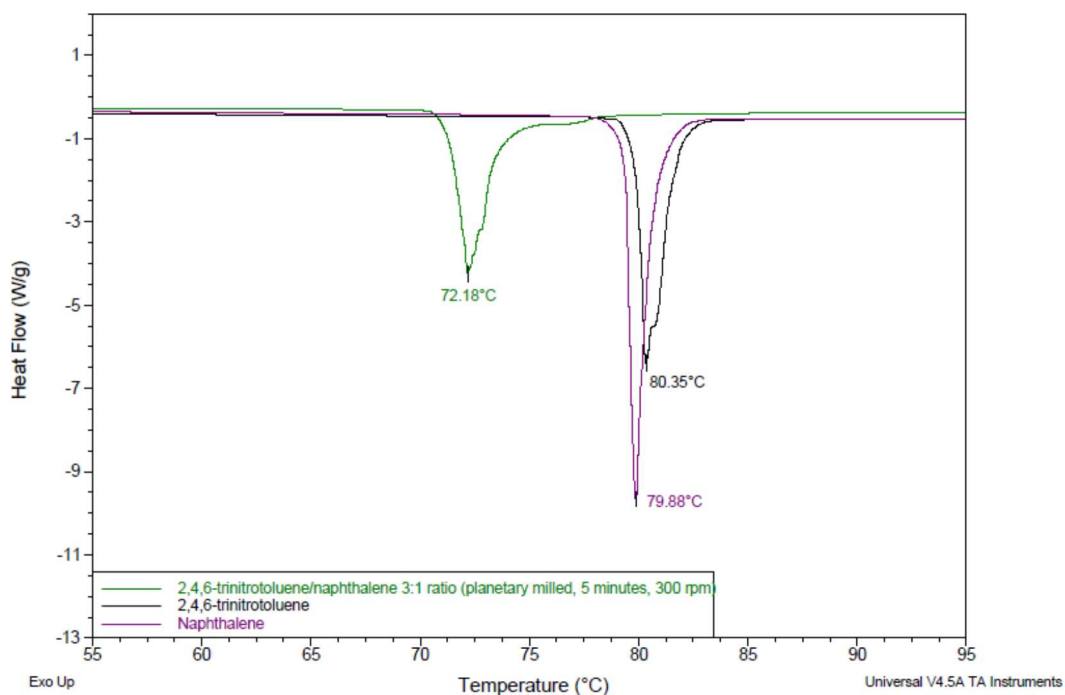


Figure A.15 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 3:1 stoichiometry.

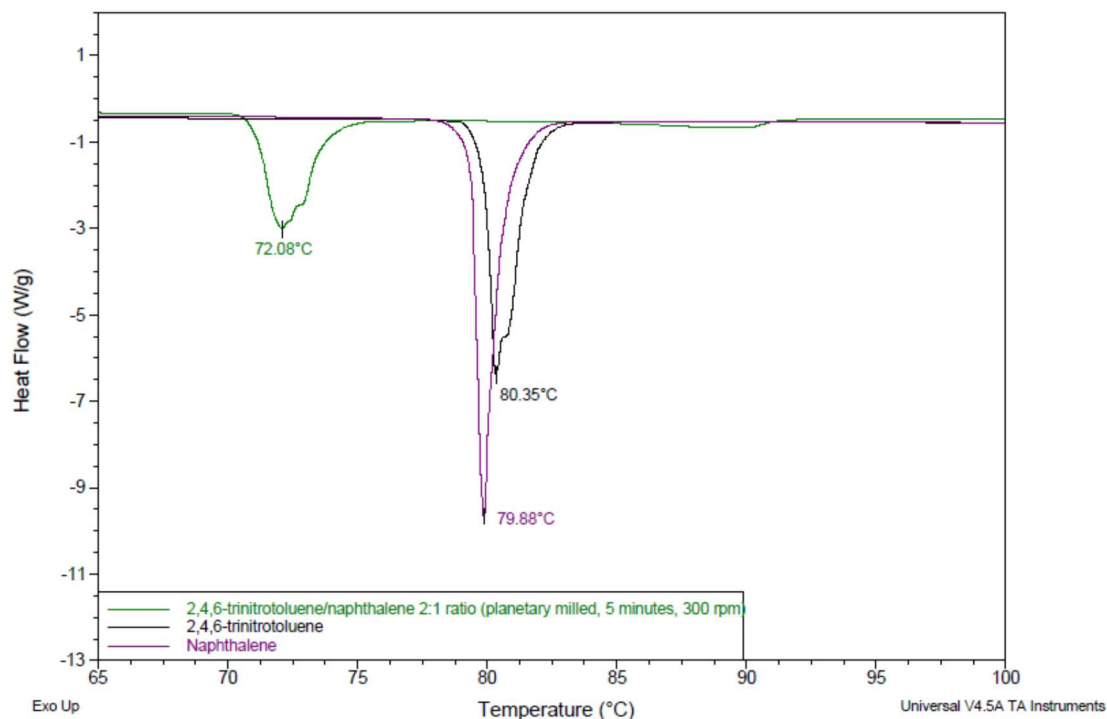


Figure A.16 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 2:1 stoichiometry.

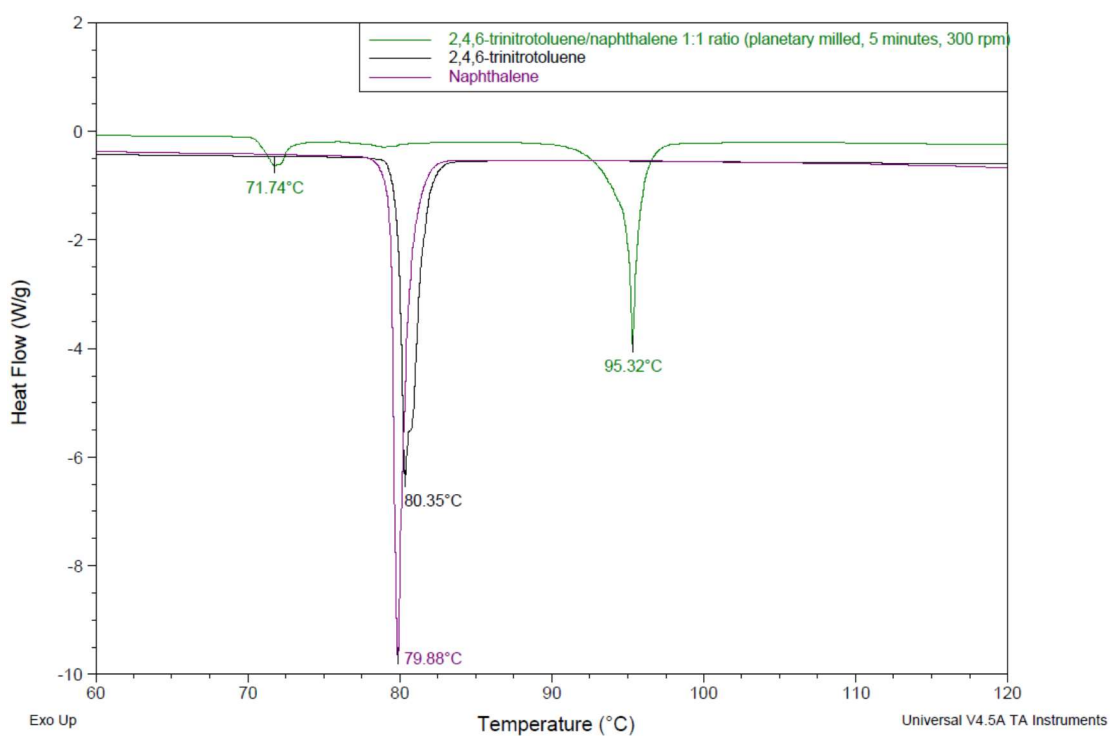


Figure A.17 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

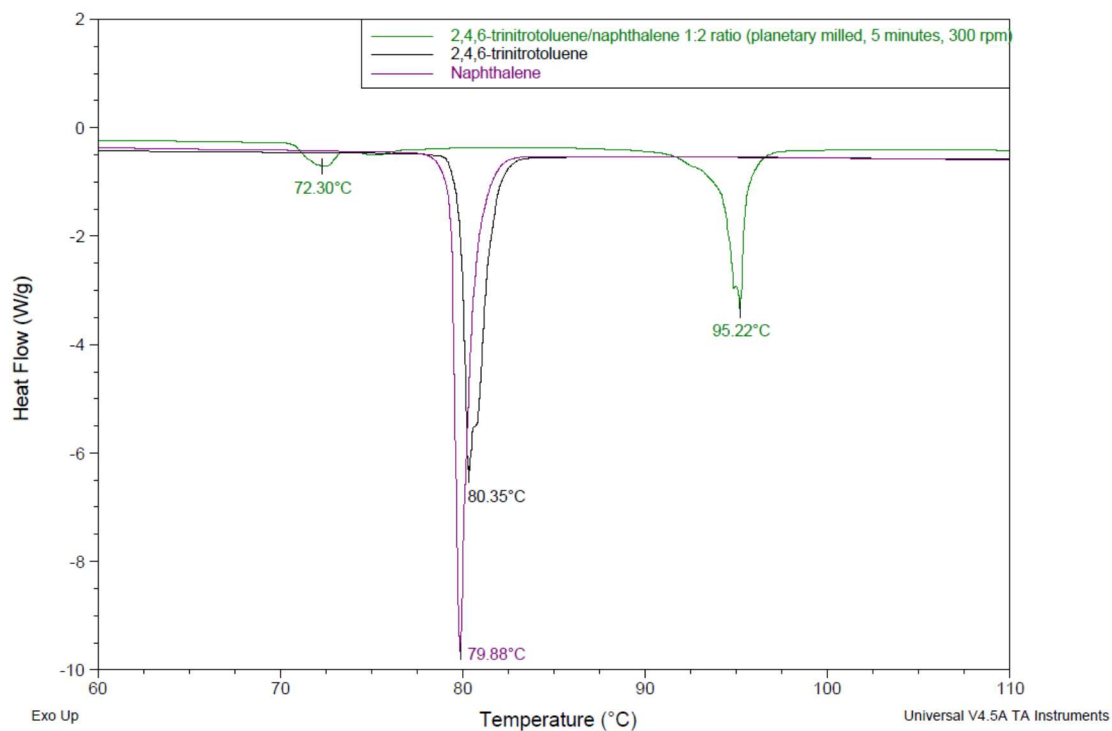


Figure A.18 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:2 stoichiometry.

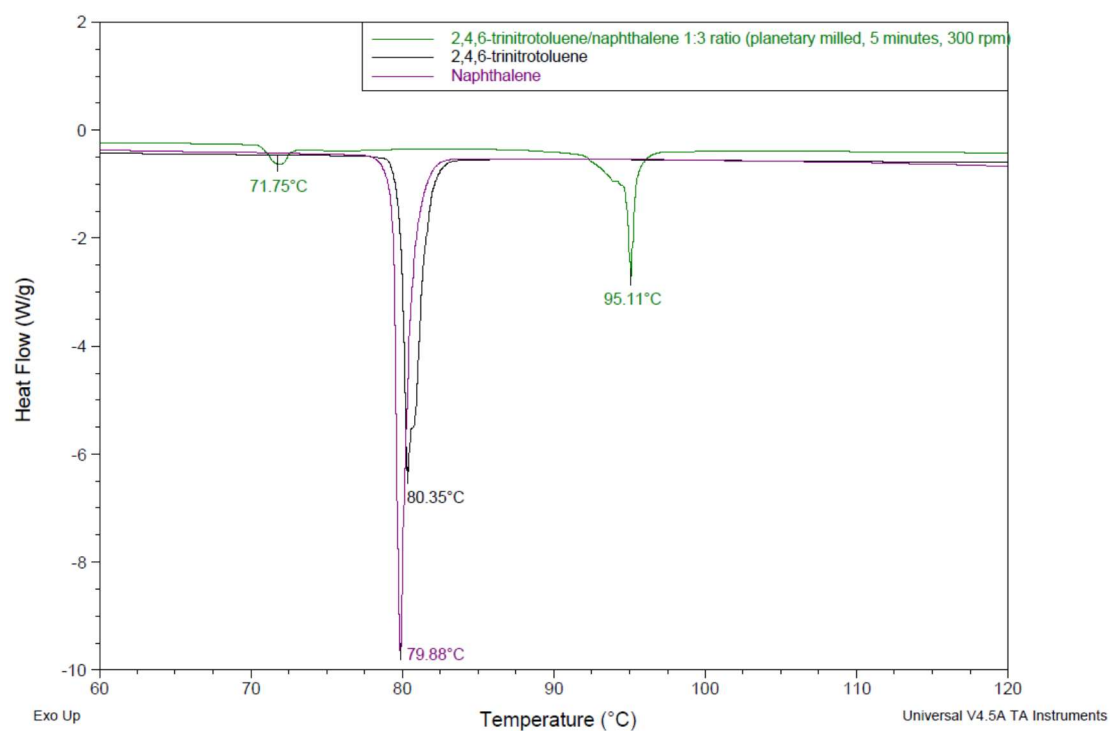


Figure A.19 - Thermal analysis of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:3 stoichiometry.

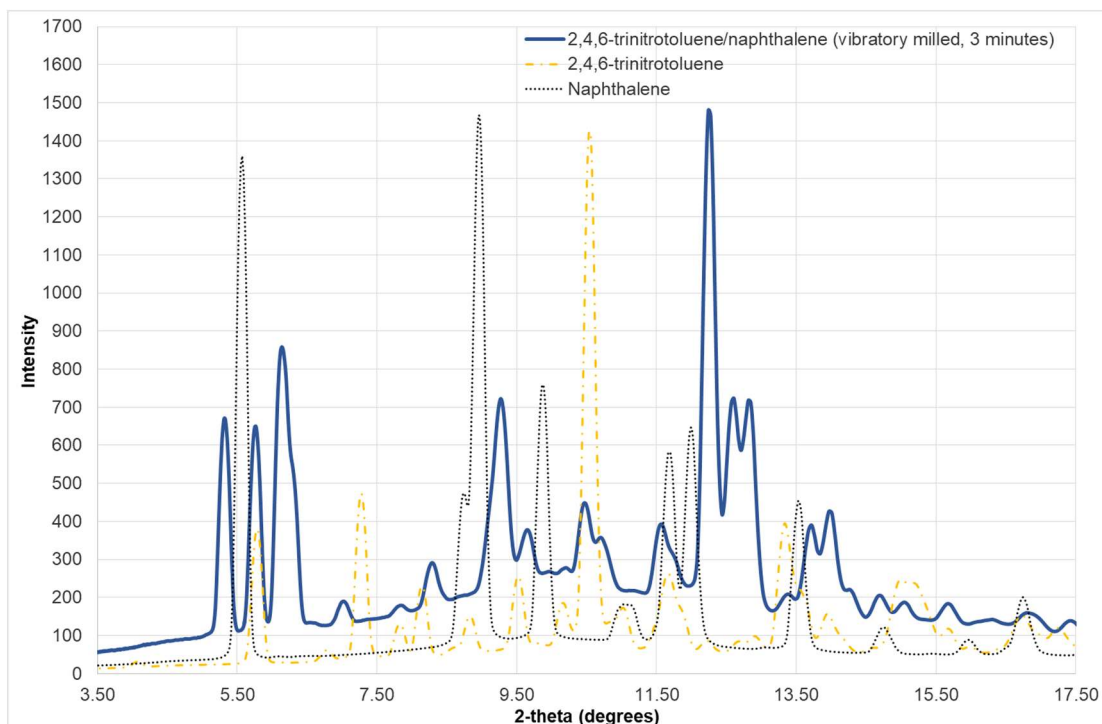


Figure A.20 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

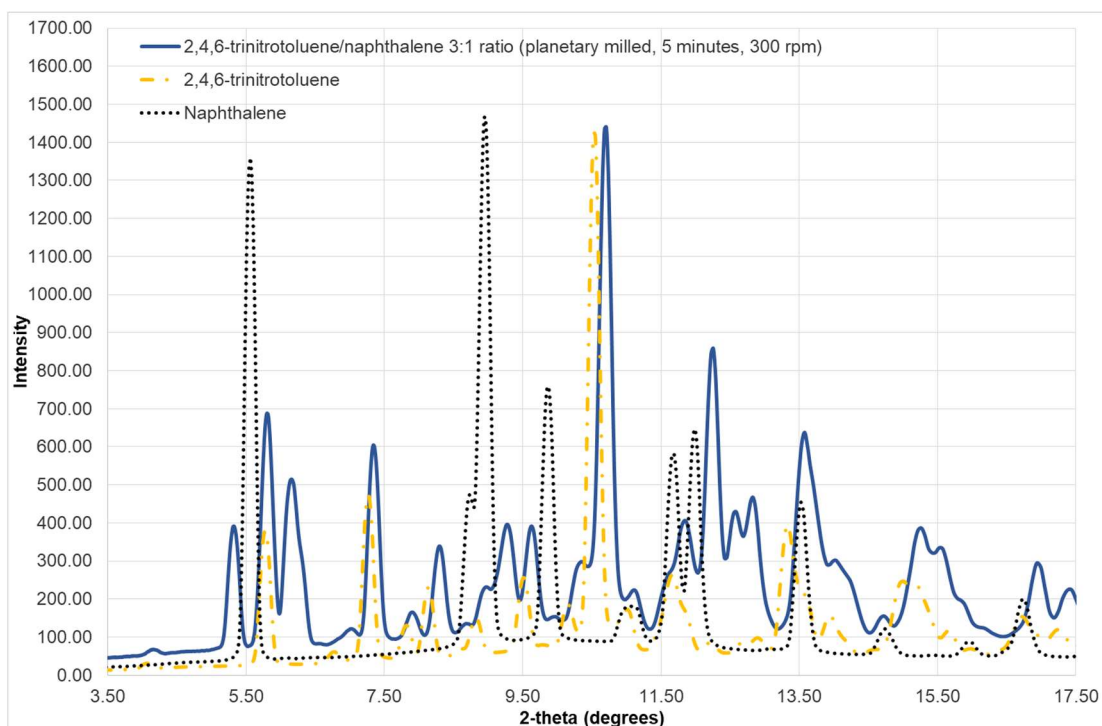


Figure A.21 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 3:1 stoichiometry.

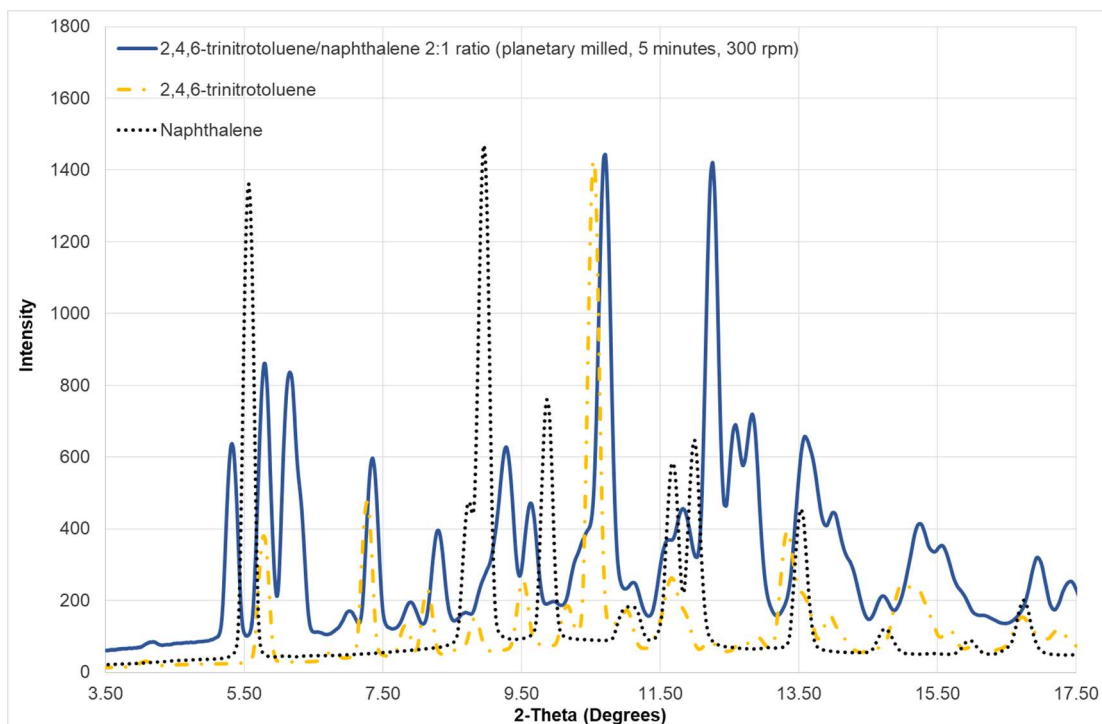


Figure A.22 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 2:1 stoichiometry.

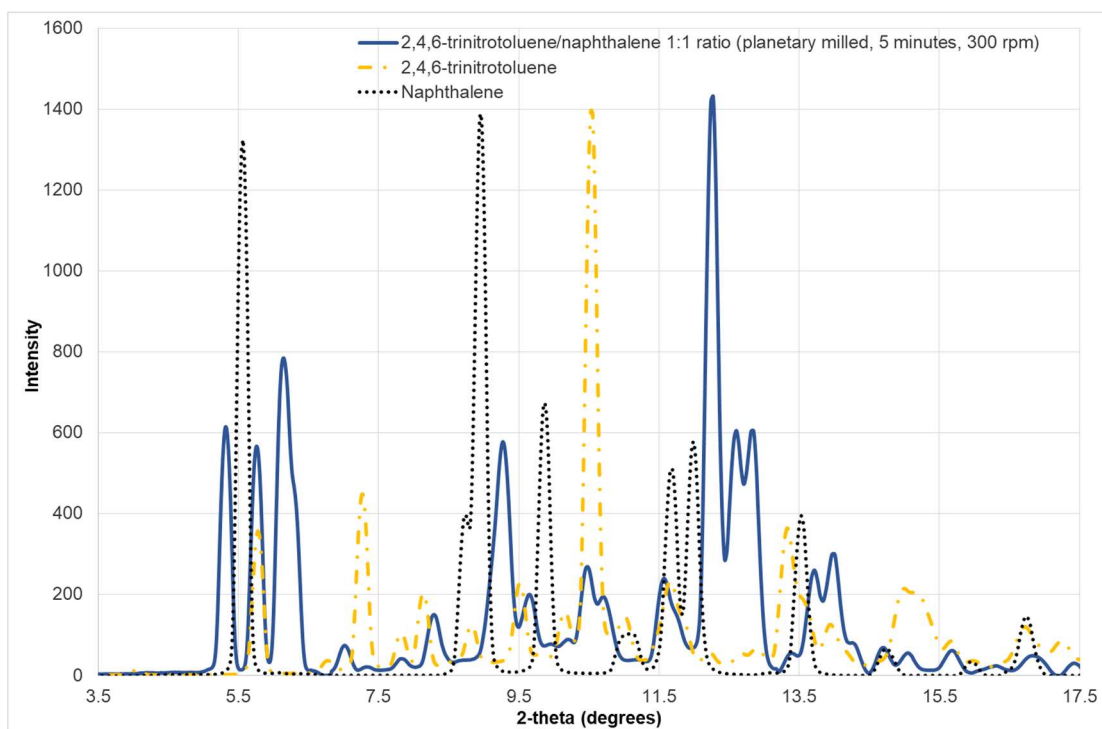


Figure A.23 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

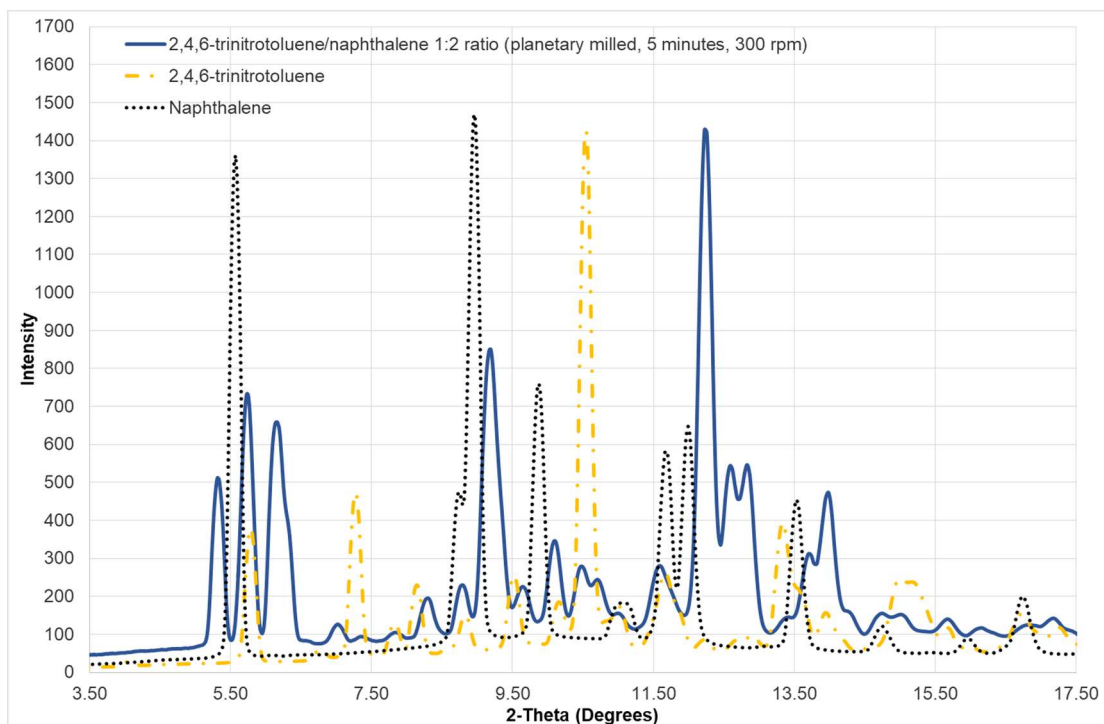


Figure A.24 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:2 stoichiometry.

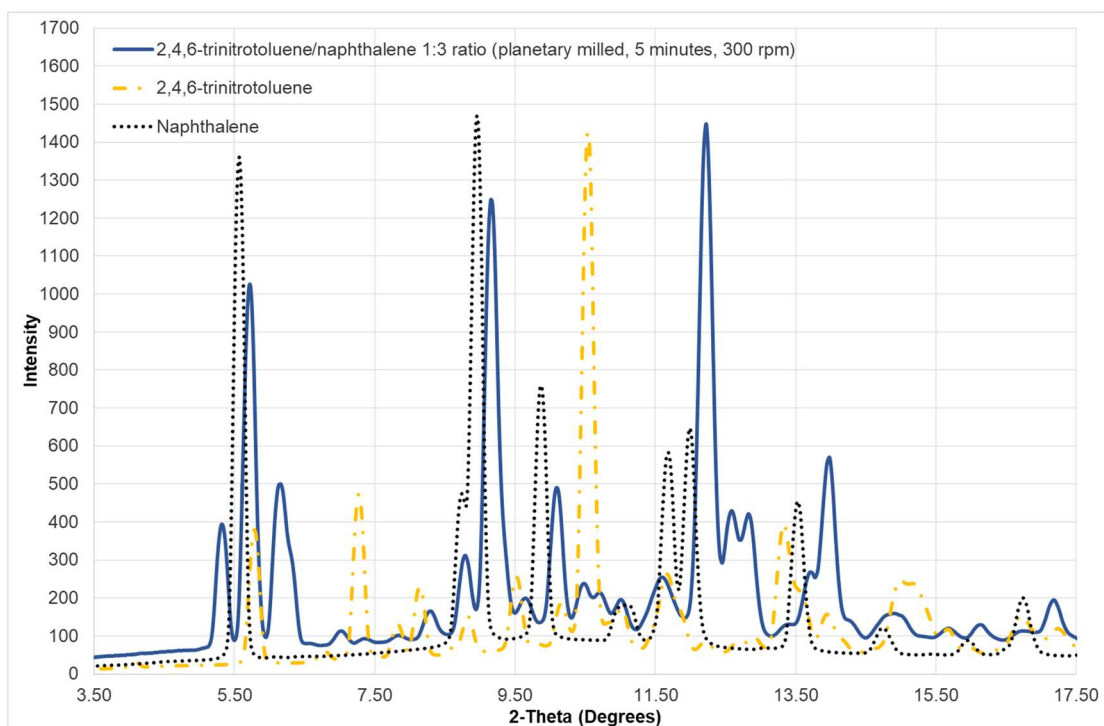


Figure A.25 - Powder x-ray pattern of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:3 stoichiometry.

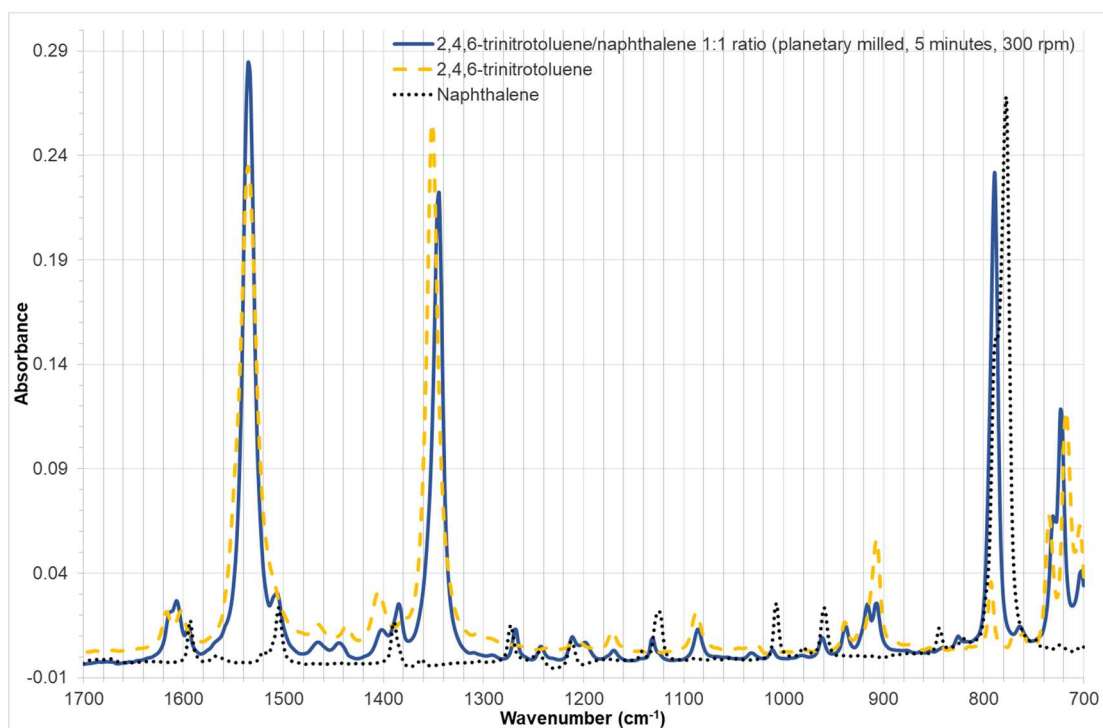


Figure A.26 - Infra-red spectra of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Table A.2 - Infrared spectra peak positions and heights of 2,4,6-trinitrotoluene/naphthalene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)
3098.89	0.02
1606.84	0.03
1595.19	0.01
1534.89	0.29
1506.74	0.03
1401.72	0.01
1384.79	0.03
1344.91	0.22
1268.36	0.01
1211.16	0.01
1085.71	0.01
961.68	0.01
938.01	0.01
916.21	0.03
907.19	0.03
825.44	0.01
789.1	0.23
763.91	0.01
730.5	0.07
722.86	0.12
702.58	0.04

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

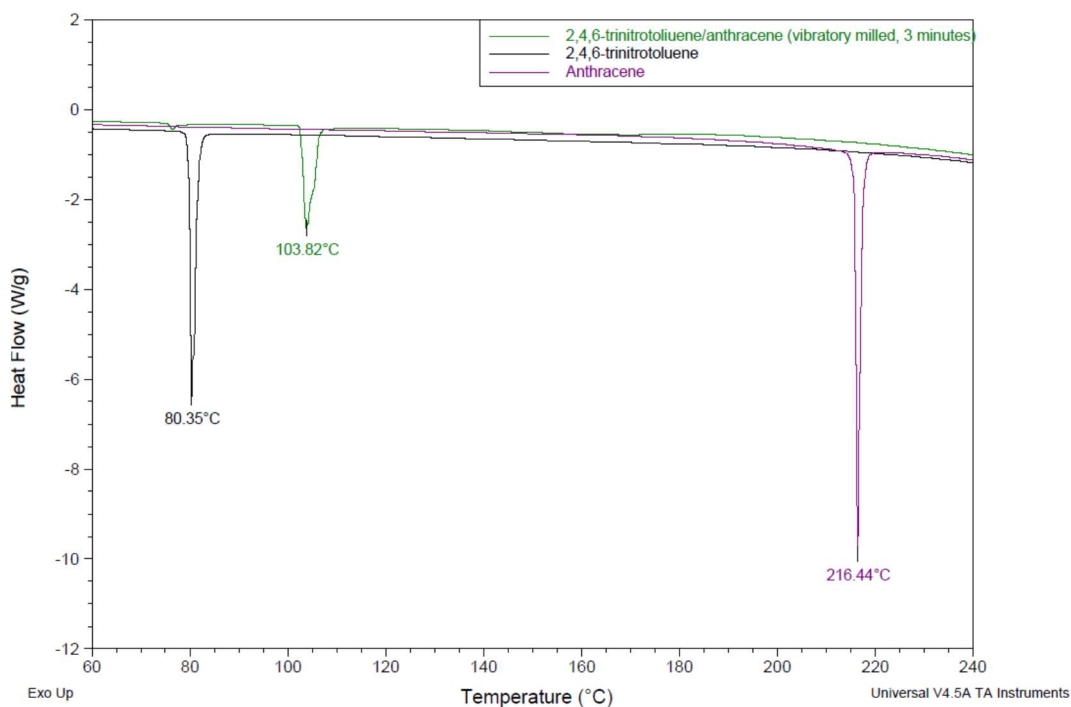


Figure A.27 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

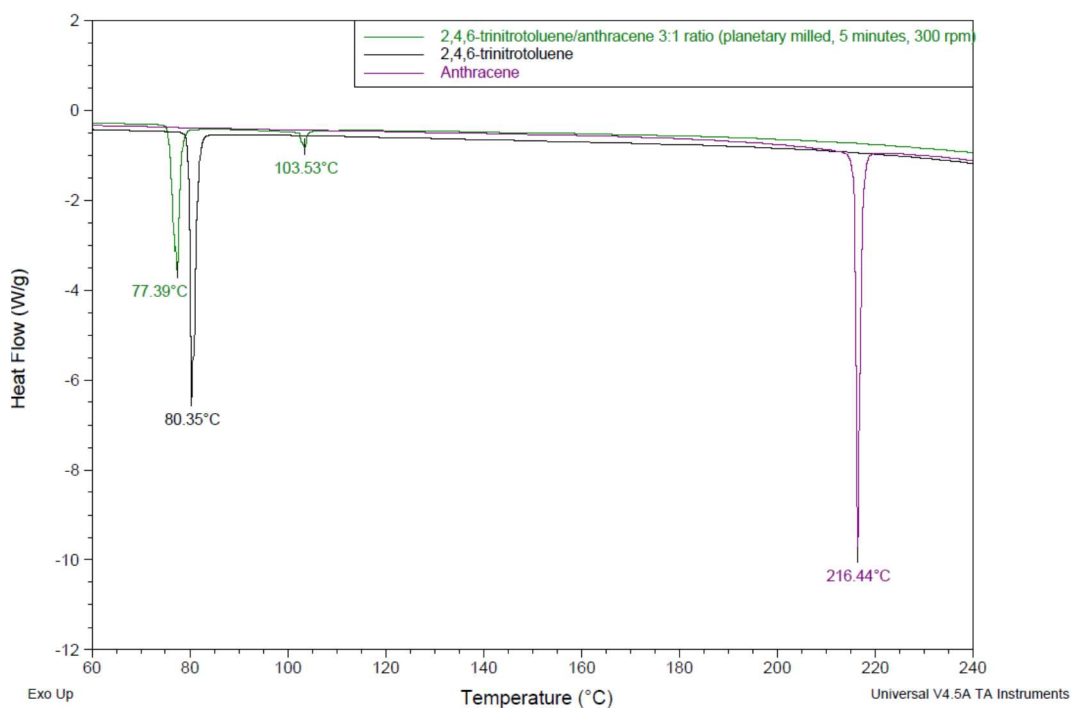


Figure A.28 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

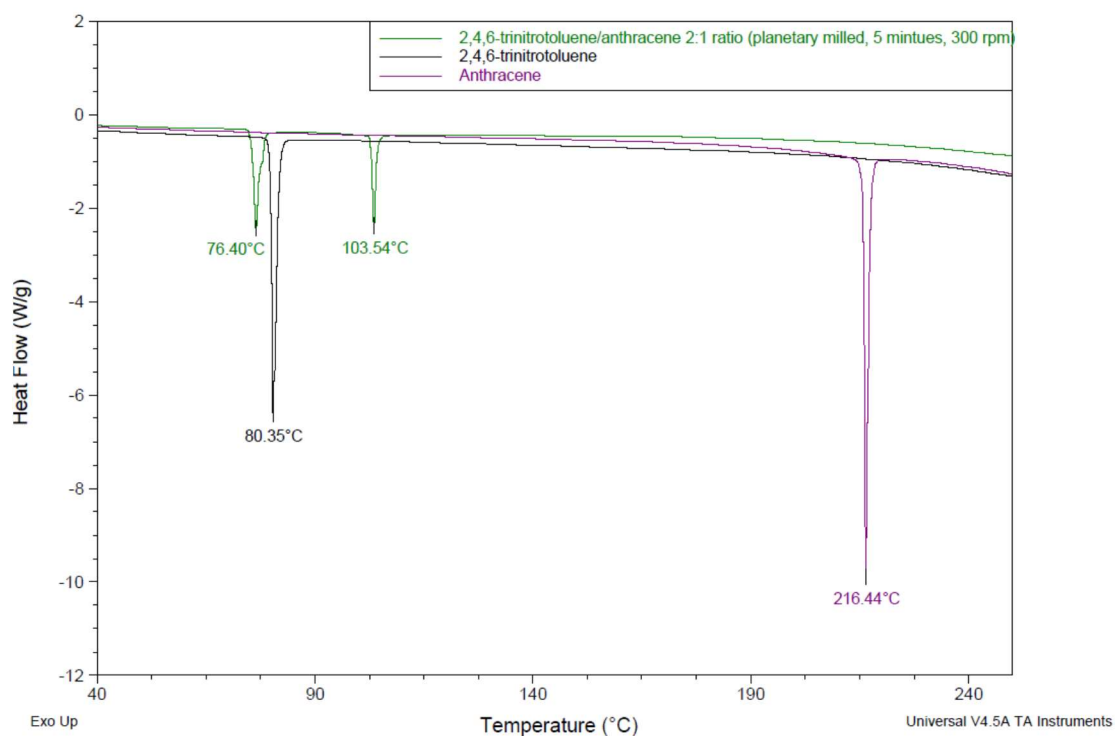


Figure A.29 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

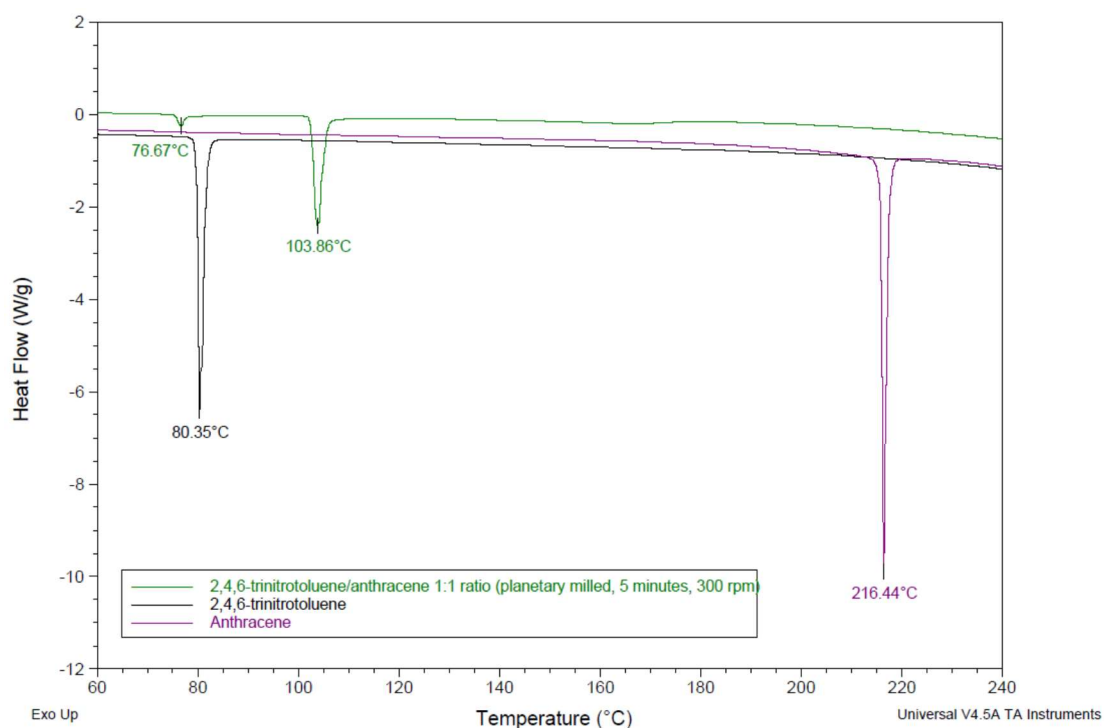


Figure A.30 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

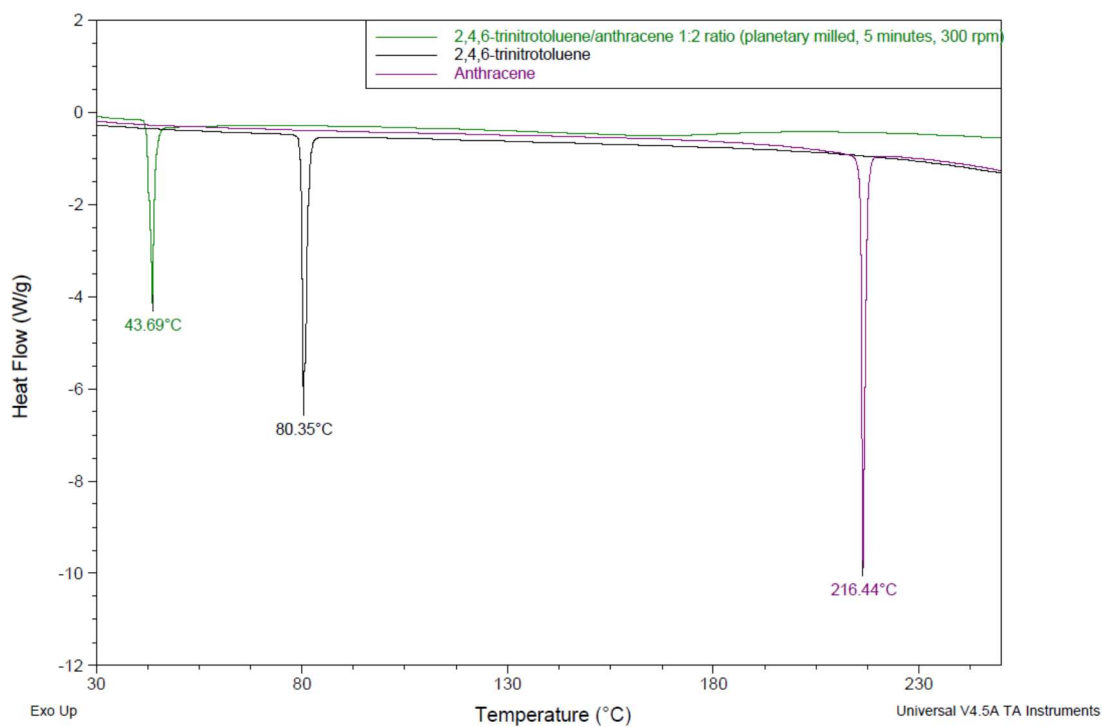


Figure A.31 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

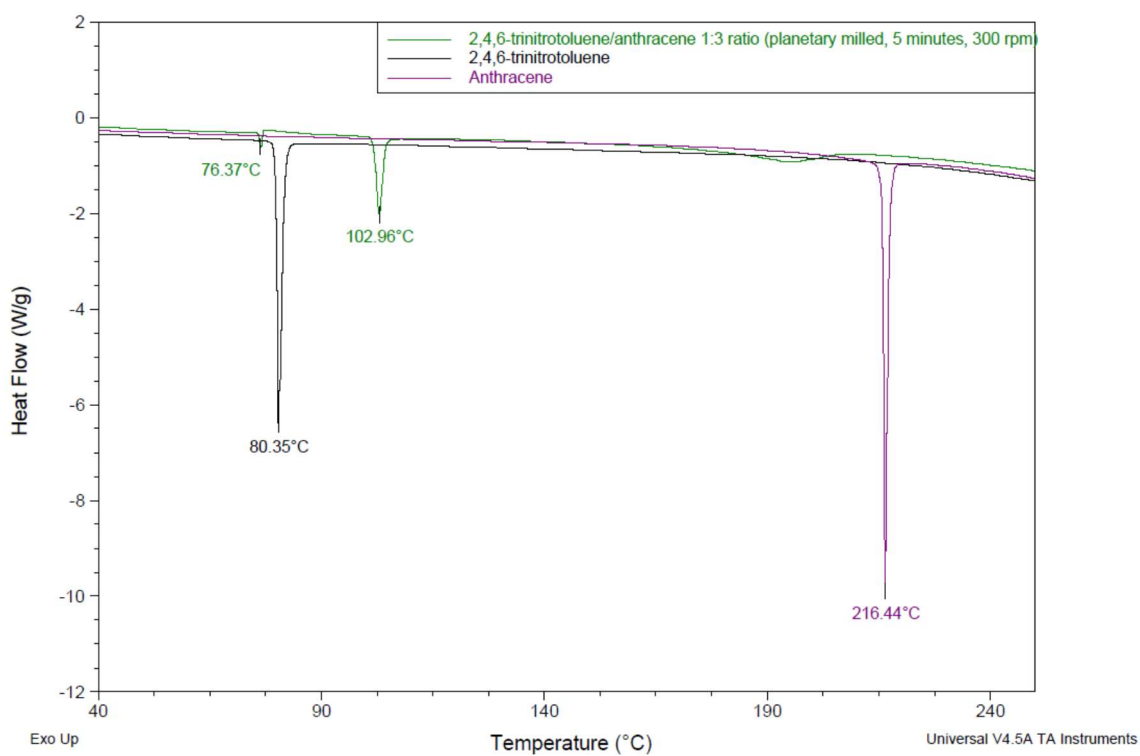


Figure A.32 - Thermal analysis of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

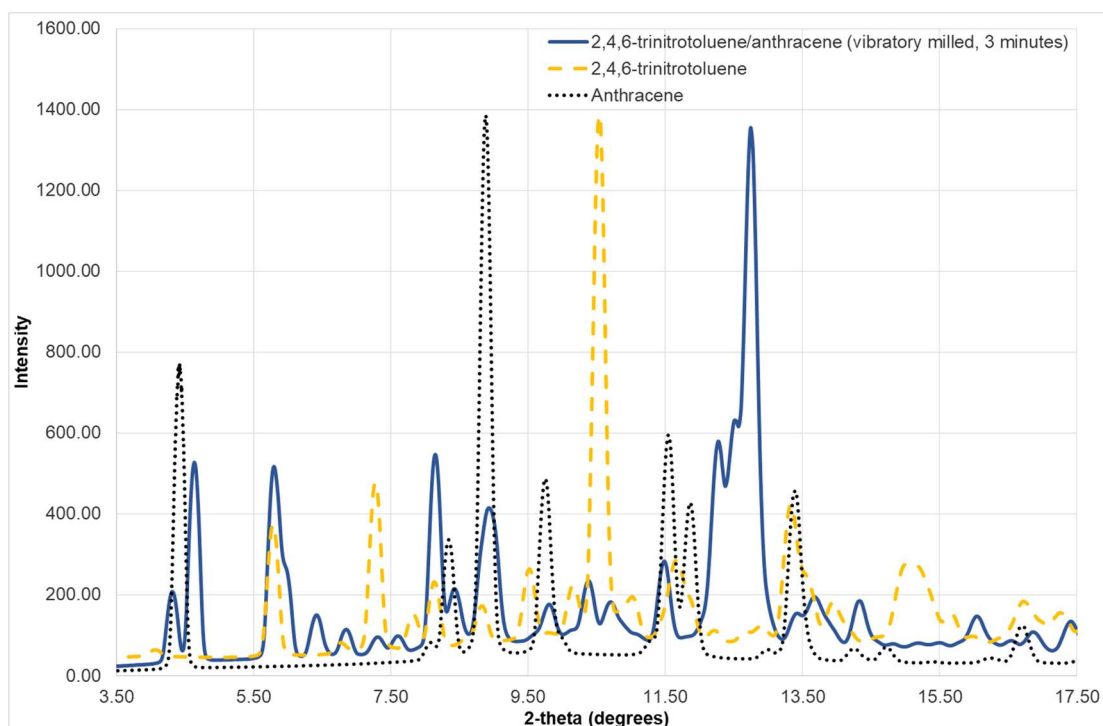


Figure A.33 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

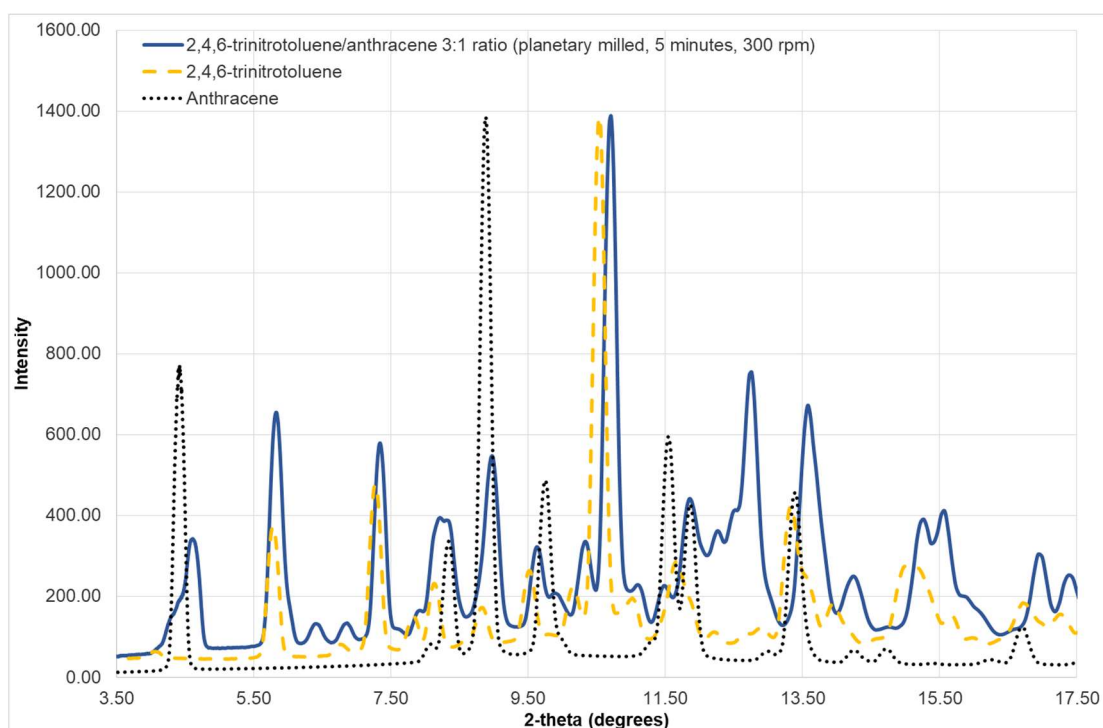


Figure A.34 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

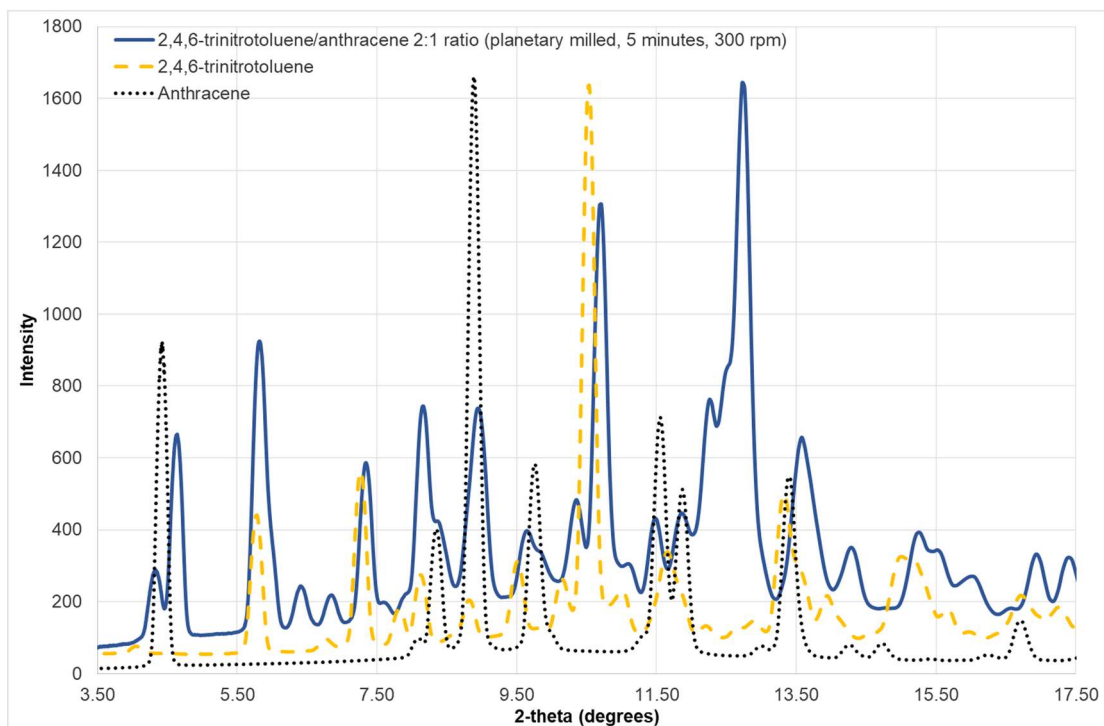


Figure A.35 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

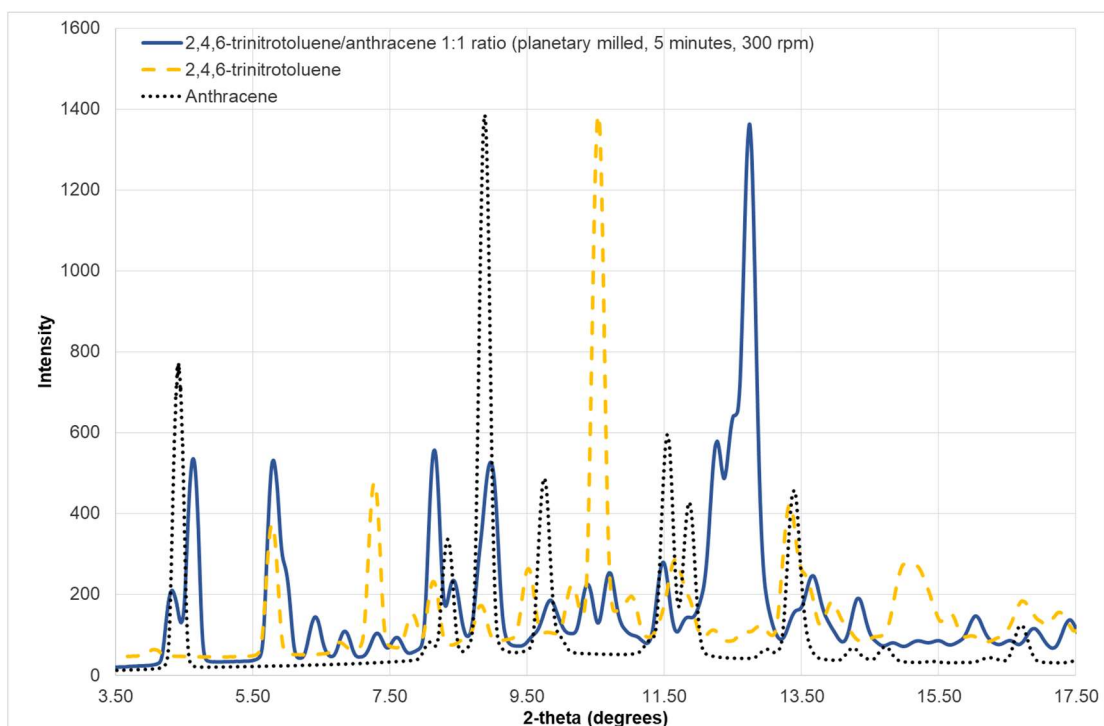


Figure A.36 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

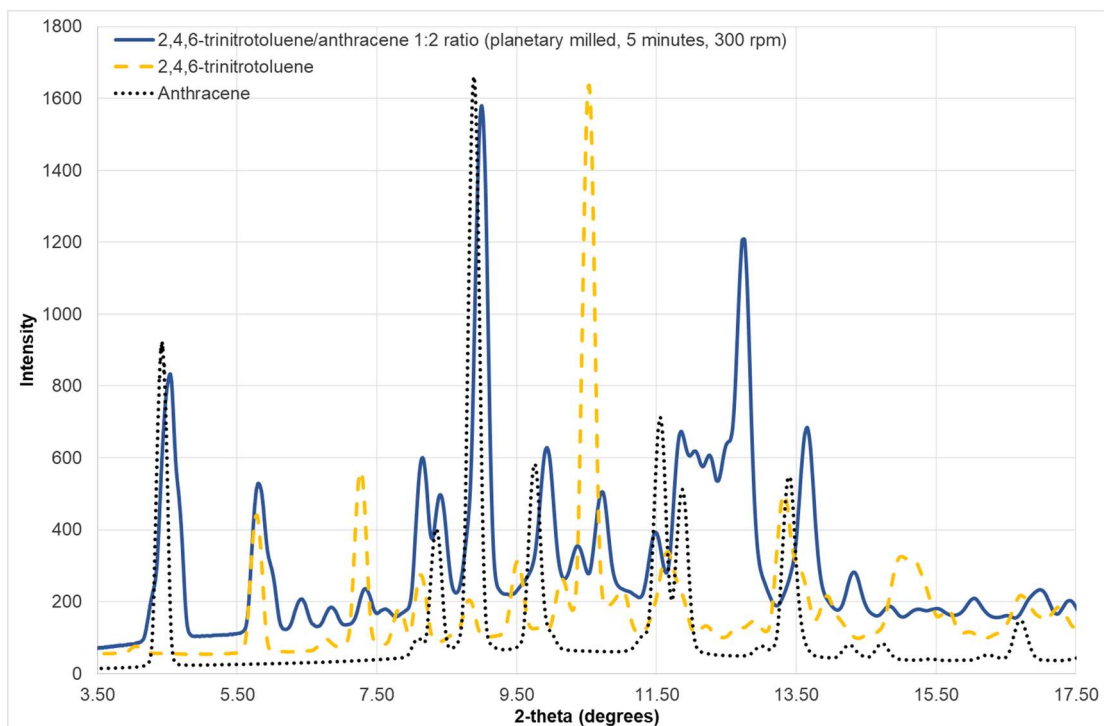


Figure A.37 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

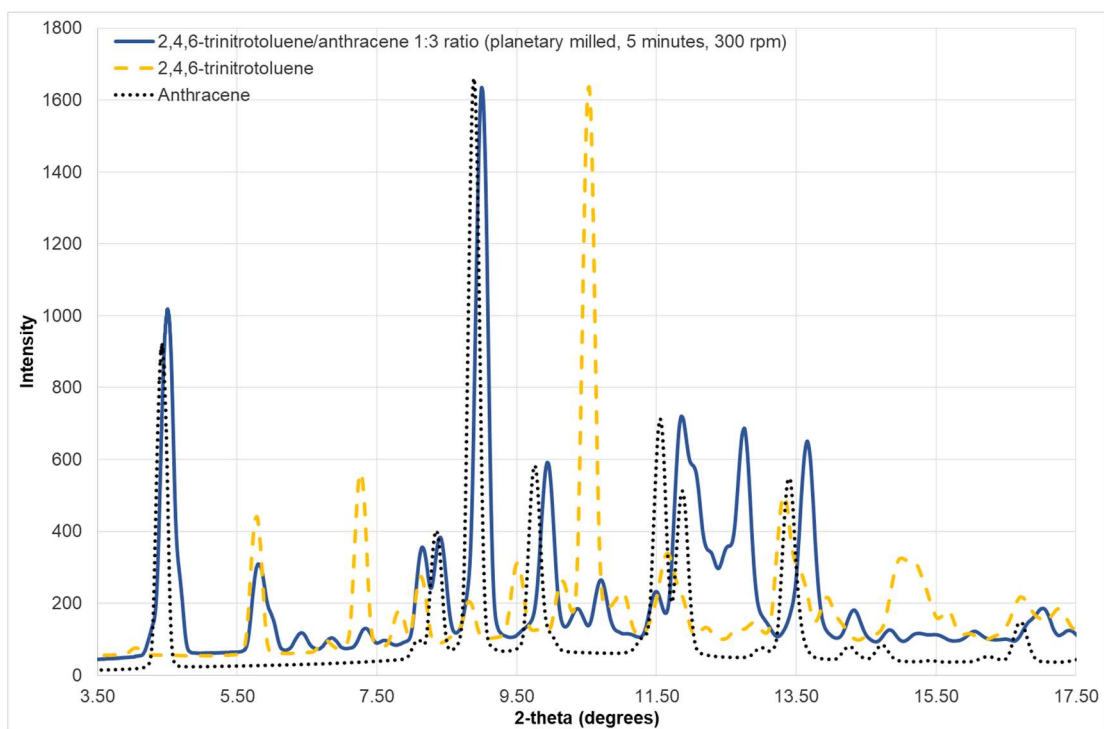


Figure A.38 - Powder x-ray pattern of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

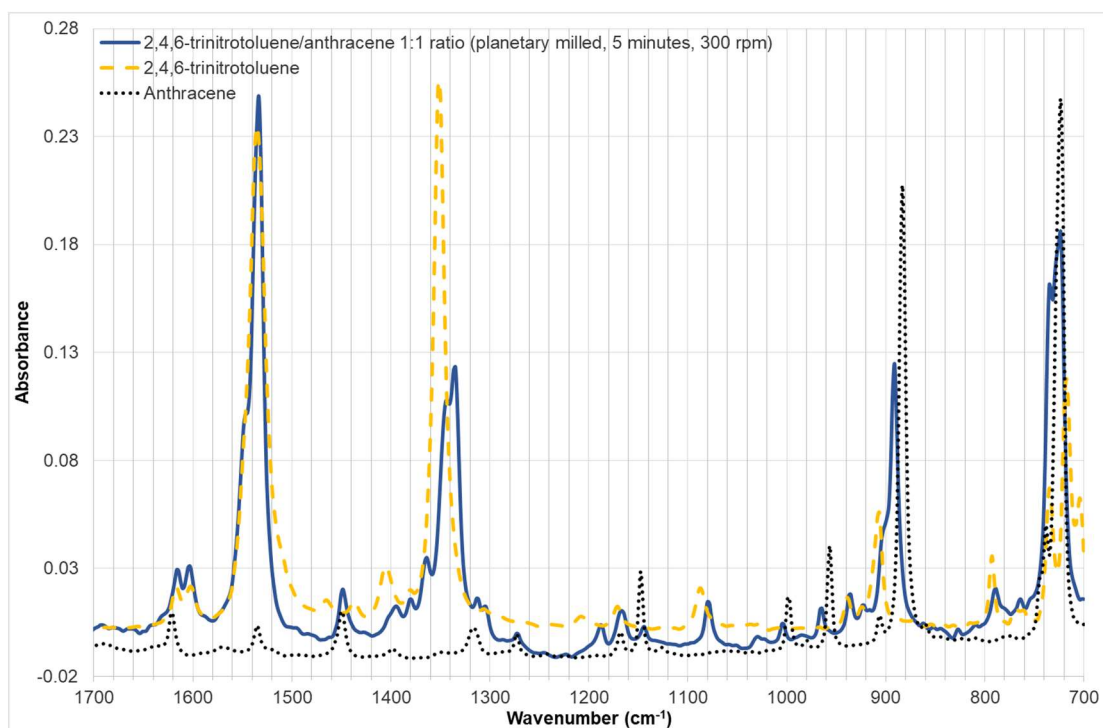


Figure A.39 - Infra-red spectra of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Table A.3 - Infrared spectra peak positions and heights of 2,4,6-trinitrotoluene/anthracene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)
3107.03	0.01
1615.7	0.01
1603.45	0.02
1533.62	0.12
1448.6	0.01
1394.71	0.01
1379.86	0.01
1363.93	0.02
1343.62	0.05
1335.42	0.06
1312.92	0.01
1305.01	0.01
1166.88	0.01
1079.53	0.01
965.05	0.01
936.08	0.01
922.69	0.01
916.36	0.01
891.33	0.06
789.14	0.01
764.03	0.01
734.27	0.08
723.83	0.09
701.68	0.01

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

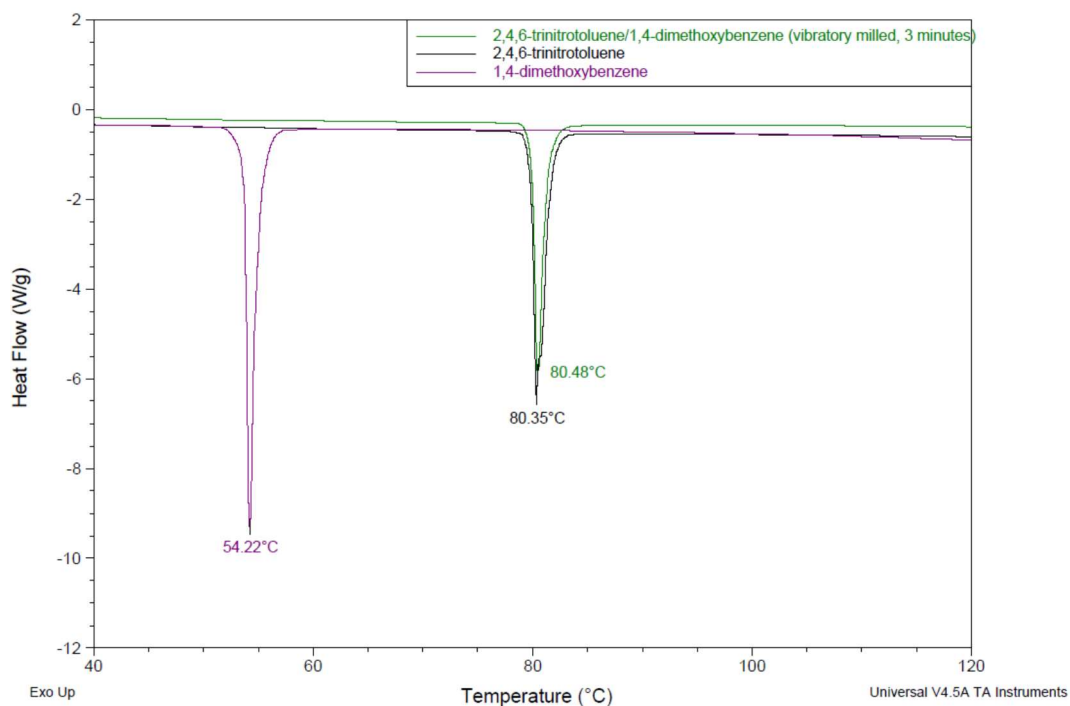


Figure A.40 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

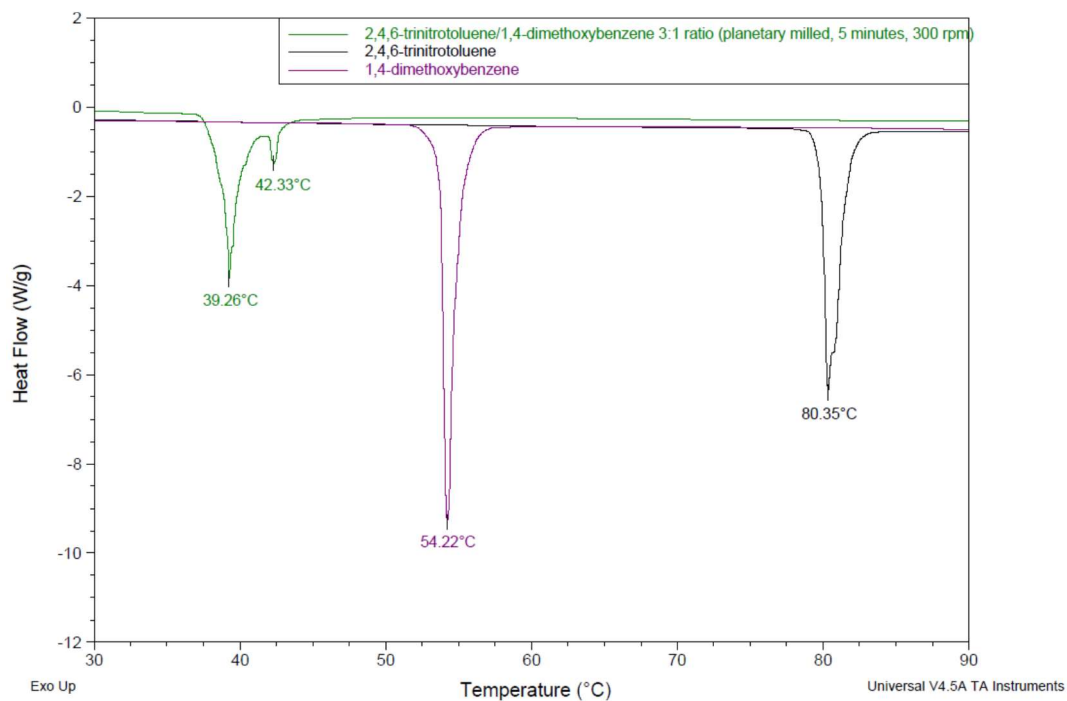


Figure A.41 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

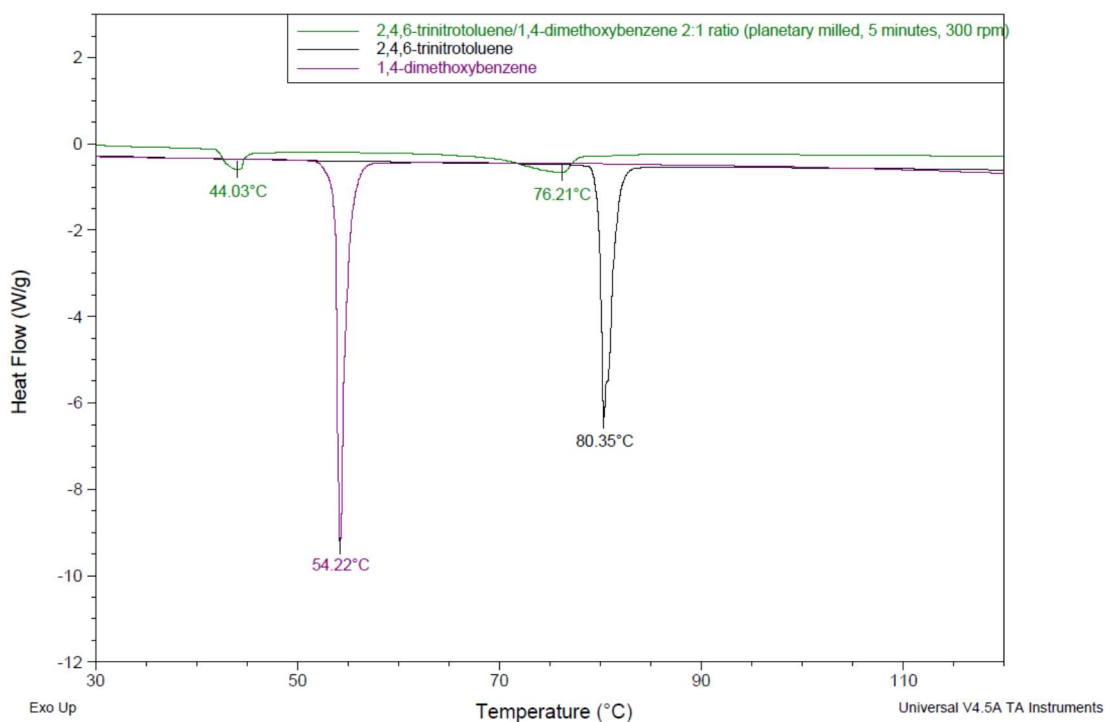


Figure A.42 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

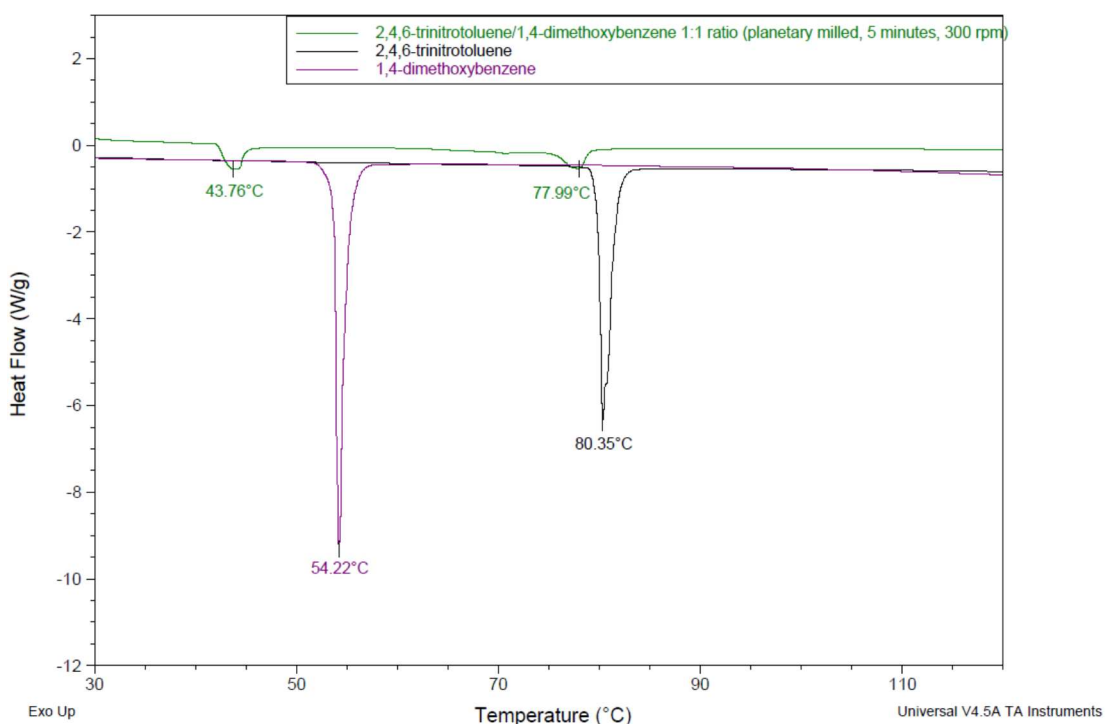


Figure A.43 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

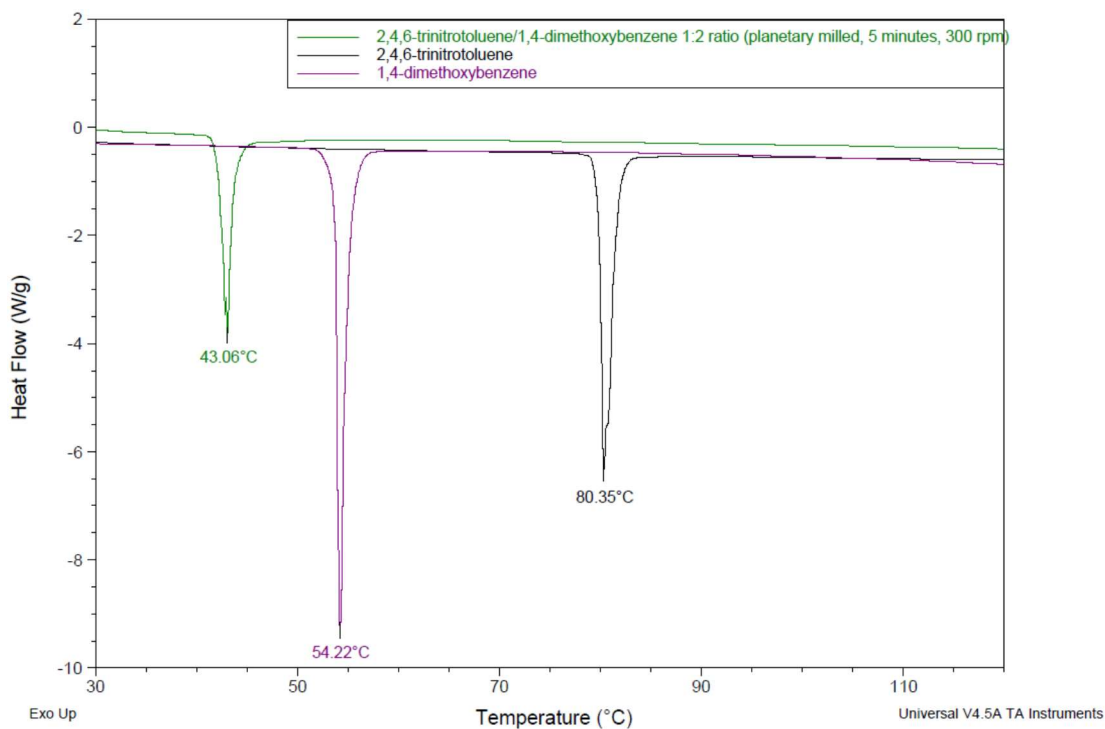


Figure A.44 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

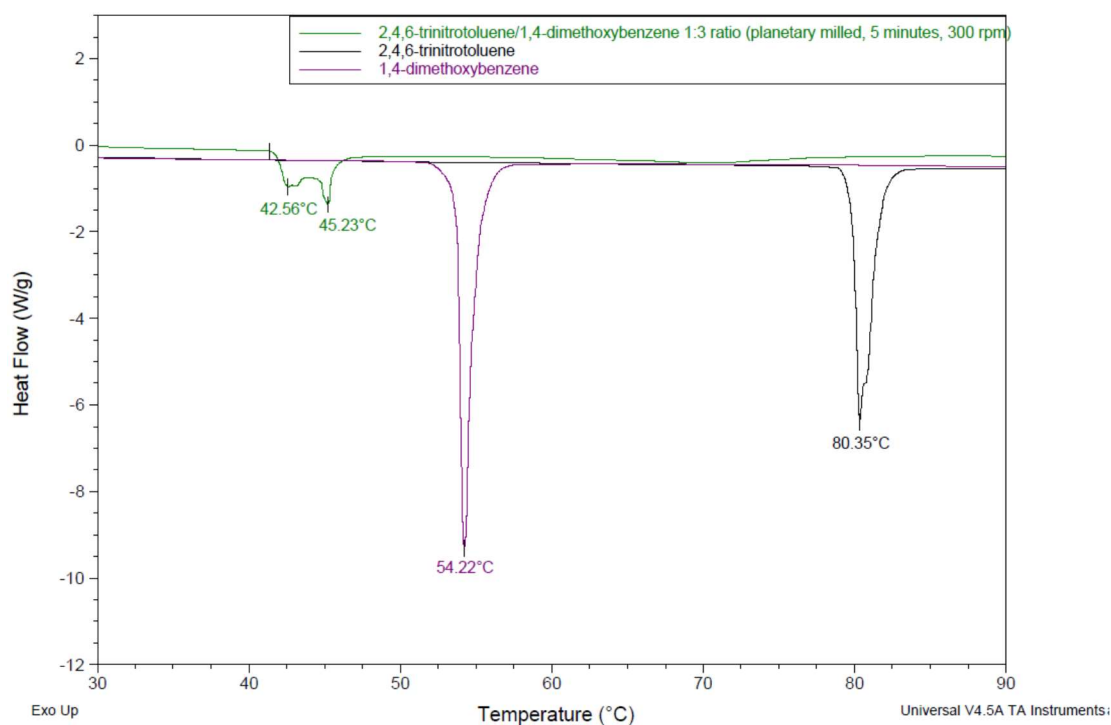


Figure A.45 - Thermal analysis of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

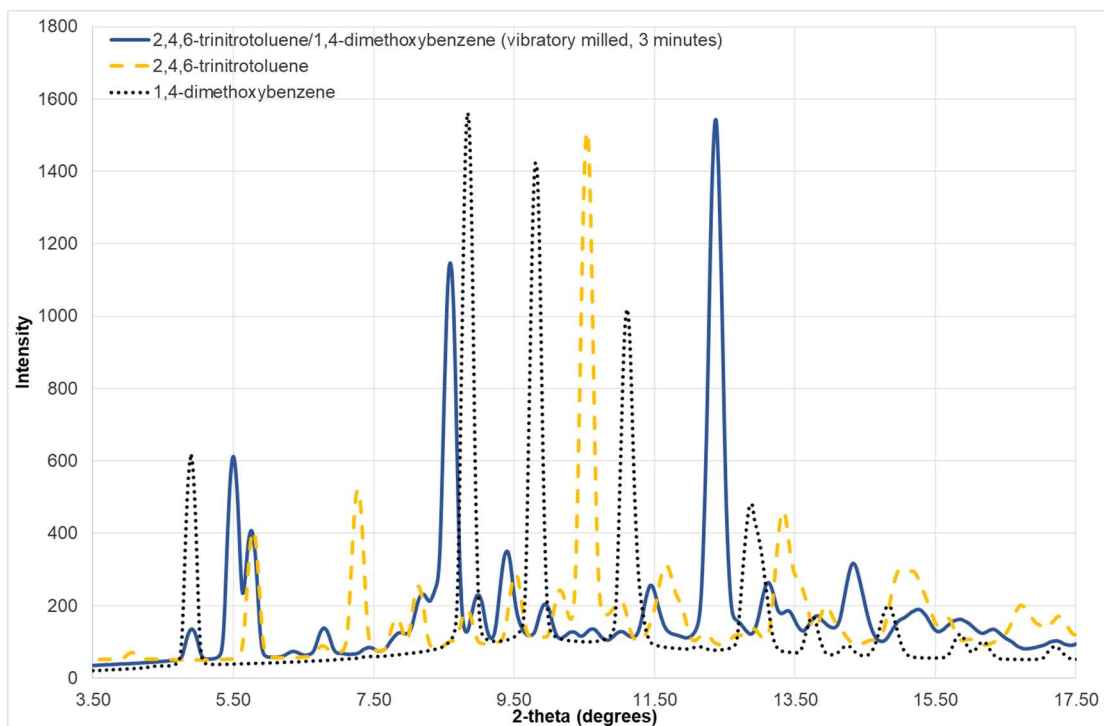


Figure A.46 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by vibratory milling for 3 minutes with a 1:1 stoichiometry.

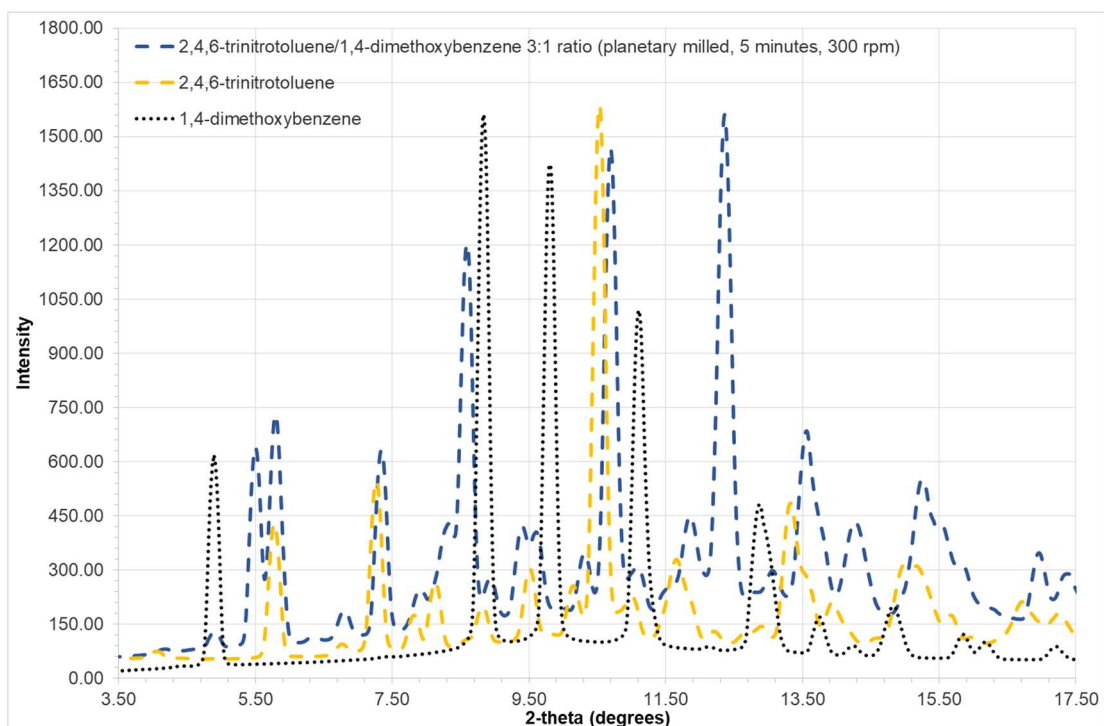


Figure A.47 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 3:1 stoichiometry.

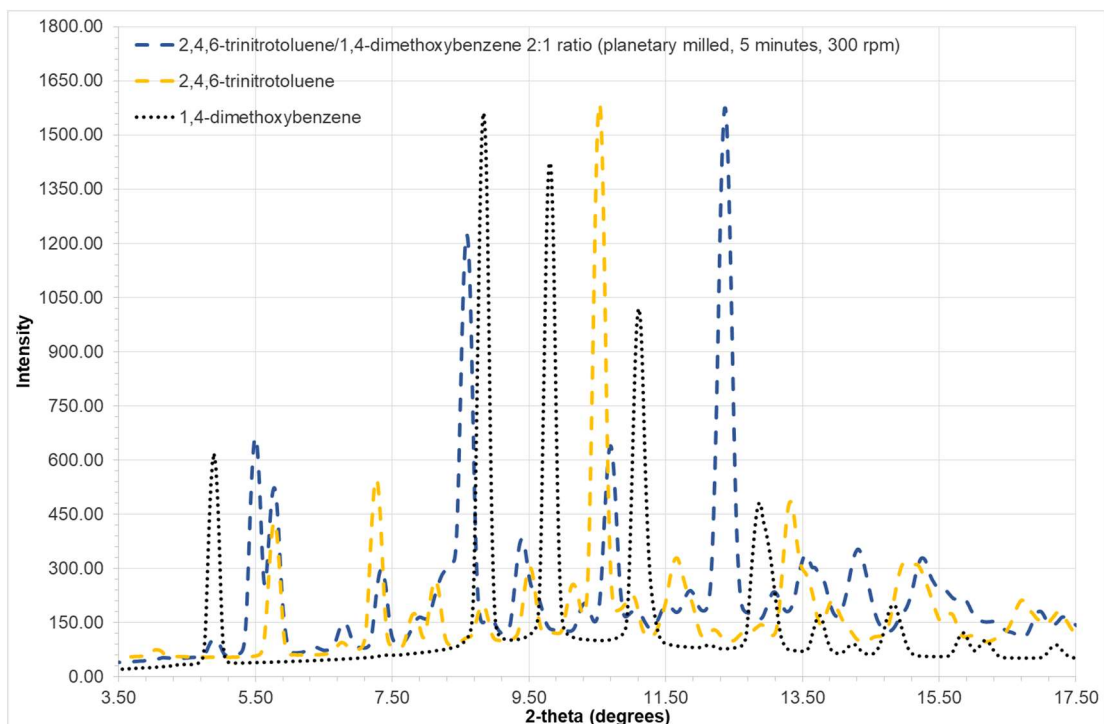


Figure A.48 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 2:1 stoichiometry.

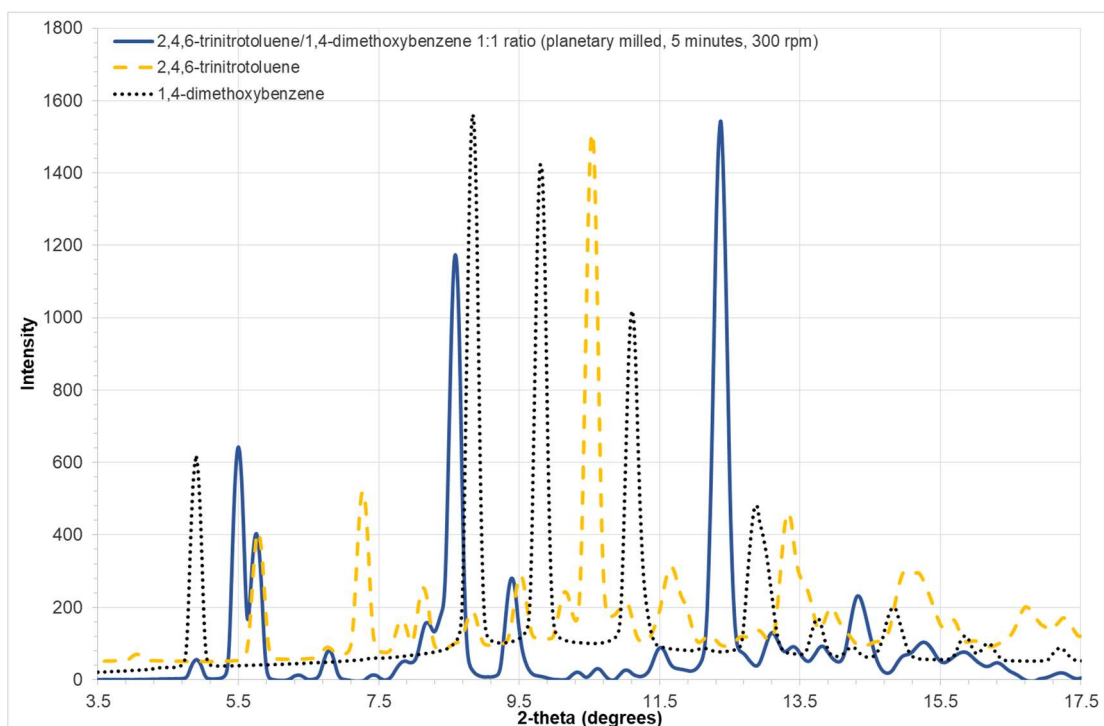


Figure A.49 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

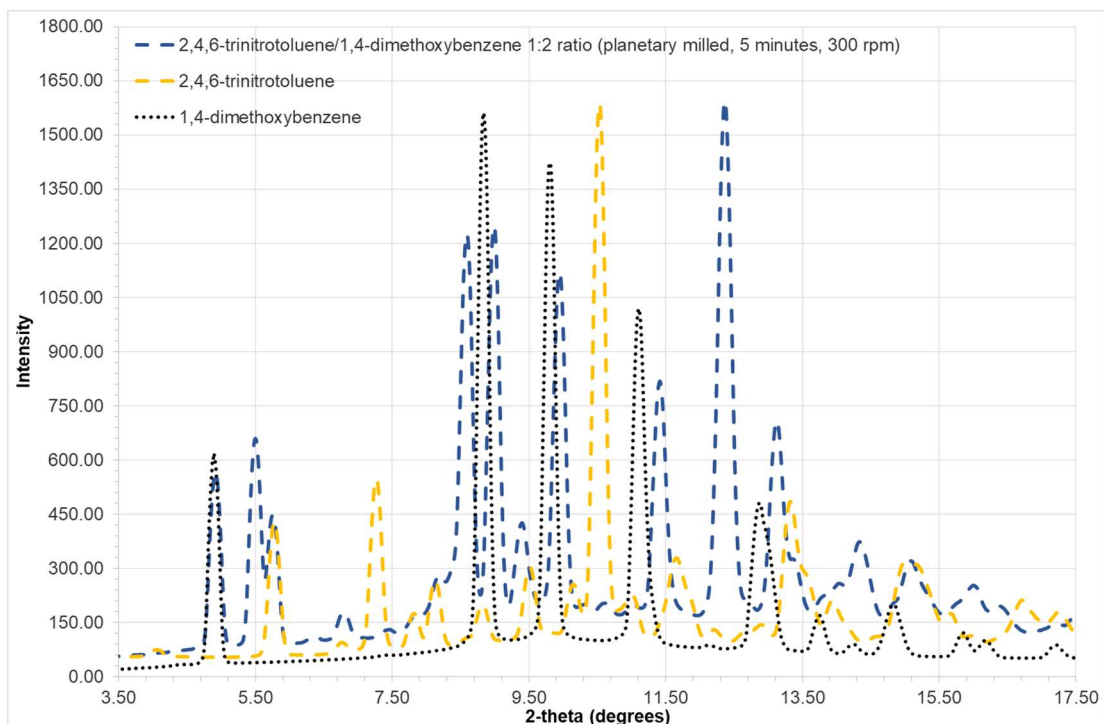


Figure A.50 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:2 stoichiometry.

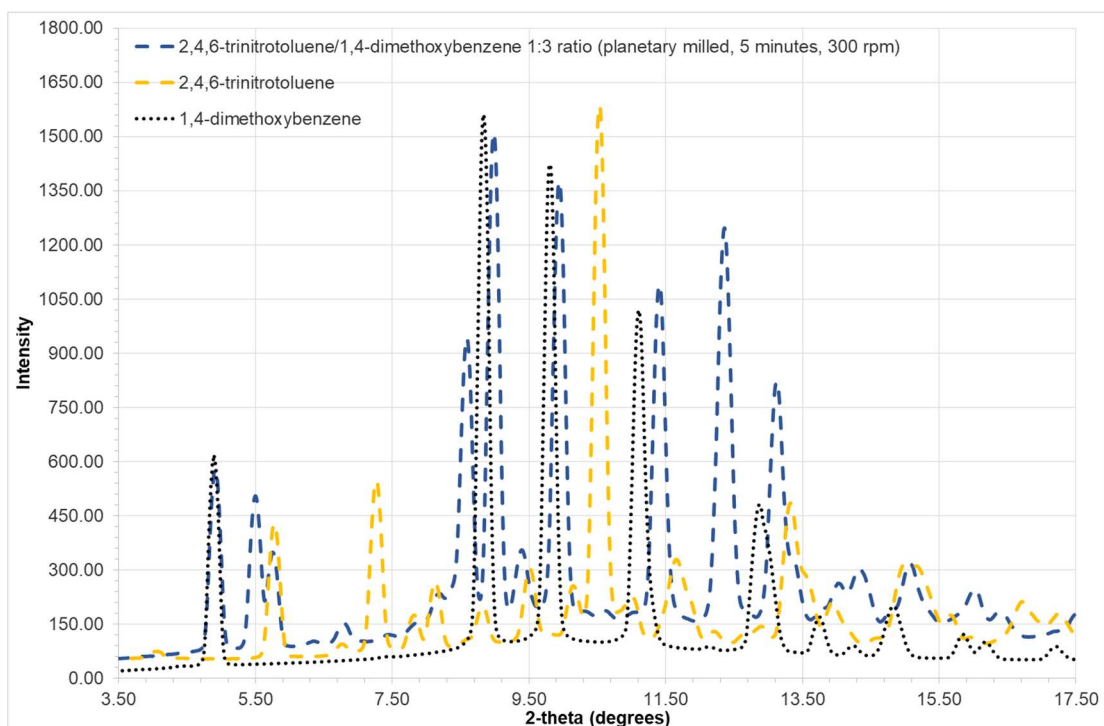


Figure A.51 - Powder x-ray pattern of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:3 stoichiometry.

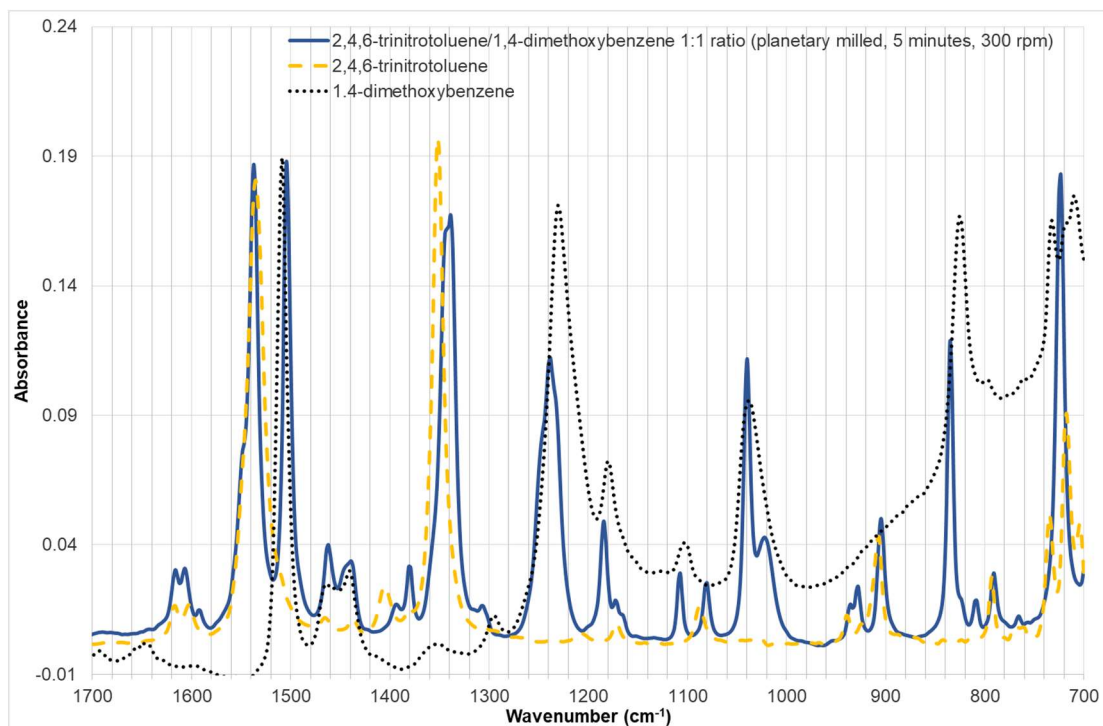


Figure A.52 – Infra-red spectra of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm with a 1:1 stoichiometry.

Table A.4 - Infrared spectra peak positions and heights of 2,4,6-trinitrotoluene/1,4-dimethoxybenzene produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)
3087.55	0.01
1616.25	0.03
1606.84	0.03
1592.56	0.01
1537.29	0.19
1504.18	0.19
1462.26	0.04
1439.38	0.03
1393.29	0.02
1380.31	0.03
1338.97	0.17
1307.13	0.02
1238.51	0.11
1184.31	0.05
1172.51	0.02
1107.47	0.03
1080.66	0.03
1039.77	0.11
1022.25	0.04
935.34	0.02
928.13	0.02
904.71	0.05
834.92	0.12
808.86	0.02

B Results 2 – Manipulation of electrostatic potential and its impact on co-crystal formation (Chapter 5)

B.1 *N*-heterocyclic co-formers investigated in this study

Co-former name (CAS No.)	Co-former name (CAS No.)
Pyrrolidine (288-13-1)	2-methylimidazole (693-98-1)
3-Pyrroline (123-75-1)	4-Methylimidazole (822-36-6)
Pyrrole (109-97-7)	Imidazol-2-amine (7720-39-0)
2-Nitropyrrole (5919-26-6)	2-Bromoimidazole (16681-56-4)
2-Methylpyrrole (636-41-9)	4-Bromoimidazole (2302-25-2)
3-Methylpyrrole (616-43-3)	2,4-Dimethylimidazole (930-62-1)
2,4-Dimethylpyrrole (625-82-1)	4,5-Dinitroimidazole (19183-14-3)
2,5-Dimethylpyrrole (625-84-3)	4,5-Dichloroimidazole (15965-30-7)
Pyrazole (288-13-1)	2,4,5-Tribromoimidazole (2034-22-2)
3-Nitropyrazole (26621-44-3)	2-Methyl-5-nitroimidazole (696-23-1)
4-Nitropyrazole (2075-46-9)	4-Methyl-5-nitroimidazole (14003-66-8)
5-Methylpyrazole (88054-14-2)	2-Bromo-5-nitroimidazole (65902-59-2)
Pyrazol-4-amine (28466-26-4)	4-Bromo-2-methylimidazole (16265-11-5)
3-Bromopyrazole (14521-80-3)	5-Bromo-4-methylimidazole (15813-08-8)
4-Bromopyrazole (2075-45-8)	4,5-Dibromo-2-methylimidazole (4002-81-7)
3,4-Dimethylpyrazole (2820-37-3)	2,5-Dibromo-4-methylimidazole (219814-29-6)
3,5-Dimethylpyrazole (67-51-6)	1,2,3-Triazole (288-35-7)
3,4,5-Tribromopyrazole (17635-44-8)	5-Nitro-1,2,3-triazole (84406-63-3)
3-Methyl-5-nitropyrazole (34334-96-8)	1,2,4-Triazole (288-88-0)
5-Methylpyrazol-3-amine (31230-17-8)	3-Methyl-1,2,4-triazole (7170-01-6)
4-Bromopyrazol-3-amine (16461-94-2)	1,2,4-Triazol-3-amine (61-82-5)
3-Bromopyrazol-5-amine	5-Bromo-1,2,4-triazole (7343-33-1)

(950739-21-6)	
3,5-Dimethylpyrazol-4-amine (5272-86-6)	1,2,4-Triazol-3,5-diamine (1455-77-2)
3,4-Dimethylpyrazol-5-amine (91159-73-8)	3,5-Dimethyl-1,2,4-triazole (7343-34-2)
3-Methyl-4-bromopyrazole (13808-64-5)	3,5-Dibromo-1,2,4-triazole (7411-23-6)
3-Bromo-5-methylpyrazole (57097-81-1)	1,2,3,4-Tetrazole (288-94-8)
4-Bromo-3,5-dimethylpyrazole (3398-16-1)	1,2,3,4-Tetrazol-5-amine (4418-61-5)
Imidazole (288-32-4)	5-Methyl-1,2,3,4-tetrazole (4076-36-2)

B.2 2-naphthol/pyrrolidine

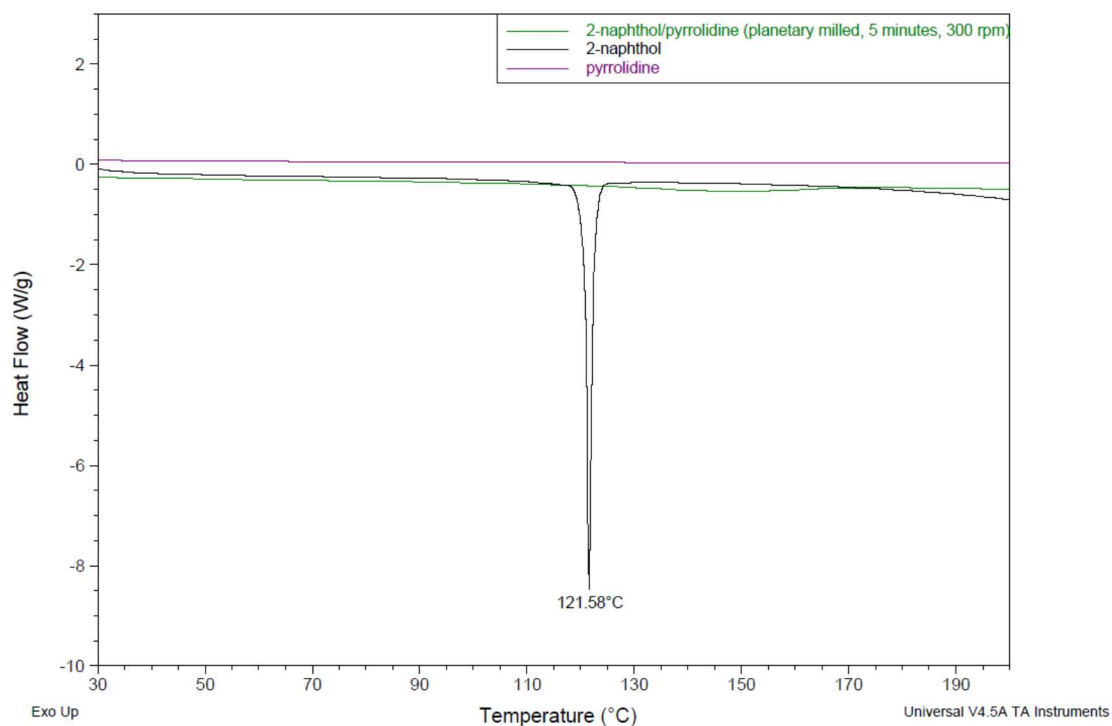


Figure B.1 - Thermal analysis of 2-naphthol/pyrrolidine produced by planetary milling for 5 minutes at 300 rpm. Pyrrolidine and the mixed system are liquids, therefore no melts are observed.

B.3 2-naphthol/3-pyrroline

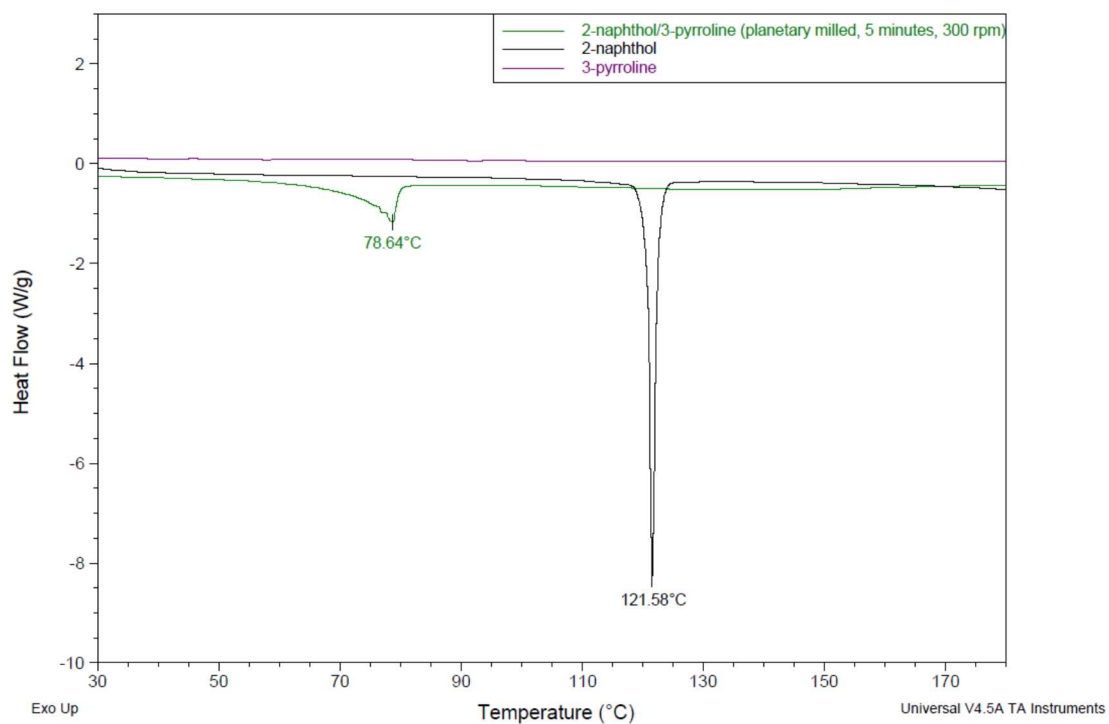


Figure B.2 - Thermal analysis of 2-naphthol/3-pyrroline produced by planetary milling for 5 minutes at 300 rpm. Pyrrole is a liquid, therefore no melt is observed.

B.4 2-naphthol/pyrrole

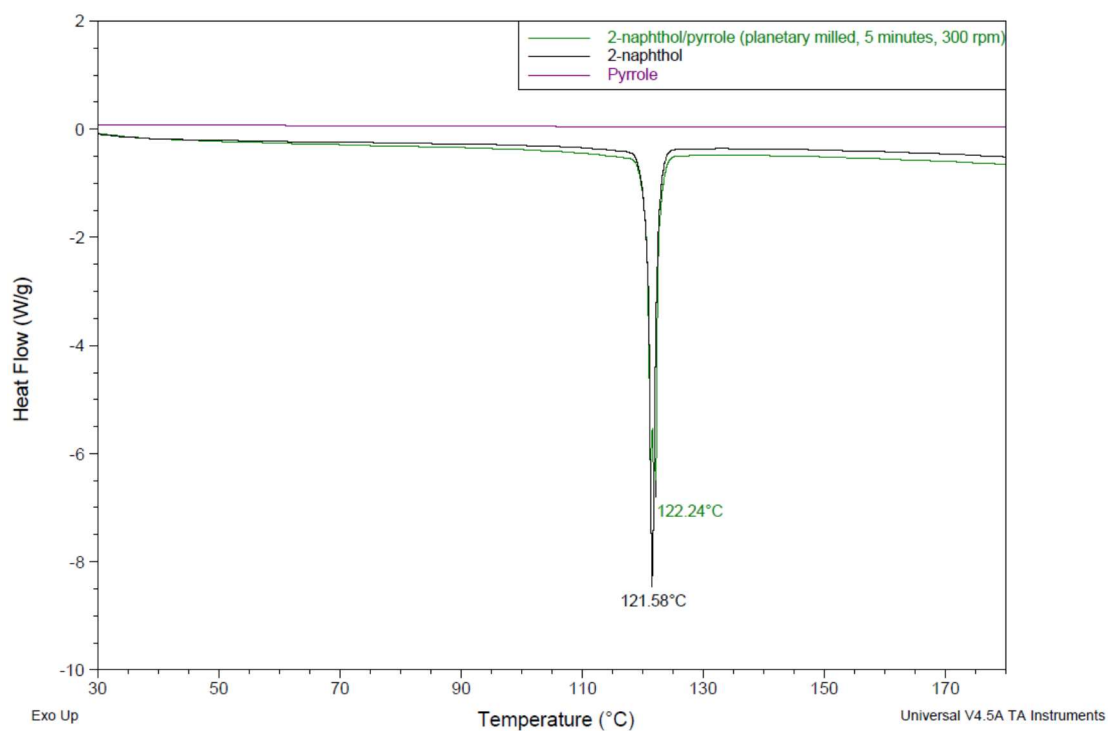


Figure B.3 – Thermal analysis of 2-naphthol/pyrrole produced by planetary milling for 5 minutes at 300 rpm. Pyrrole is a liquid, therefore no melt is observed.

B.5 2-naphthol/2-nitropyrrole

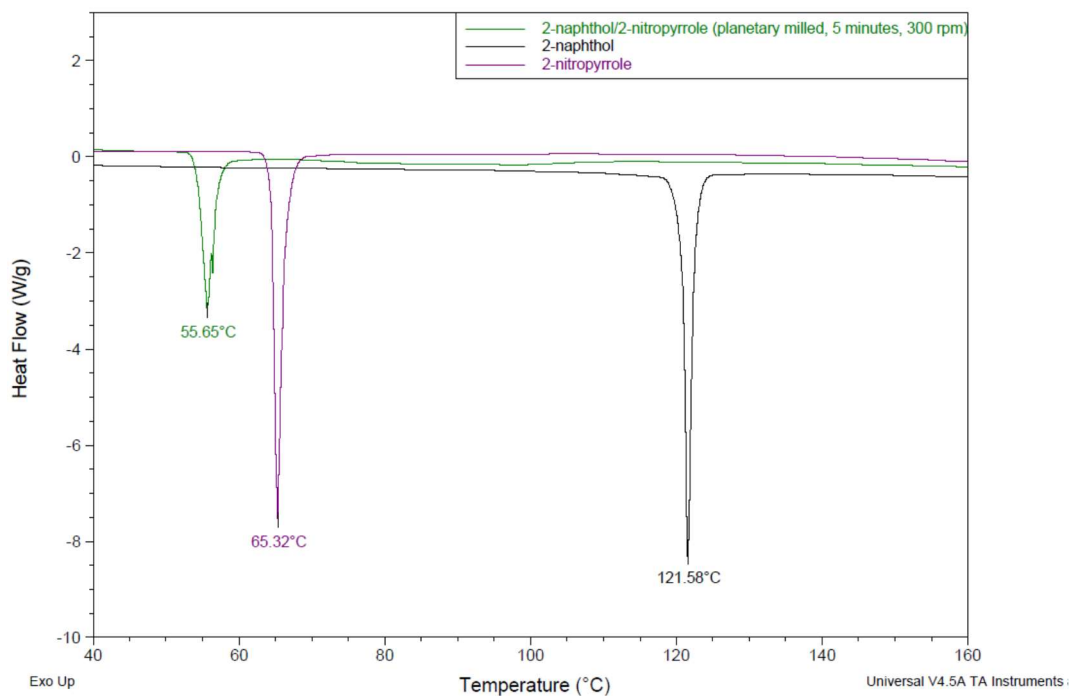


Figure B.4 – Thermal analysis of 2-naphthol/2-nitropyrrole produced by planetary milling for 5 minutes at 300 rpm.

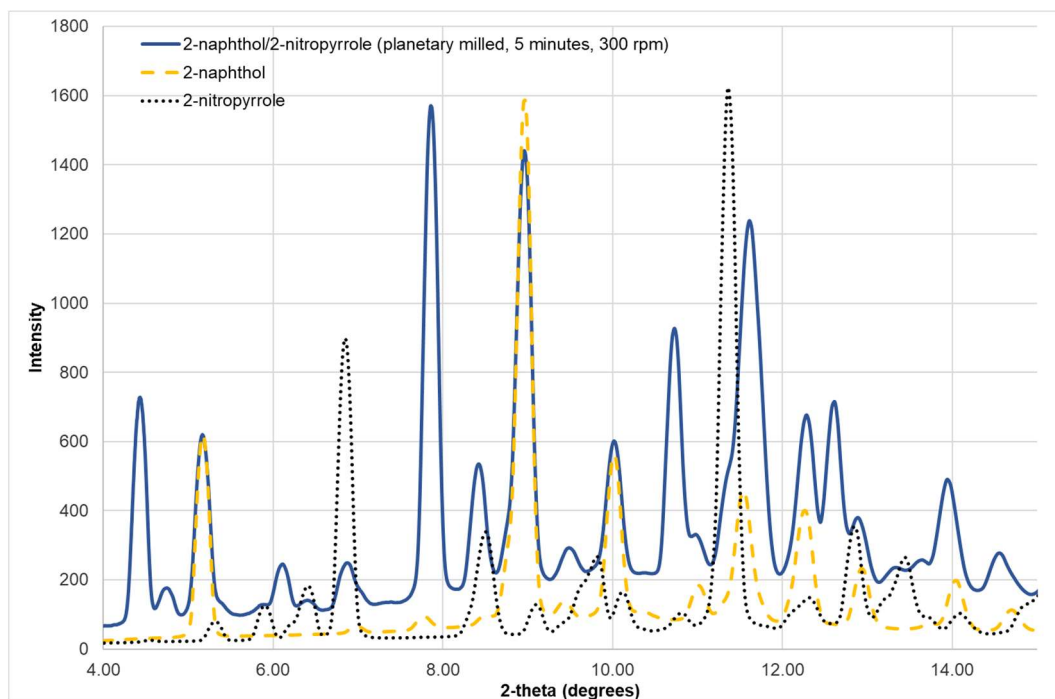


Figure B.5 - Powder x-ray pattern of 2-naphthol/2-nitropyrrole produced by planetary milling for 5 minutes at 300 rpm.

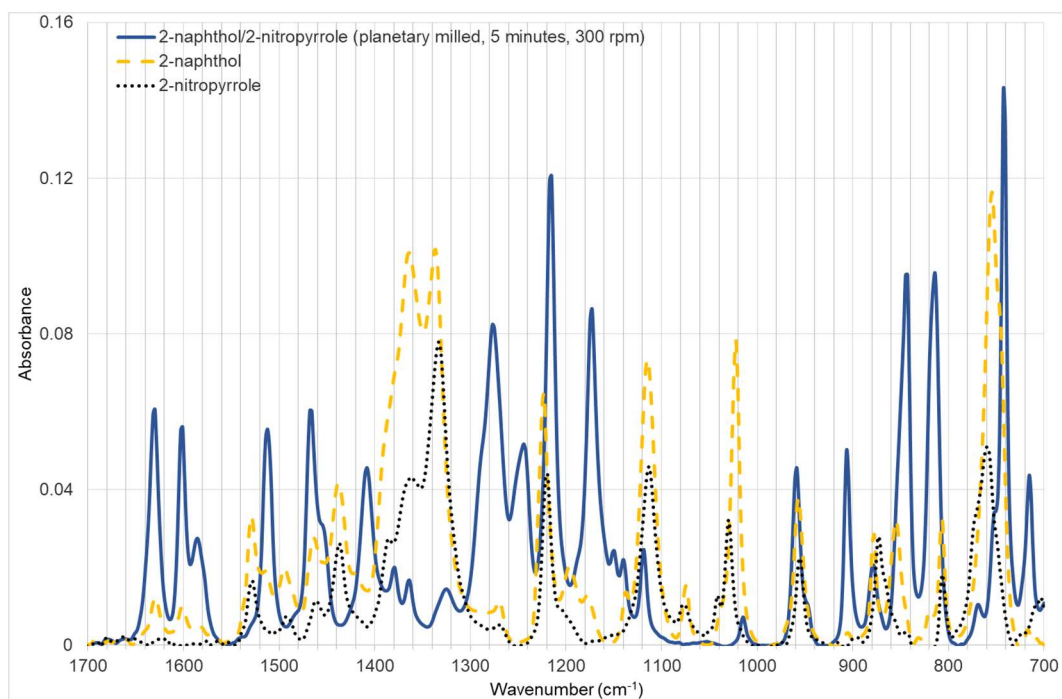


Figure B.6 – Infra-red spectra of 2-naphthol/2-nitropyrrole produced by planetary milling for 5 minutes at 300 rpm.

Table B.1 - Infrared spectra peak positions and heights of 2-naphthol/2-nitropyrrole produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)	Peak Position (cm ⁻¹)	Peak Height (Absorbance)
3242.59	0.04	1178.14	0.03
3142.1	0.01	1137.2	0.03
3129.22	0.01	1114.8	0.15
1629.56	0.01	1074.45	0.04
1601.05	0.01	1022.37	0.16
1529.06	0.06	956.87	0.08
1514.41	0.03	904.87	0.01
1494.38	0.03	877.98	0.06
1463.76	0.05	854.64	0.07
1438.1	0.08	830.95	0.02
1422.06	0.04	819.45	0.03
1363.97	0.2	806.65	0.08
1336.69	0.2	790.41	0.02
1269.57	0.03	754.46	0.25
1223.28	0.14	716.8	0.04
1196.04	0.05	707.47	0.04

B.6 2-naphthol/2-methylpyrrole

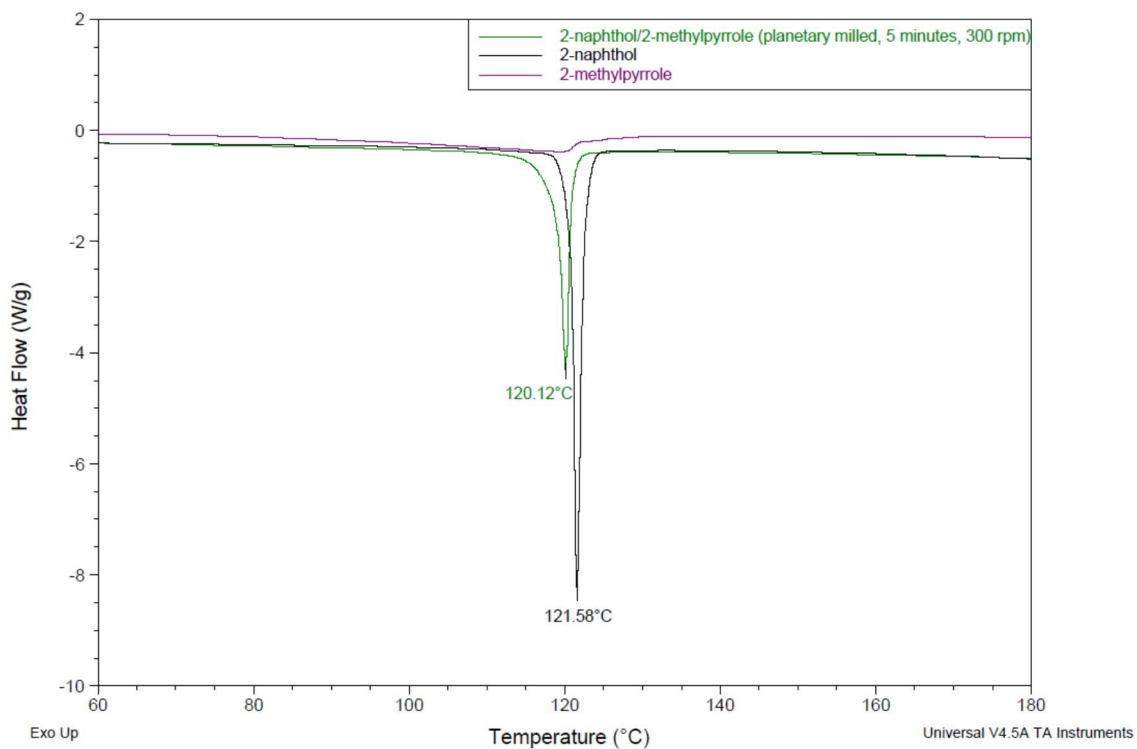


Figure B.7 - Thermal analysis of 2-naphthol/2-methylpyrrole produced by planetary milling for 5 minutes at 300 rpm. 2-methylpyrrole is a liquid and showed no melt.

B.7 2-naphthol/3-methylpyrrole

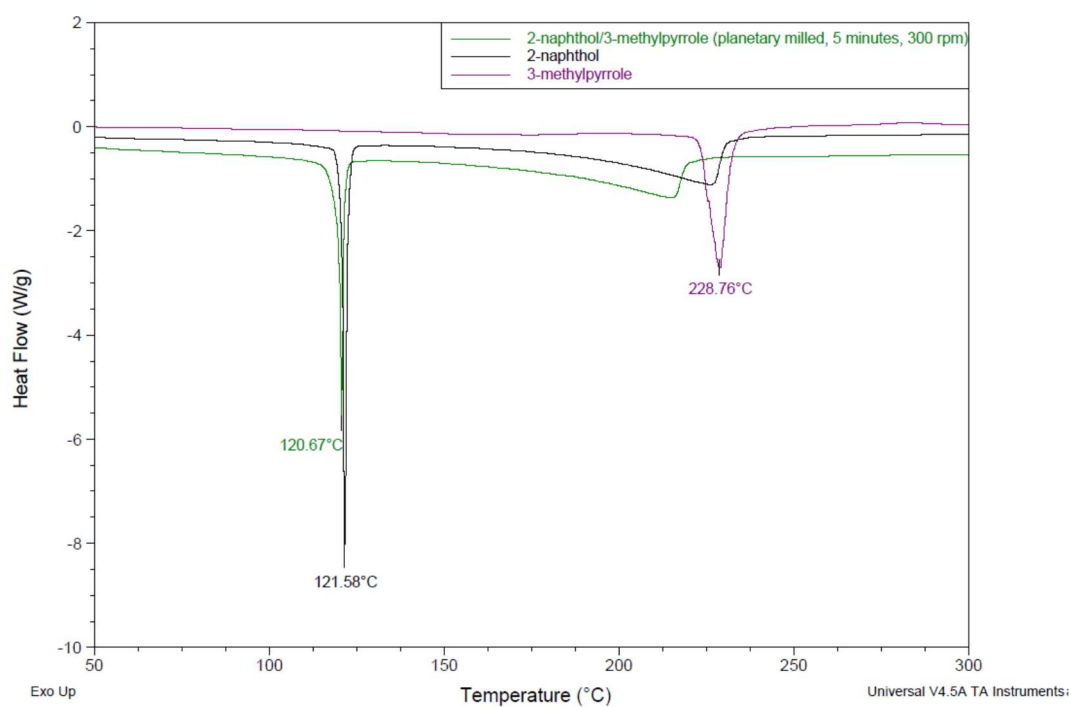


Figure B.8 - Thermal analysis of 2-naphthol/3-methylpyrrole produced by planetary milling for 5 minutes at 300 rpm.

B.8 2-naphthol/2,4-dimethylpyrrole

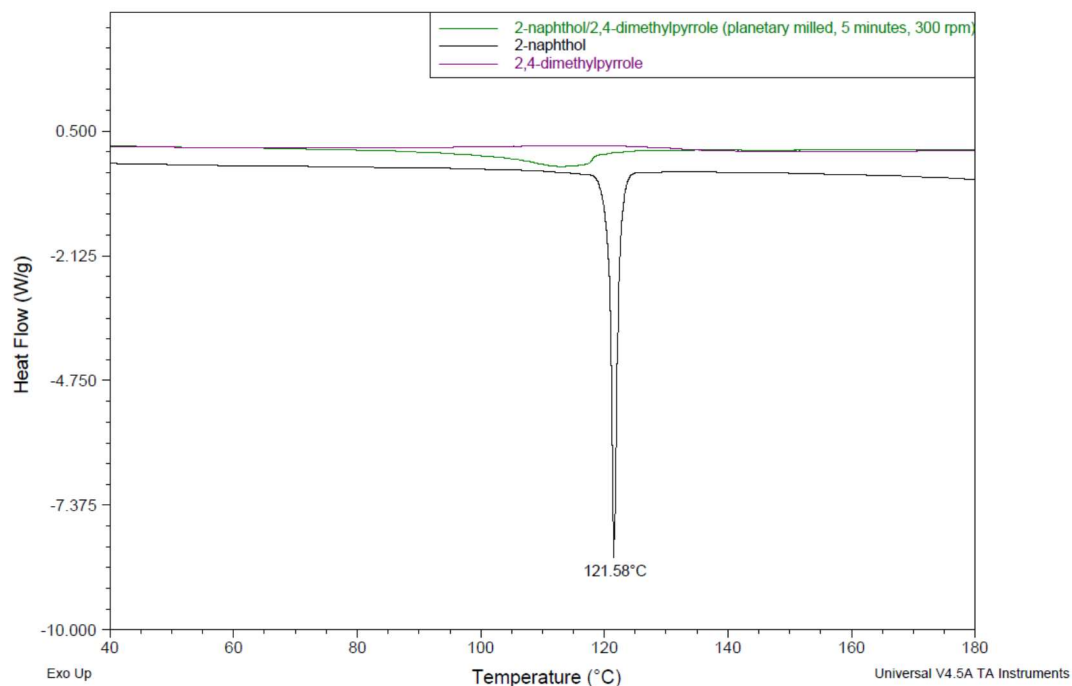


Figure B.9 - Thermal analysis of 2-naphthol/2,4-dimethylpyrrole produced by planetary milling for 5 minutes at 300 rpm. 2,4-dimethylpyrazole is a liquid and did not display a melt.

B.9 2-naphthol/2,5-dimethylpyrrole

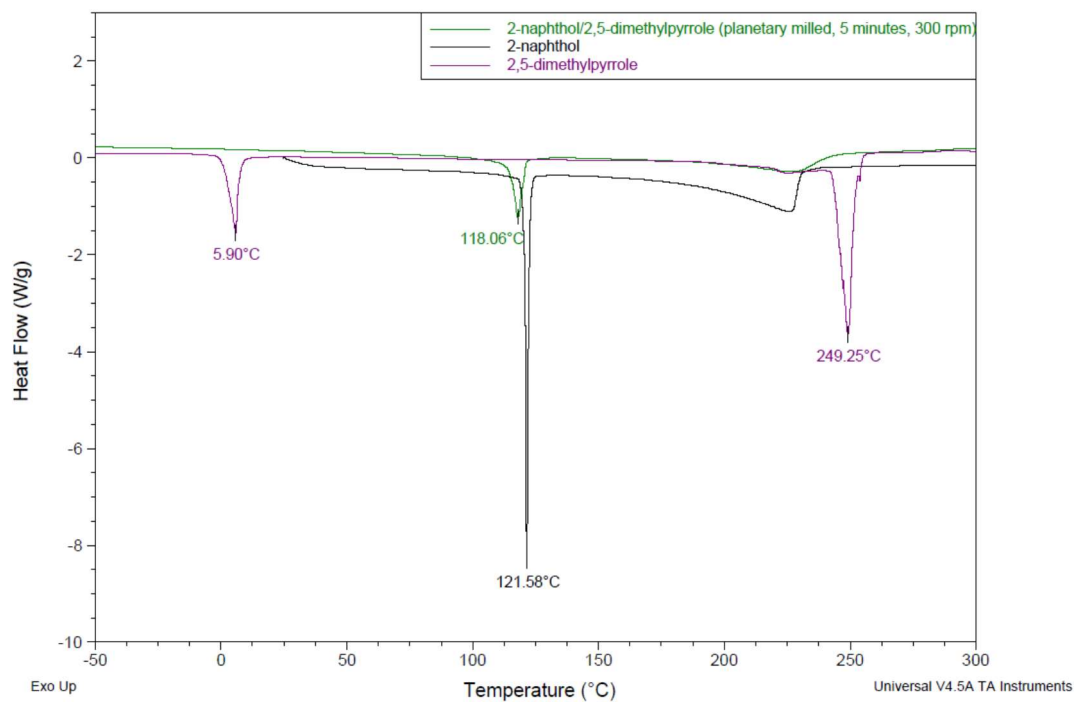


Figure B.10 - Thermal analysis of 2-naphthol/2,5-dimethylpyrrole produced by planetary milling for 5 minutes at 300 rpm.

B.10 2-naphthol/pyrazole

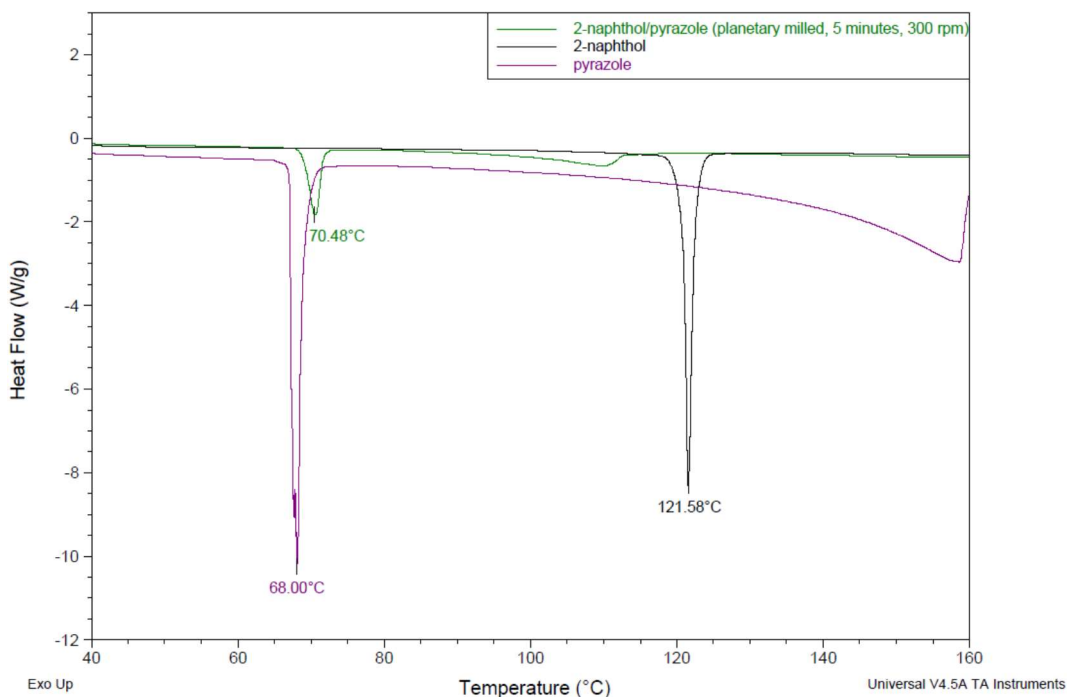


Figure B.11 – Thermal analysis of 2-naphthol/pyrazole produced by planetary milling for 5 minutes at 300 rpm.

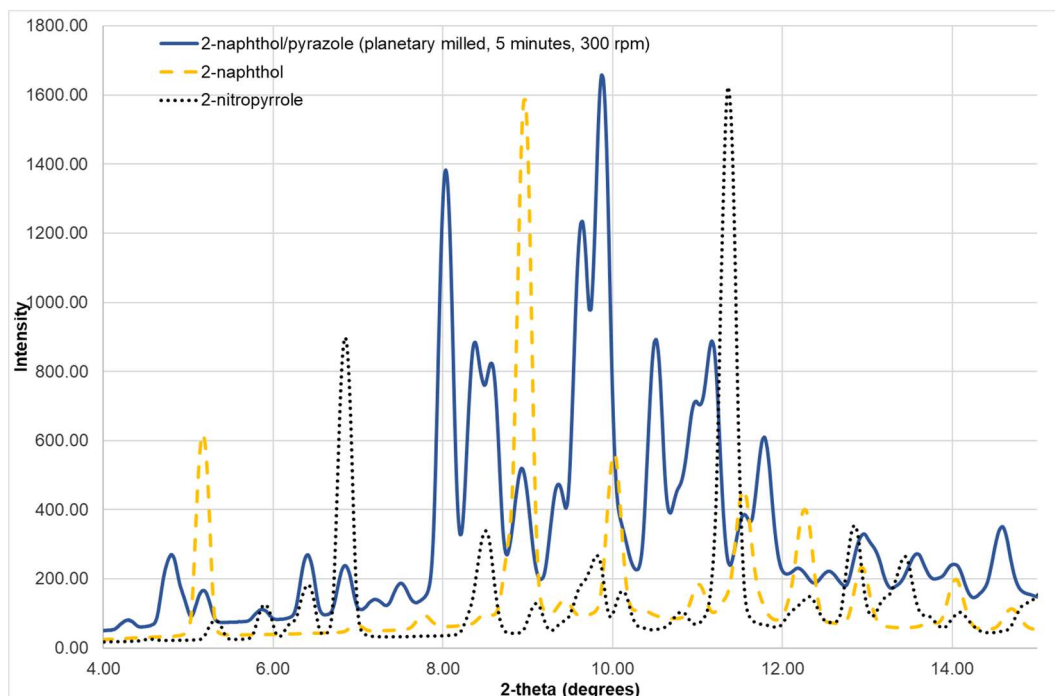


Figure B.12 - Powder x-ray pattern of 2-naphthol/pyrazole produced by planetary milling for 5 minutes at 300 rpm.

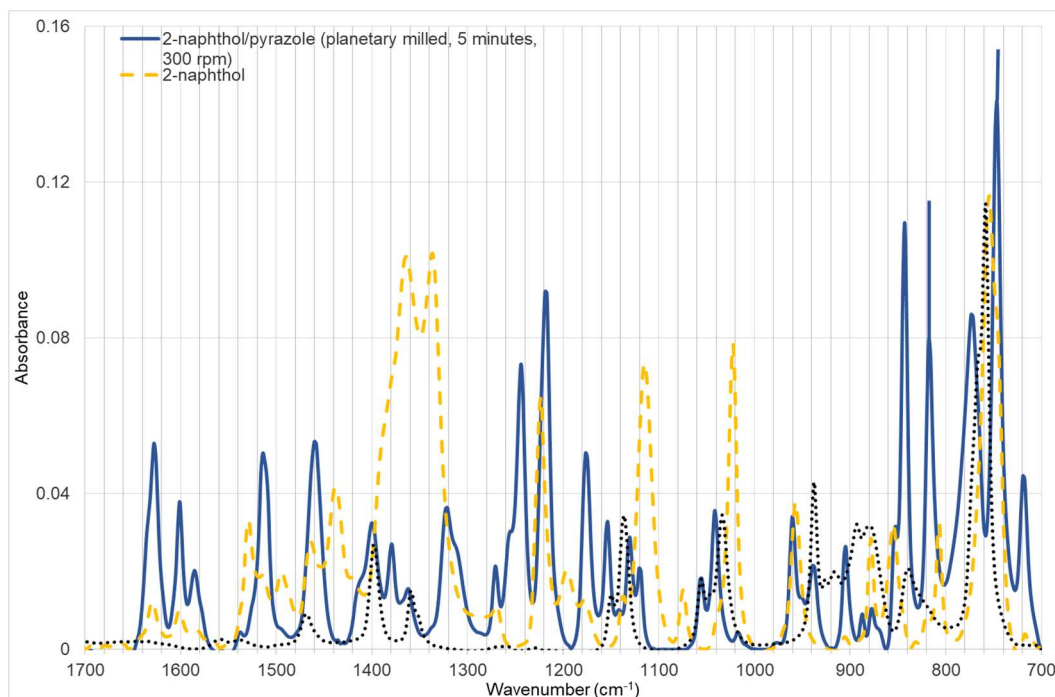


Figure B.13 – Infra-red spectra of 2-naphthol/pyrazole produced by planetary milling for 5 minutes at 300 rpm.

Table B.2 - Infrared spectra peak positions and heights of 2-naphthol/pyrazole produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)	Peak Position (cm ⁻¹)	Peak Height (Absorbance)
3281.05	0.02	1130.58	0.03
1627.71	0.05	1120.12	0.02
1600.98	0.04	1055.74	0.02
1585.47	0.02	1041.42	0.03
1513.79	0.05	960.3	0.04
1459.63	0.06	938.61	0.03
1399.83	0.04	904.87	0.03
1379.36	0.03	887.27	0.02
1362.19	0.02	877.4	0.02
1321.77	0.04	852.48	0.04
1270.88	0.02	843.03	0.12
1254.86	0.03	817.37	0.09
1244.11	0.08	772.81	0.1
1218.29	0.1	746.74	0.16
1176.09	0.05	718.77	0.06
1153.76	0.03		

B.11 2-naphthol/3-nitropyrazole

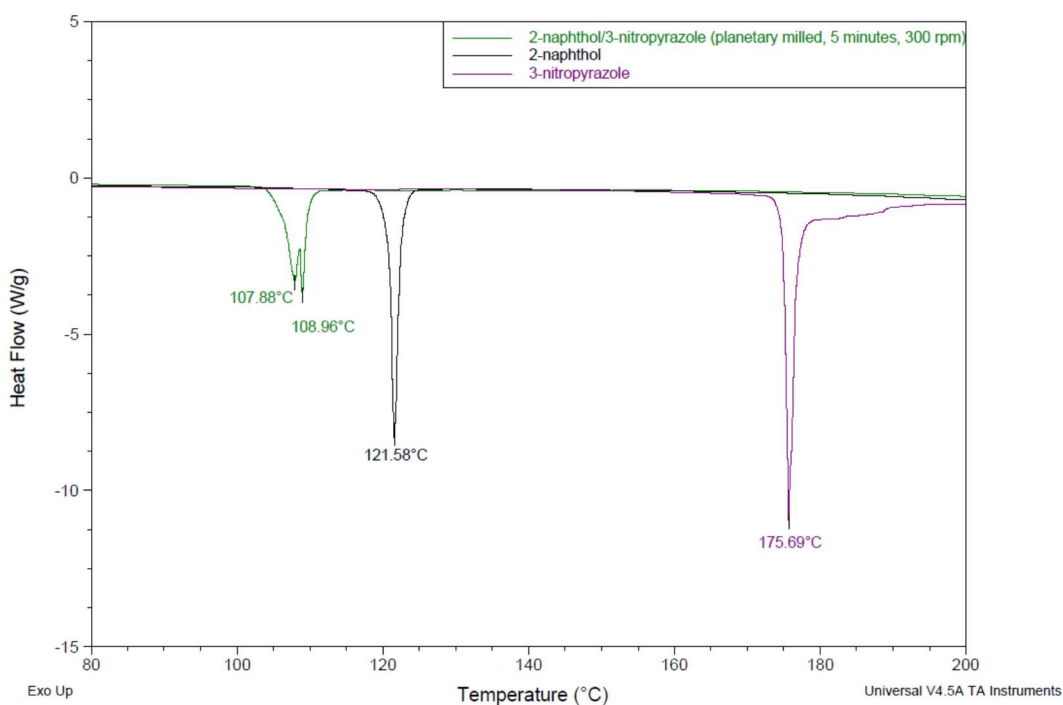


Figure B.14 - Thermal analysis of 2-naphthol/3-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

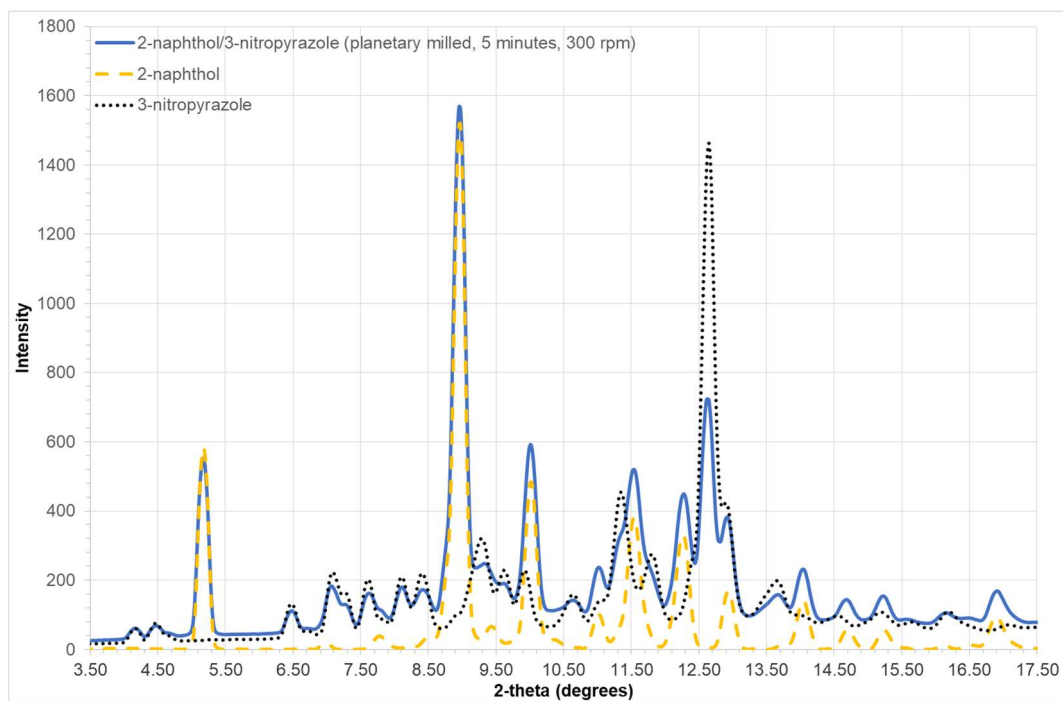


Figure B.15 – Powder x-ray pattern of 2-naphthol/3-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.12 2-naphthol/4-nitropyrazole

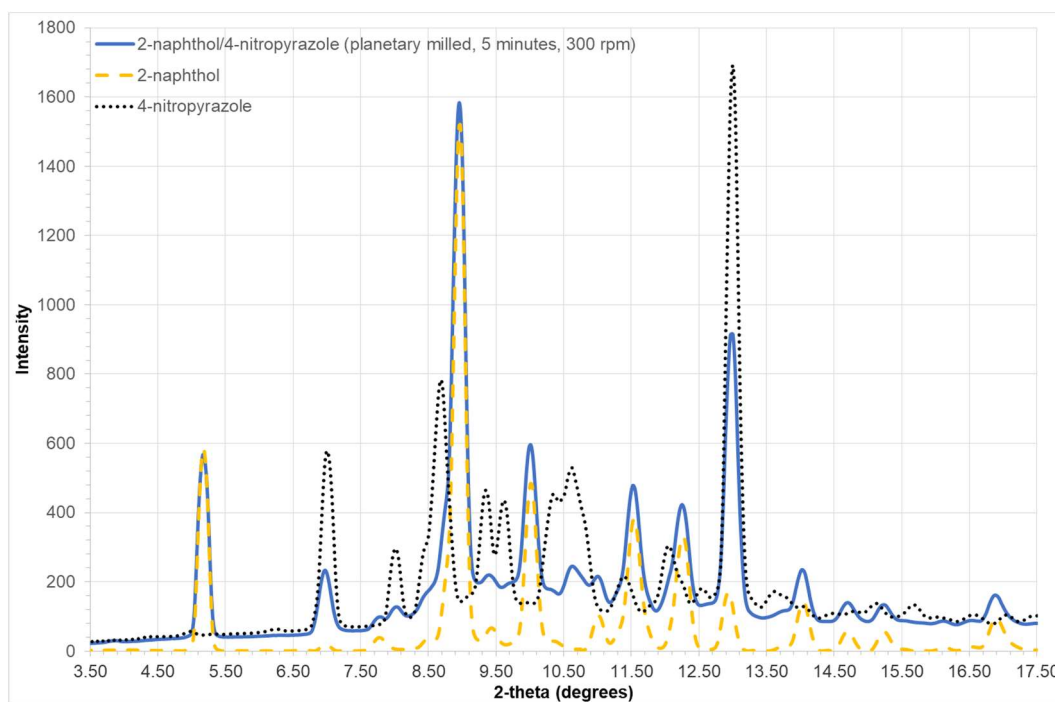


Figure B.16 - Powder x-ray pattern of 2-naphthol/4-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.13 2-naphthol/5-methylpyrazole

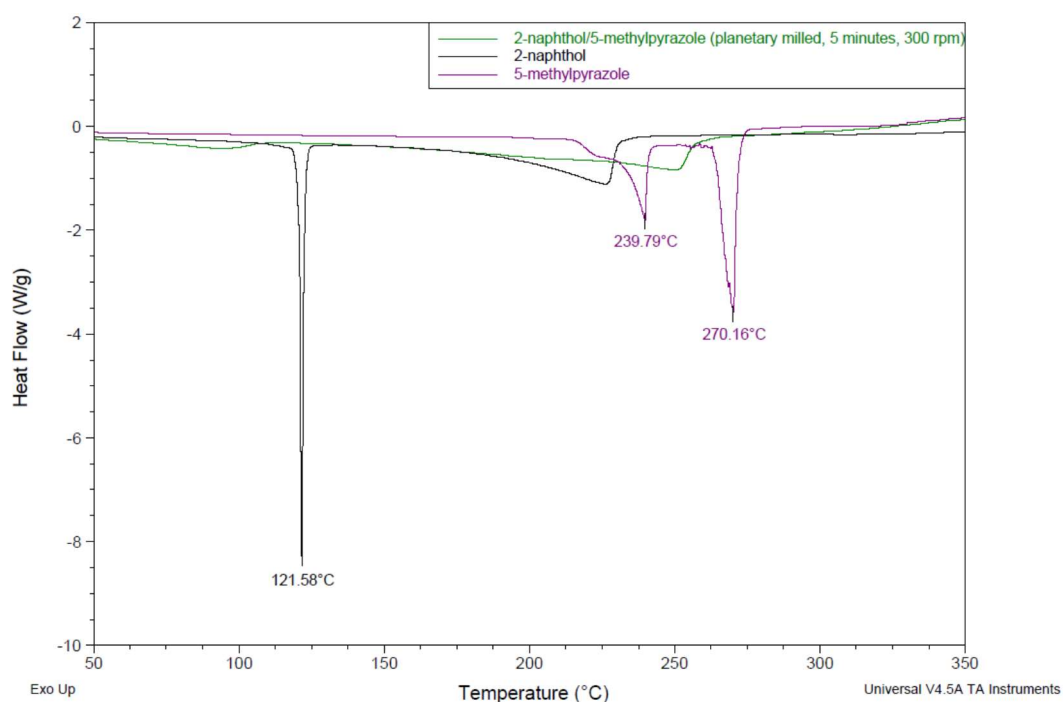


Figure B.17 - Thermal analysis of 2-naphthol/5-methylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.14 2-naphthol/pyrazol-4-amine

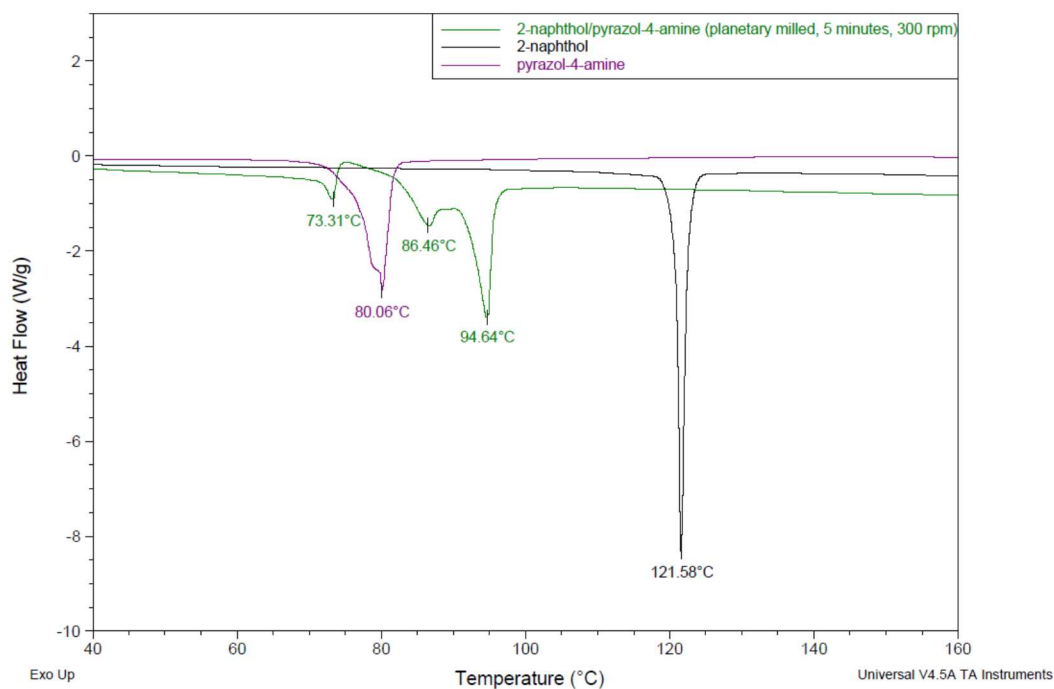


Figure B.18 - Thermal analysis of 2-naphthol/pyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

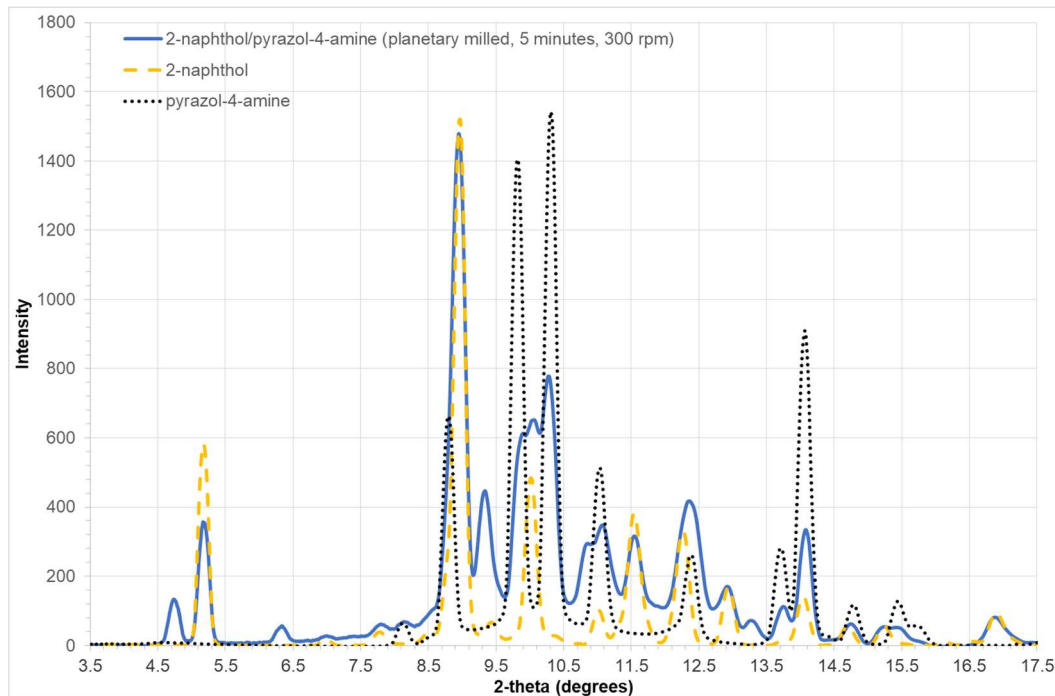


Figure B.19 – Powder x-ray pattern of 2-naphthol/pyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

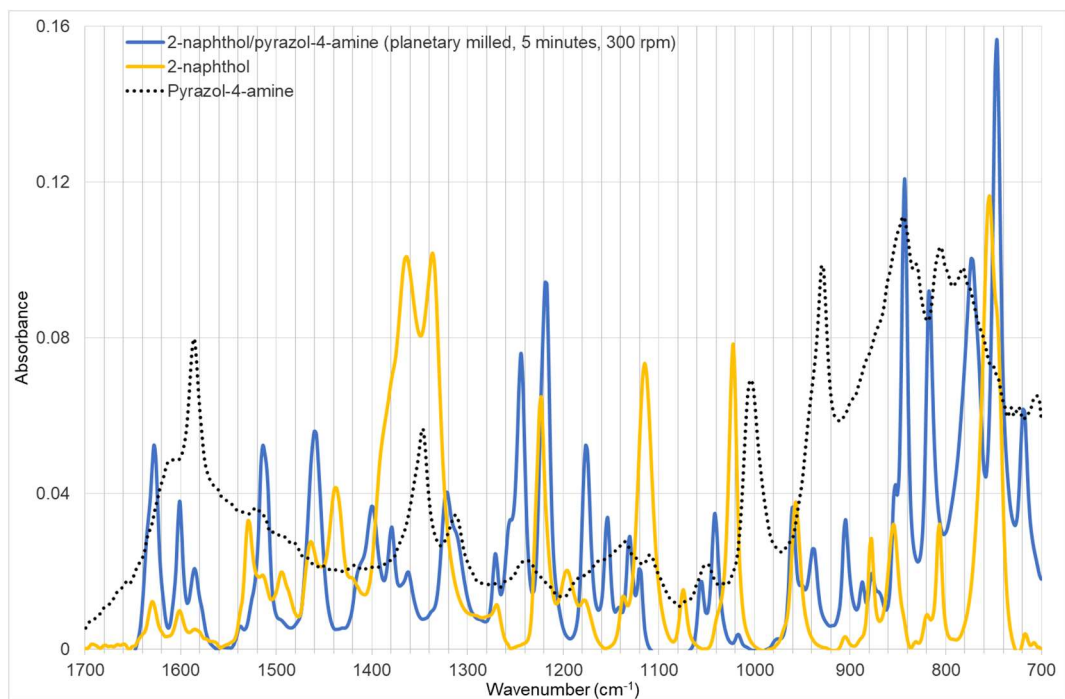


Figure B.20 - Infrared spectra of 2-naphthol/pyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Table B.3 - Infrared spectra peak positions and heights of 2-naphthol/pyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)
1631.21	0.05
1602.2	0.04
1586.97	0.02
1558.35	-0.01
1512.87	0.02
1467.34	0.03
1408.64	0.01
1323.03	-0.01
1274.77	0.02
1250.09	0.04
1217.22	0.07
1174.04	0.03
1151.06	-0.01
1140.46	-0.01
1118.65	-0.01
1014.23	-0.01
1002.5	0
958.91	0.05
929.79	0.01
906.1	0.04
878.06	0.02
843.65	0.13
814.6	0.12
742.03	0.18
715.57	0.07

B.15 2-naphthol/3-bromopyrazole

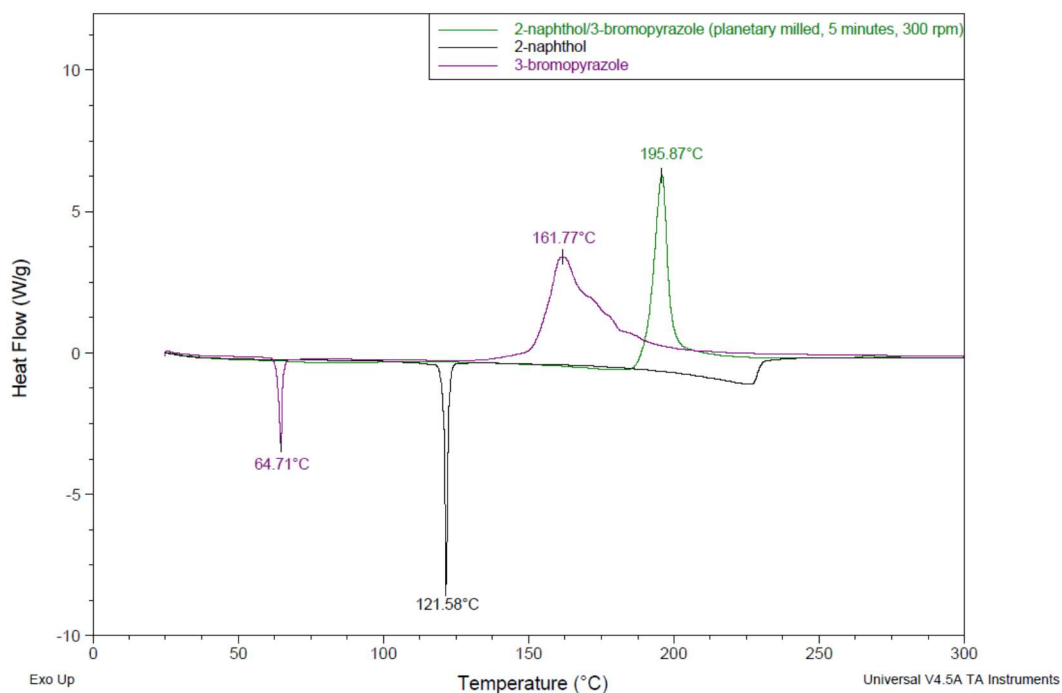


Figure B.21 - Thermal analysis of 2-naphthol/3-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

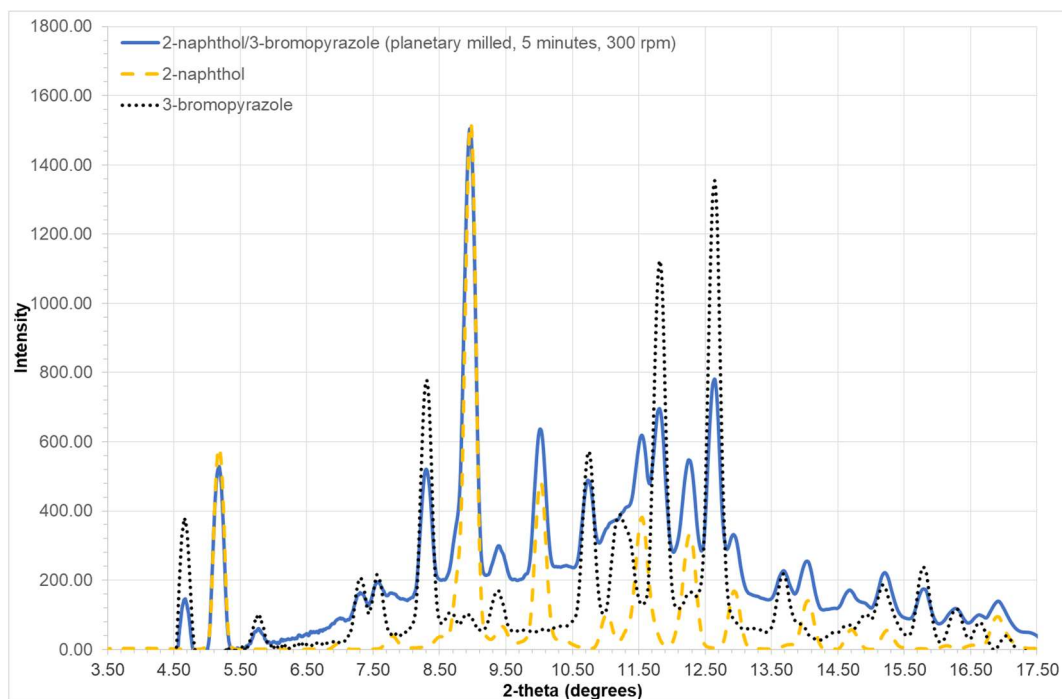


Figure B.22 – Powder x-ray pattern of 2-naphthol/3-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.16 2-naphthol/4-bromopyrazole

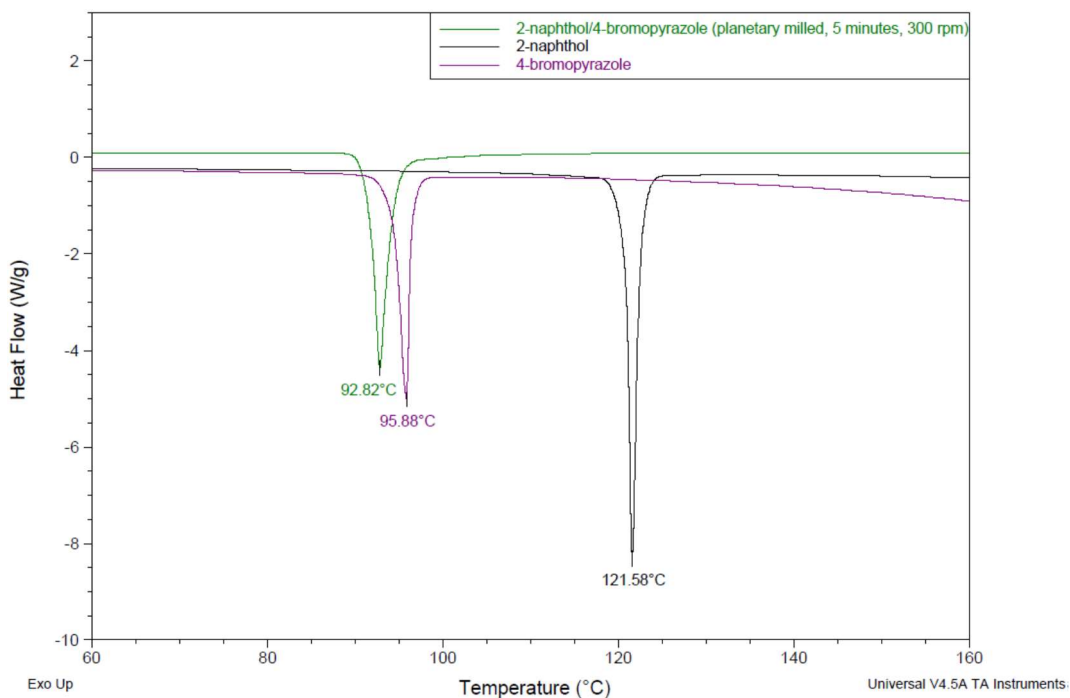


Figure B.23 - Thermal analysis of 2-naphthol/4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

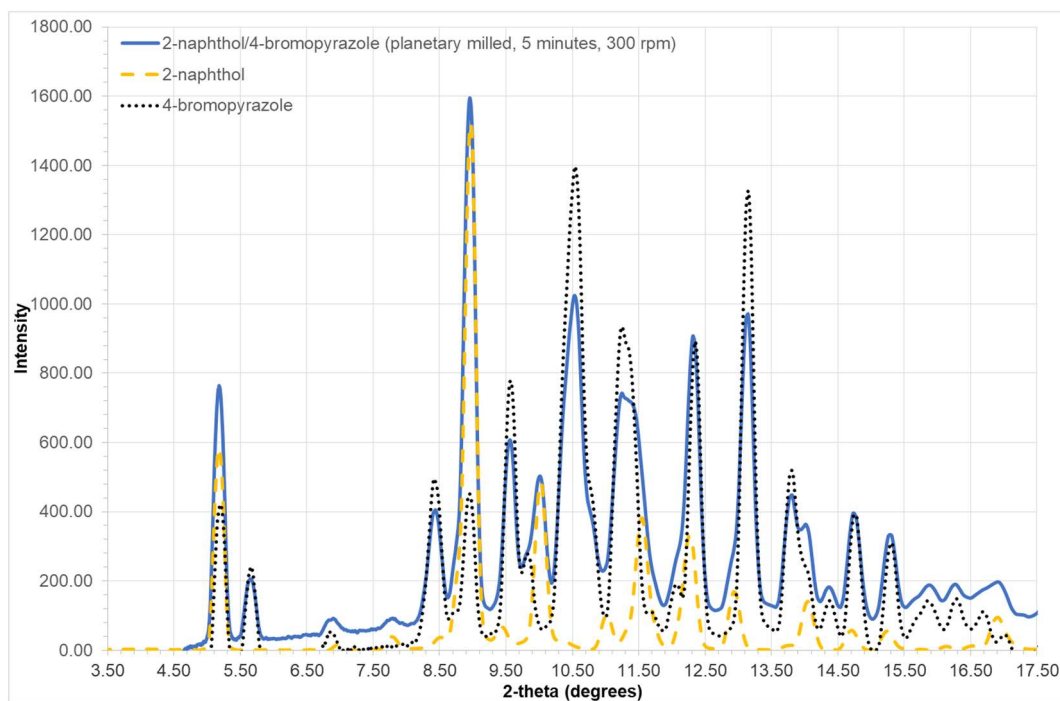


Figure B.24 – Powder x-ray pattern of 2-naphthol/4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.17 2-naphthol/3,4-dimethylpyrazole

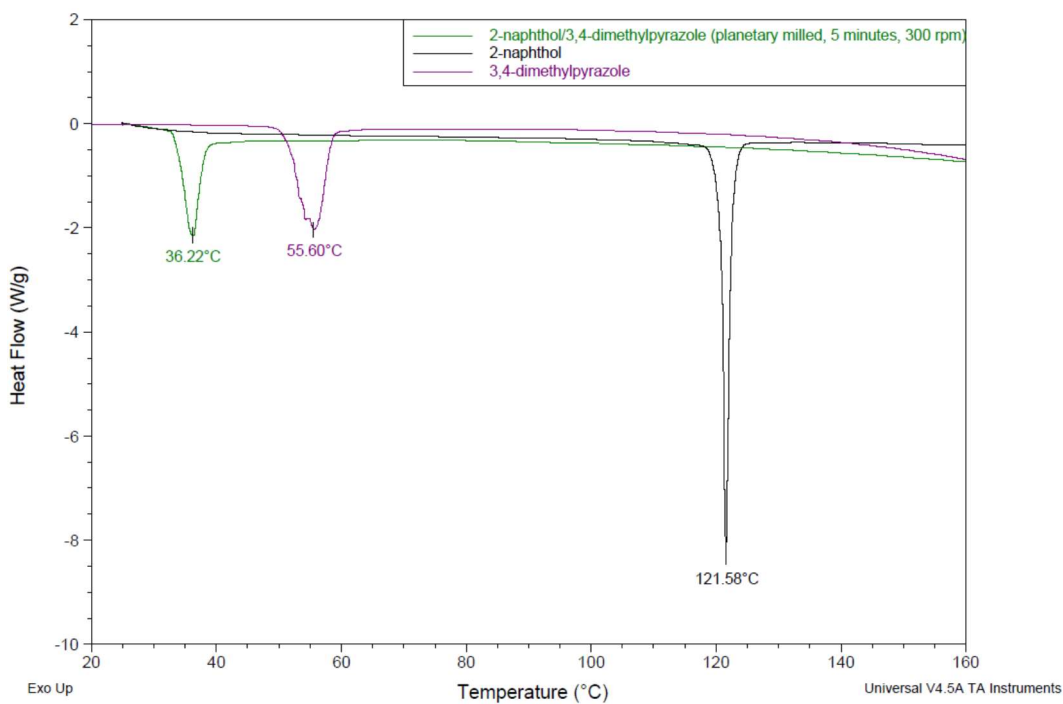


Figure B.25 - Thermal analysis of 2-naphthol/3,4-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

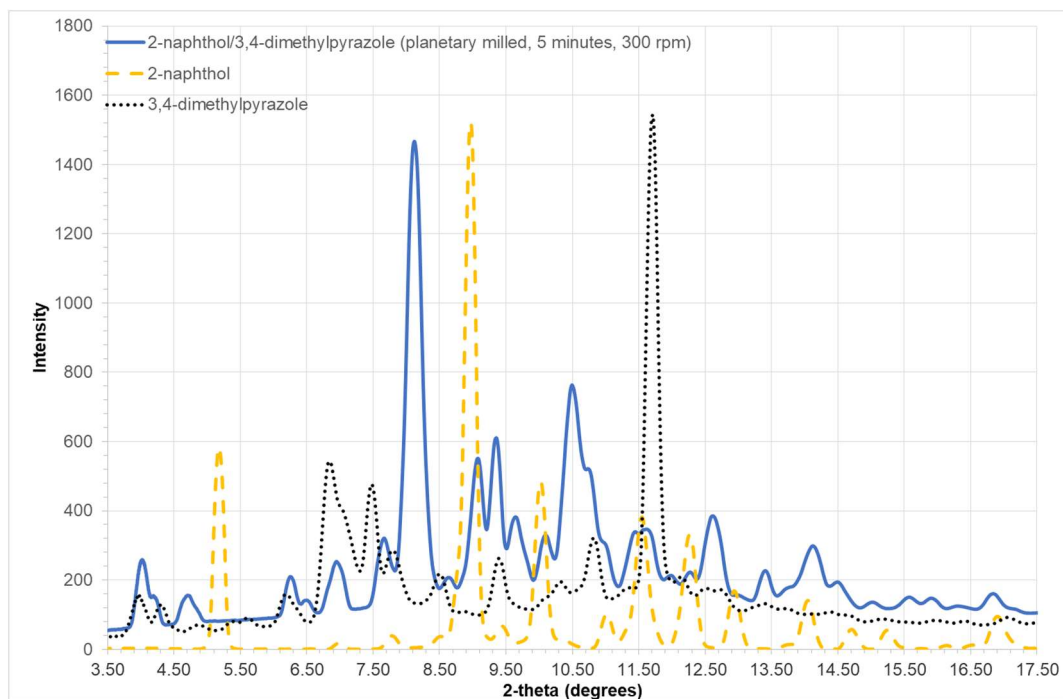


Figure B.26 – Powder x-ray pattern of 2-naphthol/3,4-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

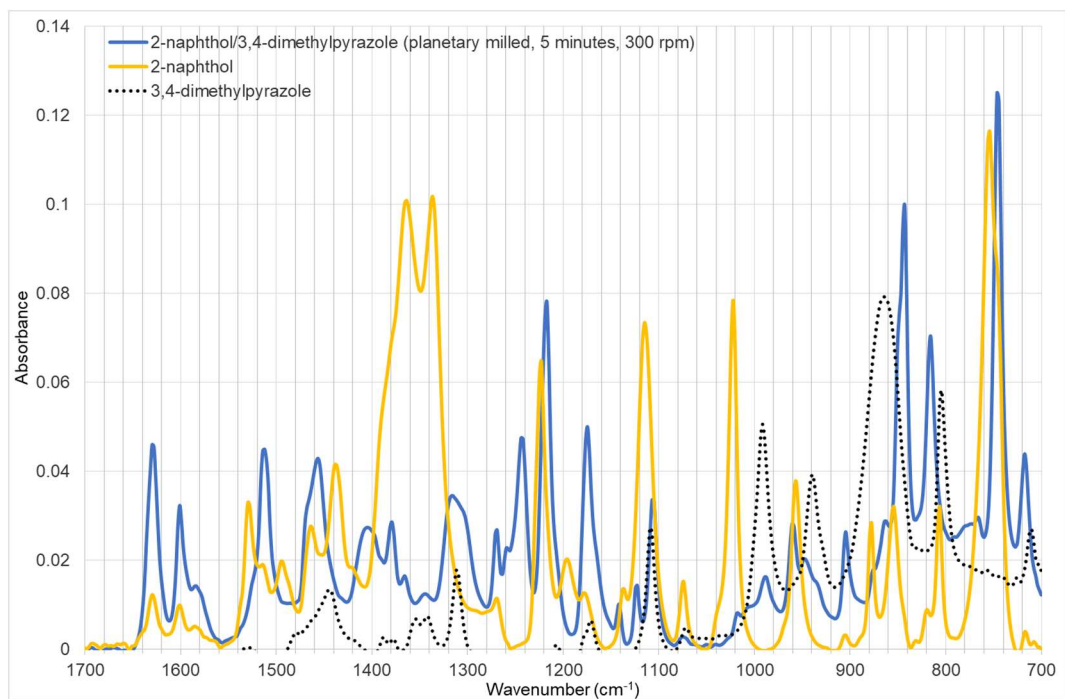


Figure B.27 – Infra-red spectra of 2-naphthol/3,4-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

Table B.4- Infrared spectra peak positions and heights of 2-naphthol/3,4-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)	Peak Position (cm ⁻¹)	Peak Height (Absorbance)
3262.11	0.03	1141.84	0.01
1629.17	0.05	1123.14	0.01
1600.9	0.03	1106.42	0.03
1584.2	0.01	1017.73	0.01
1512.72	0.05	988.68	0.02
1485.56	0.01	960.06	0.03
1456.55	0.04	947.5	0.02
1404.47	0.03	904.6	0.03
1379.36	0.03	862.94	0.03
1365.86	0.02	843.34	0.1
1344.37	0.01	816.03	0.07
1315.82	0.03	790.6	0.03
1269.65	0.03	773.28	0.03
1258.83	0.02	766.3	0.03
1243.37	0.05	745.77	0.13
1217.49	0.08	717.46	0.04
1174.82	0.05		

B.18 2-naphthol/3,5-dimethylpyrazole

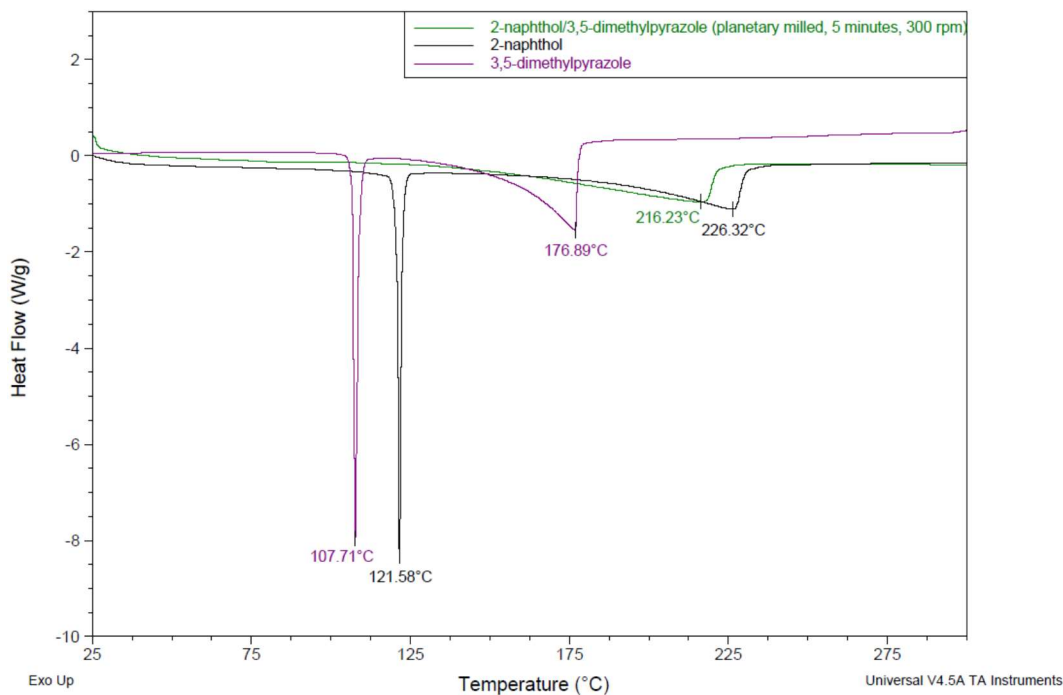


Figure B.28 - Thermal analysis of 2-naphthol/3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm. No melt is observed for the mixed system

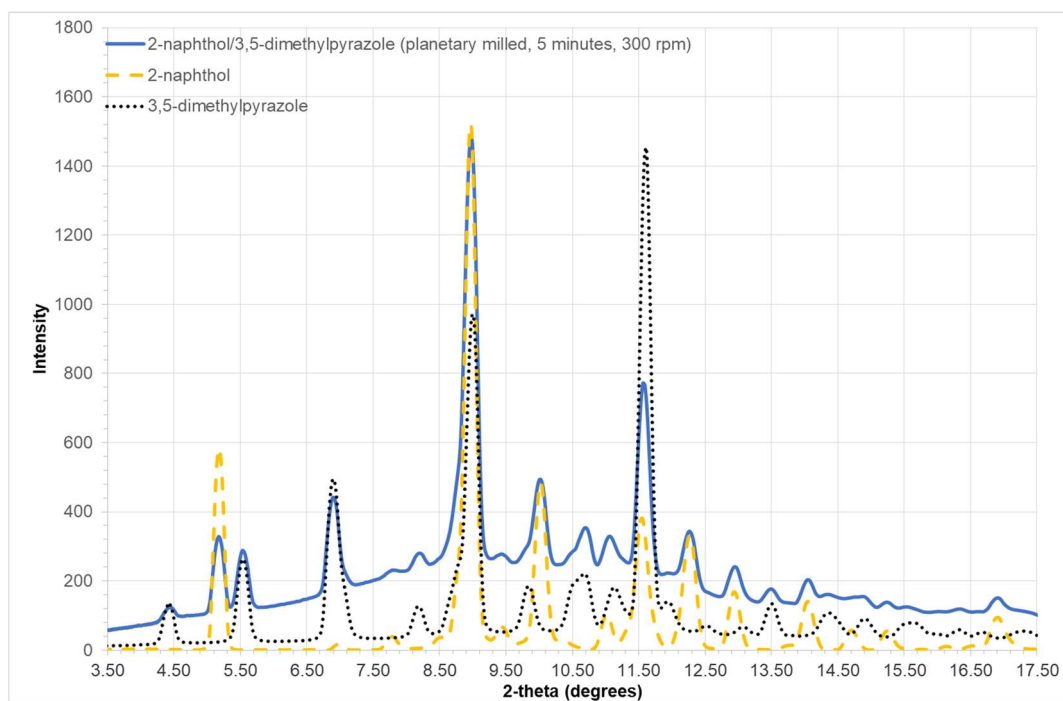


Figure B.29 – Powder x-ray pattern of 2-naphthol/3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.19 2-naphthol/3,4,5-tribromopyrazole

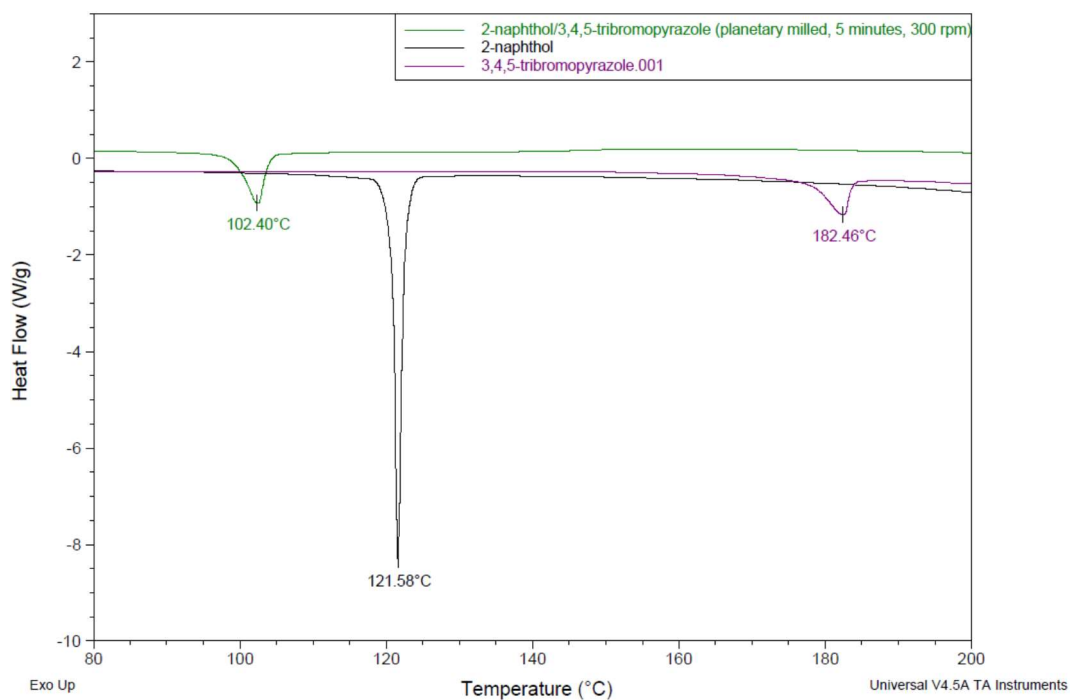


Figure B.30 - Thermal analysis of 2-naphthol/3,4,5-tribromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

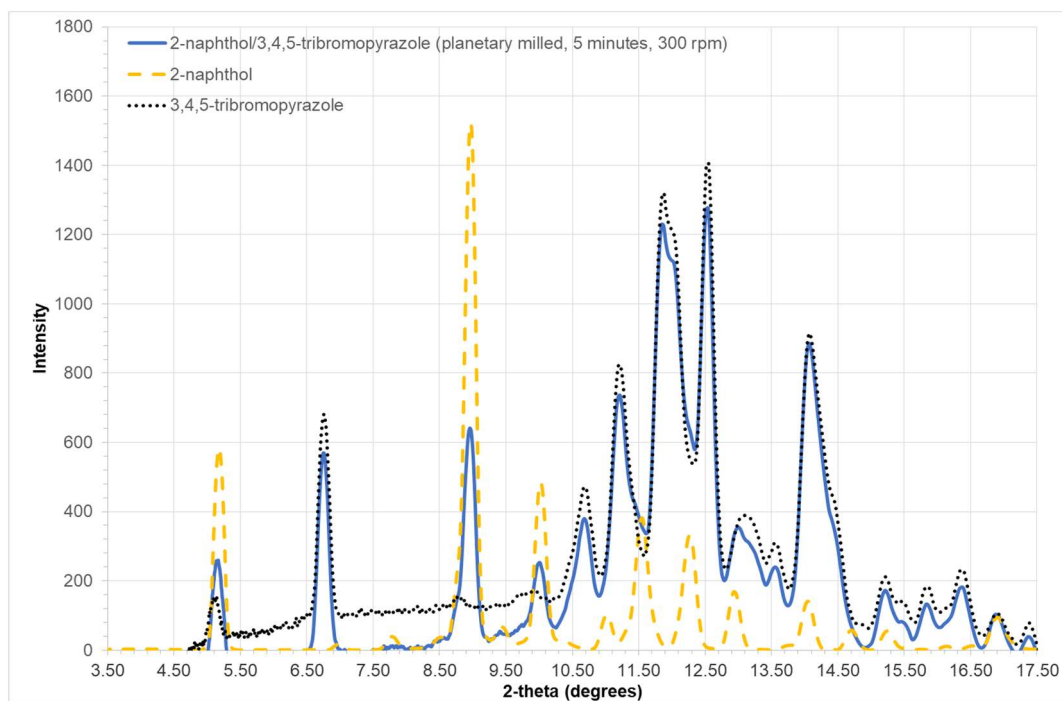


Figure B.31 – Powder x-ray pattern of 2-naphthol/3,4,5-tribromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.20 2-naphthol/3-methyl-5-nitropyrazole

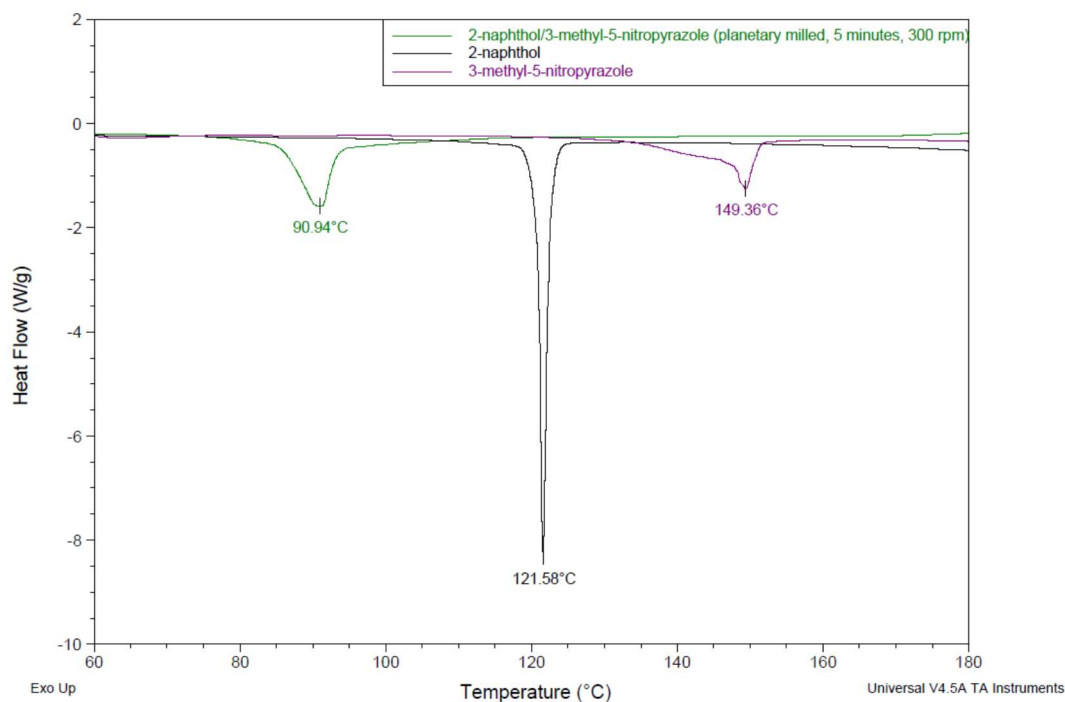


Figure B.32 - Thermal analysis of 2-naphthol/3-methyl-5-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

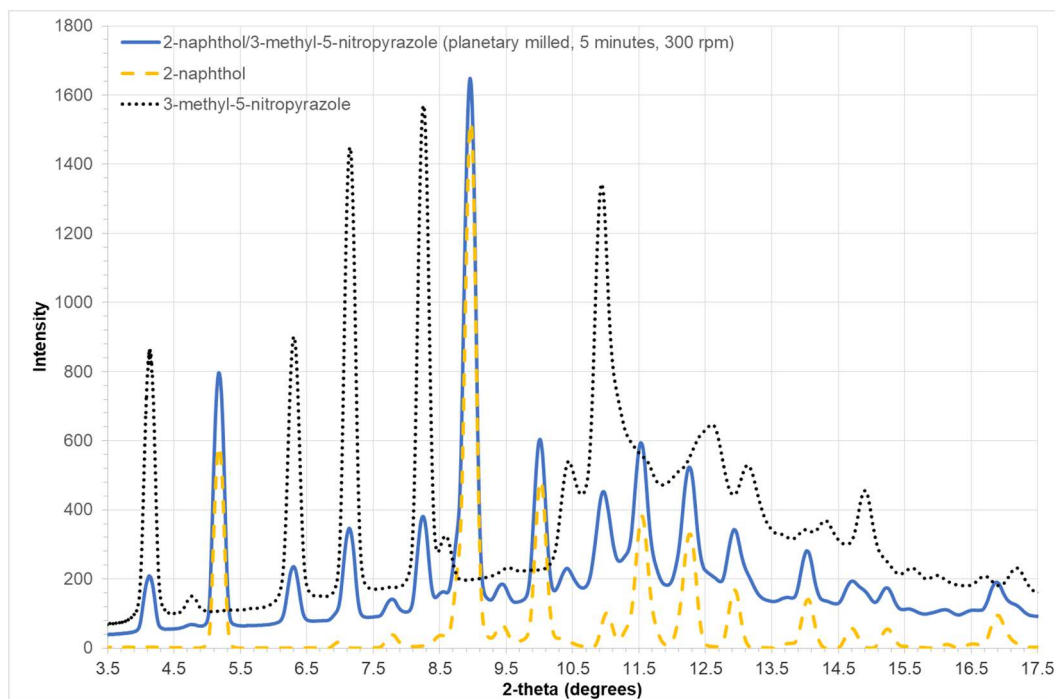


Figure B.33 – Powder x-ray pattern of 2-naphthol/3-methyl-5-nitropyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.21 2-naphthol/5-methylpyrazol-3-amine

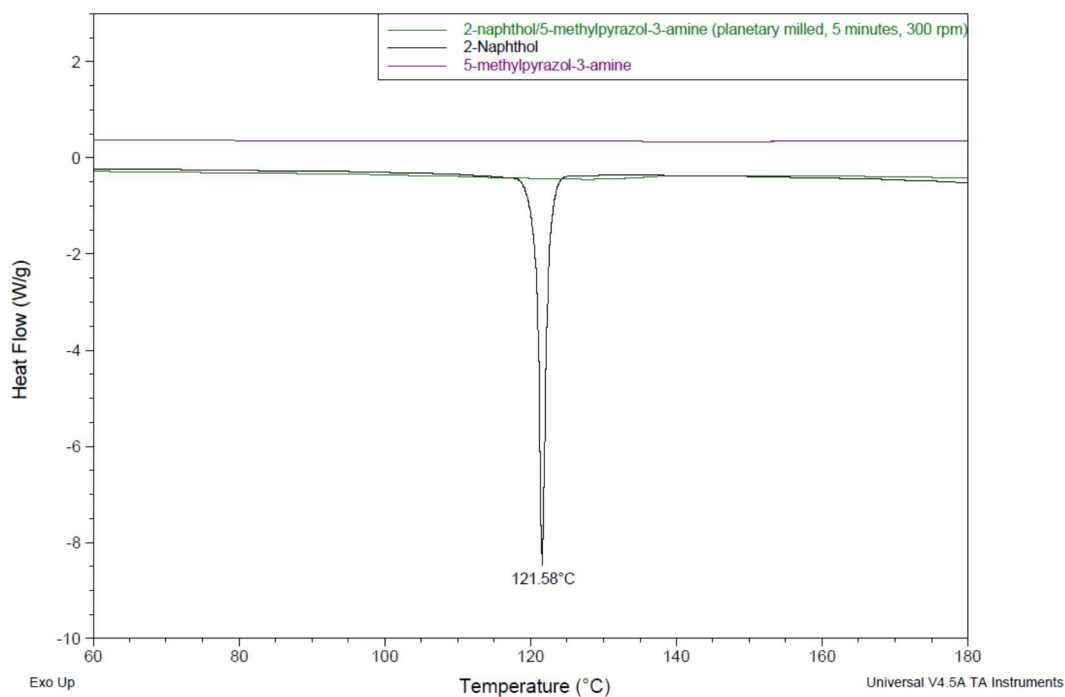


Figure B.34 - Thermal analysis of 2-naphthol/5-methylpyrazol-3-amine produced by planetary milling for 5 minutes at 300 rpm. Both 5-methylpyrazol-3-amine and the mixed system are liquids and did not display melts.

B.22 2-naphthol/4-bromopyrazol-3-amine

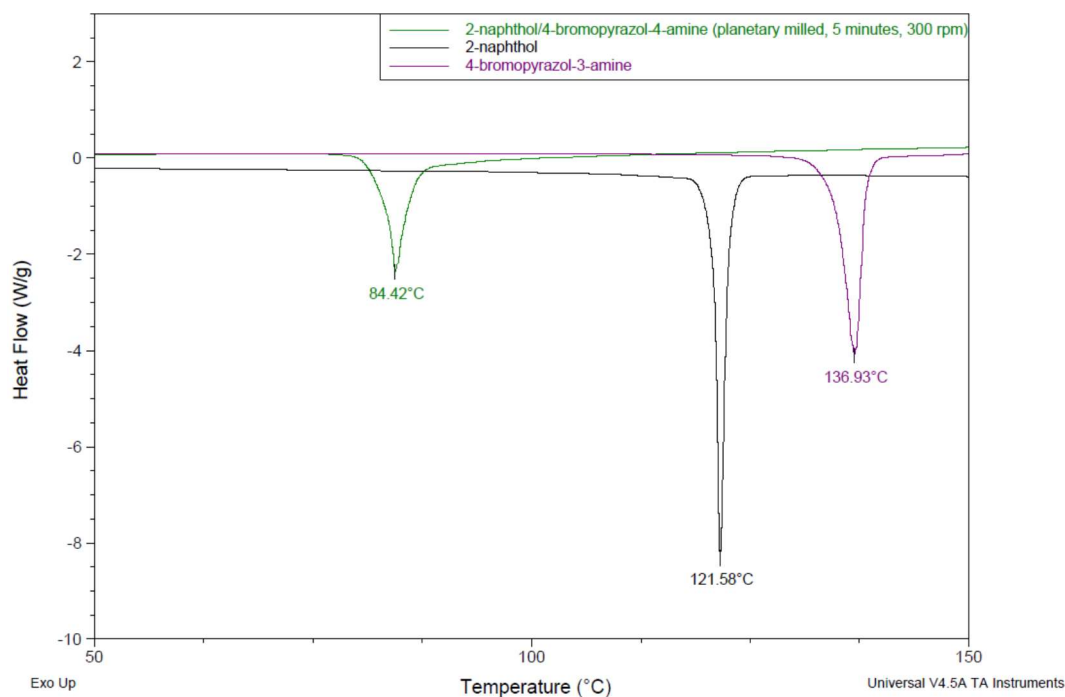


Figure B.35 - Thermal analysis of 2-naphthol/4-bromopyrazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

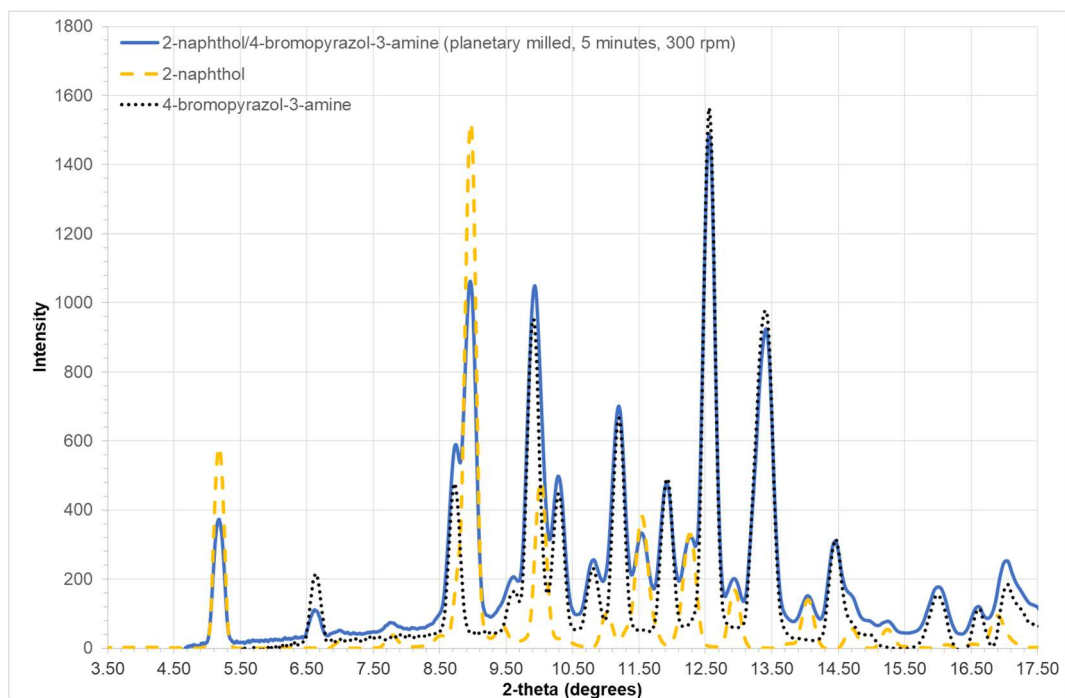


Figure B.36 – Powder x-ray pattern of 2-naphthol/4-bromopyrazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

B.23 2-naphthol/3-bromopyrazol-5-amine

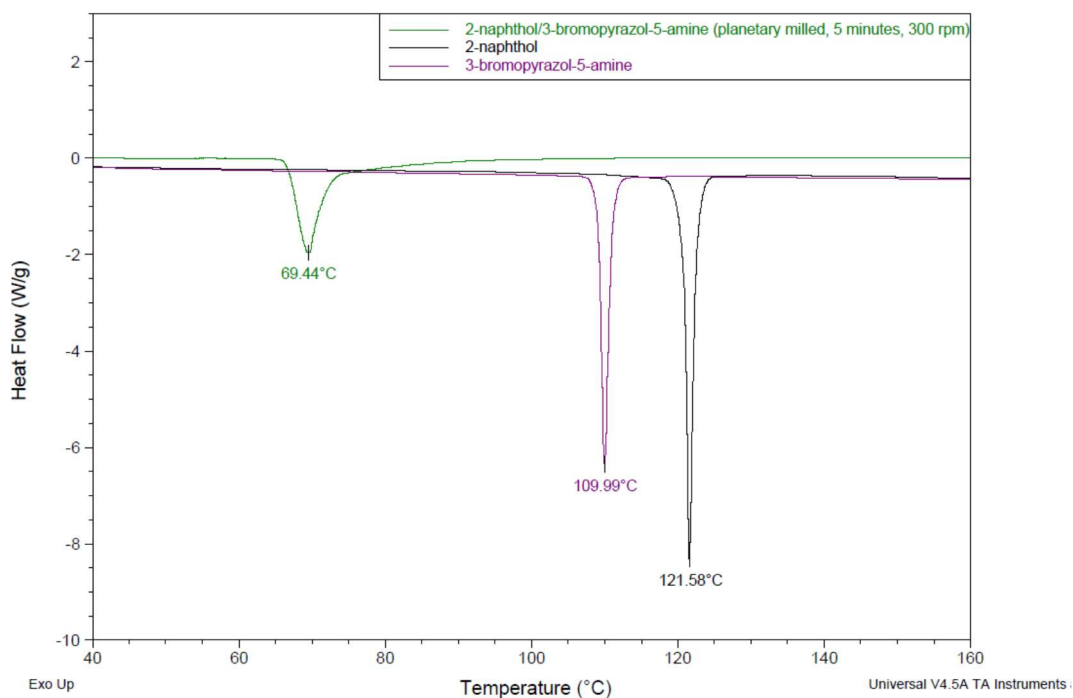


Figure B.37 - Thermal analysis of 2-naphthol/3-bromopyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

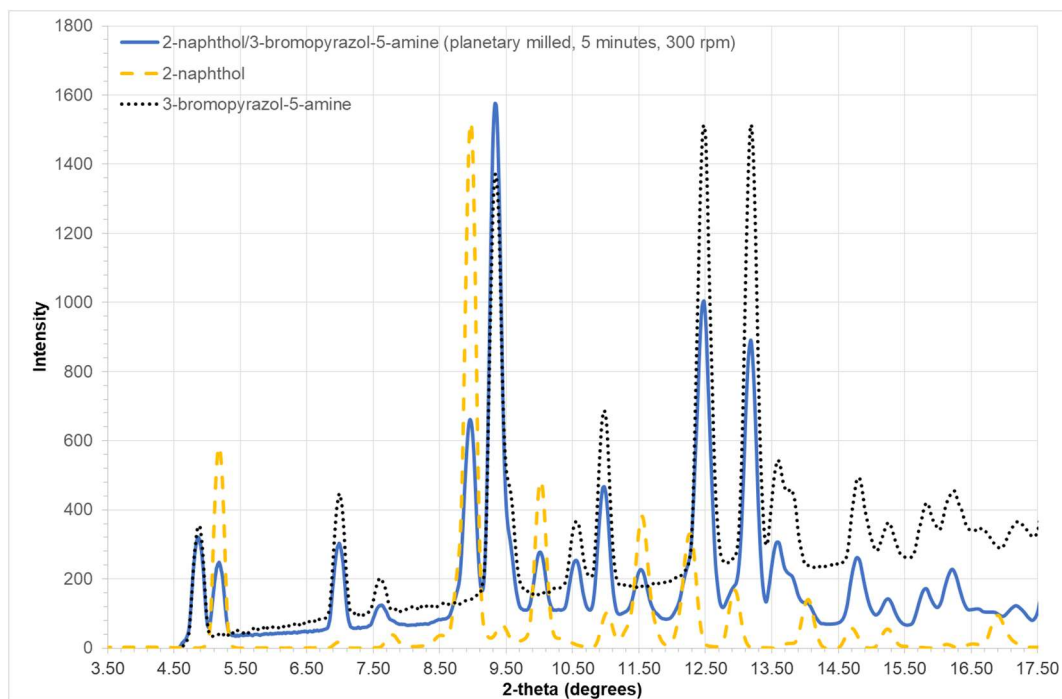


Figure B.38 – Powder x-ray pattern of 2-naphthol/3-bromopyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

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

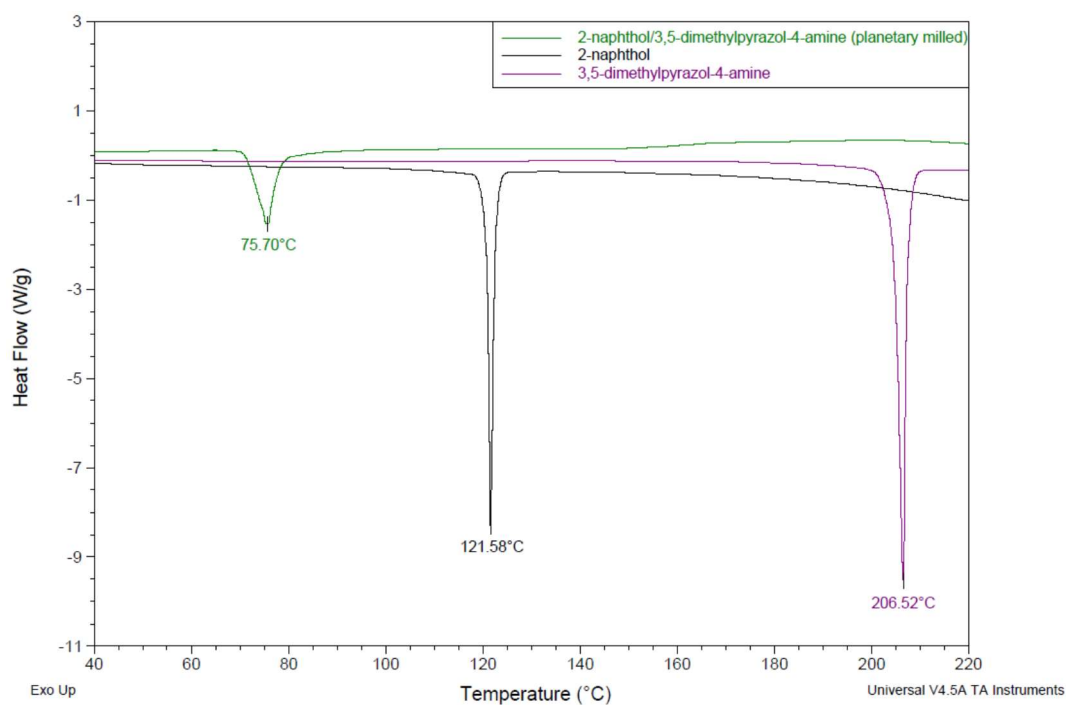


Figure B.39 - Thermal analysis of 2-naphthol/3,5-dimethylpyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

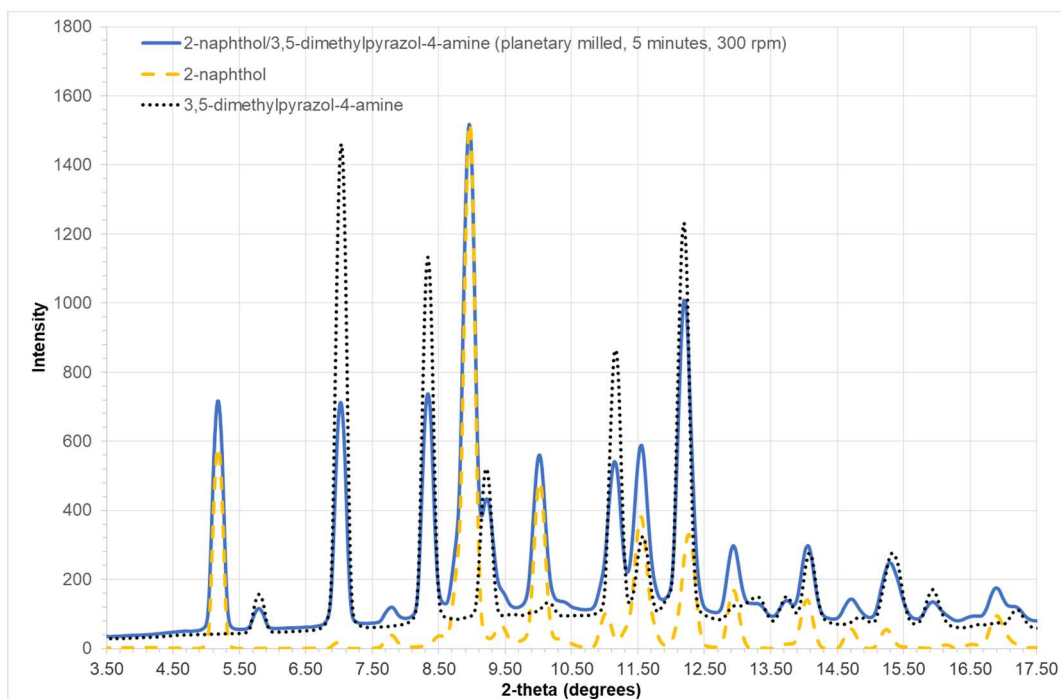


Figure B.40 – Powder x-ray pattern of 2-naphthol/3,5-dimethylpyrazol-4-amine produced by planetary milling for 5 minutes at 300 rpm.

B.25 2-naphthol/3,4-dimethylpyrazol-5-amine

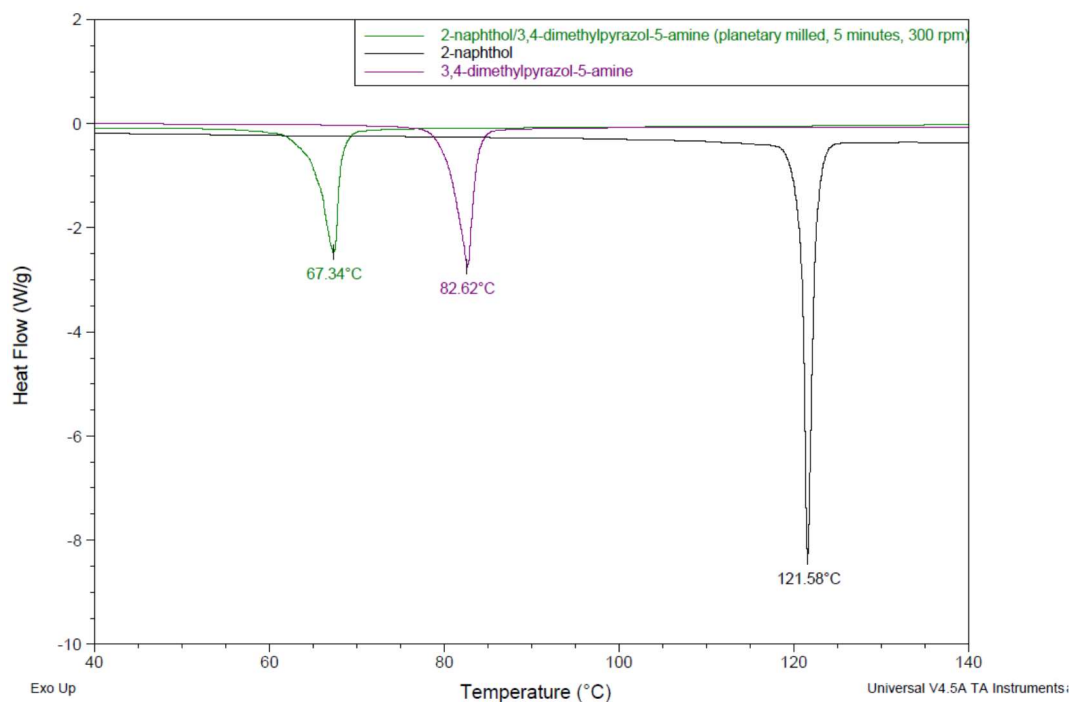


Figure B.41 - Thermal analysis of 2-naphthol/3,4-dimethylpyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

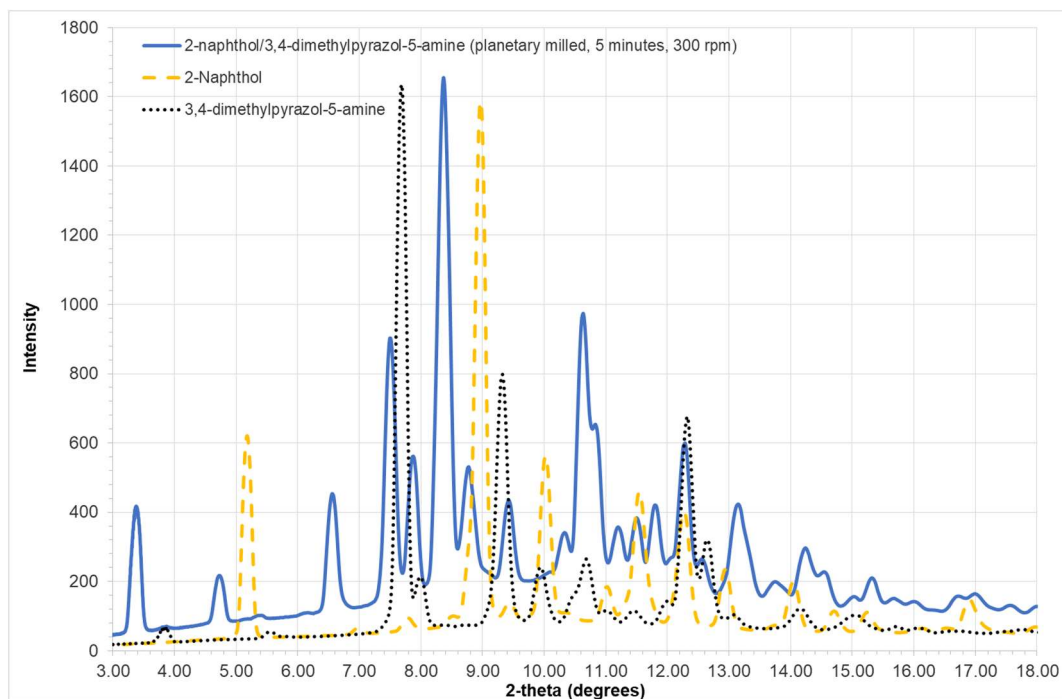


Figure B.42 – Powder x-ray pattern of 2-naphthol/3,4-dimethylpyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

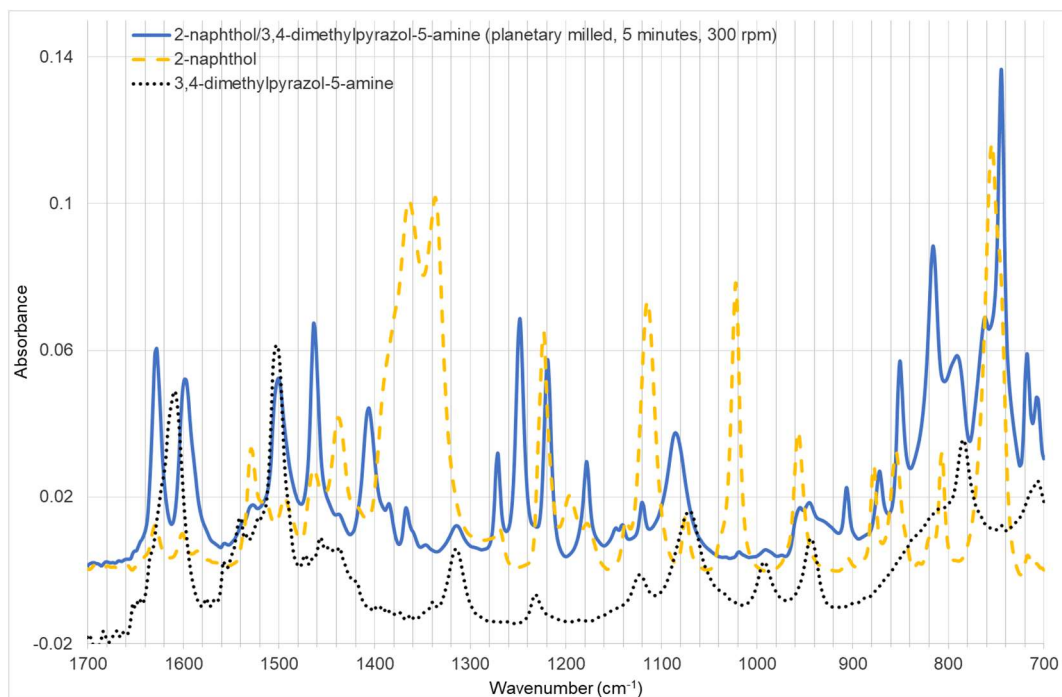


Figure B.43 – Infrared spectra of 2-naphthol/3,4-dimethylpyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

Table B.5 - Infrared spectra peak positions and heights of 2-naphthol/3,4-dimethylpyrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Positions (cm ⁻¹)	Peak Height (Absorbance)	Peak Positions (cm ⁻¹)	Peak Height (Absorbance)
3389.11	0.02	1178.37	0.03
3321.95	0.01	1147.51	0.01
1628.41	0.06	1141.06	0.01
1598.35	0.05	1120.23	0.02
1556.73	0.01	1085.44	0.04
1527.49	0.02	991.16	0.01
1500.76	0.05	954.86	0.02
1463.52	0.07	945.33	0.02
1437.73	0.02	906.41	0.02
1406.28	0.04	871.92	0.03
1385.22	0.02	850.55	0.06
1367.12	0.02	815.87	0.09
1346.68	0.01	790.95	0.06
1314.17	0.01	761.59	0.07
1271.3	0.03	744.62	0.14
1248.16	0.07	717.62	0.06
1219.11	0.06	707.35	0.05

B.26 2-naphthol/3-methyl-4-bromopyrazole

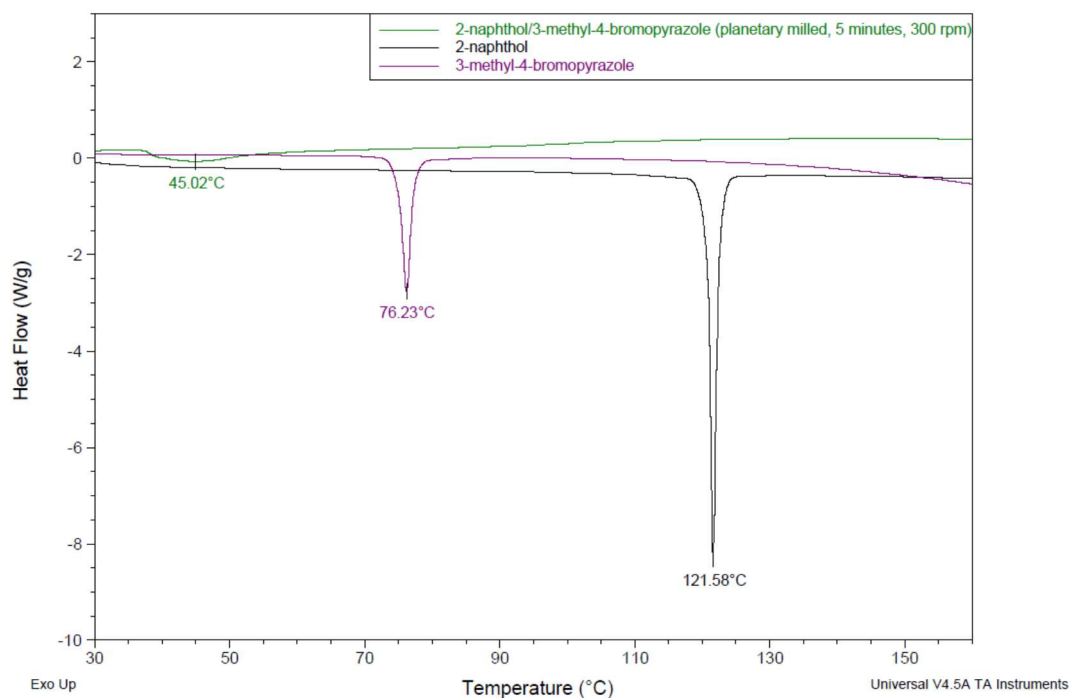


Figure B.44 - Thermal analysis of 2-naphthol/3-methyl-4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

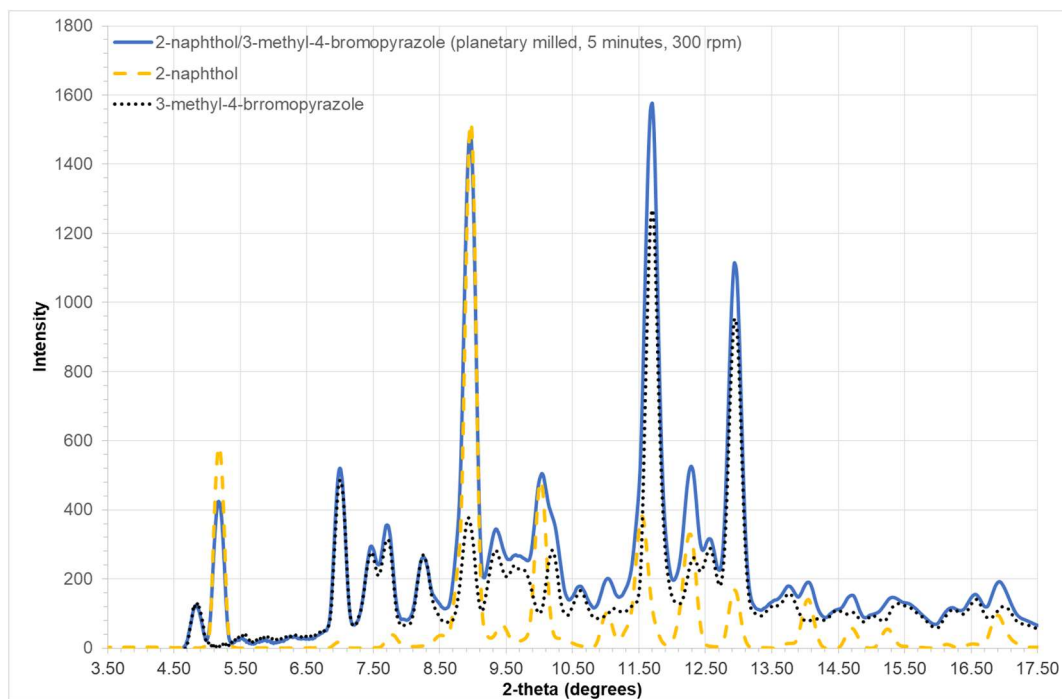


Figure B.45 – Powder x-ray pattern of 2-naphthol/3-methyl-4-bromopyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.27 2-naphthol/3-bromo-5-methylpyrazole

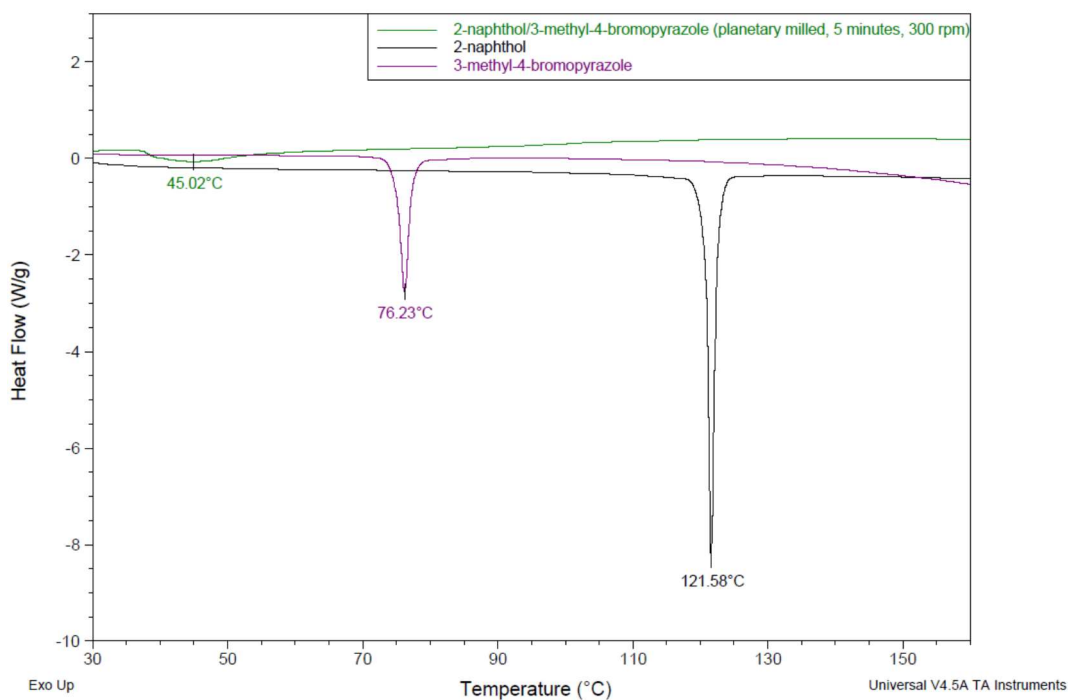


Figure B.46 - Thermal analysis of 2-naphthol/3-bromo-5-methylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

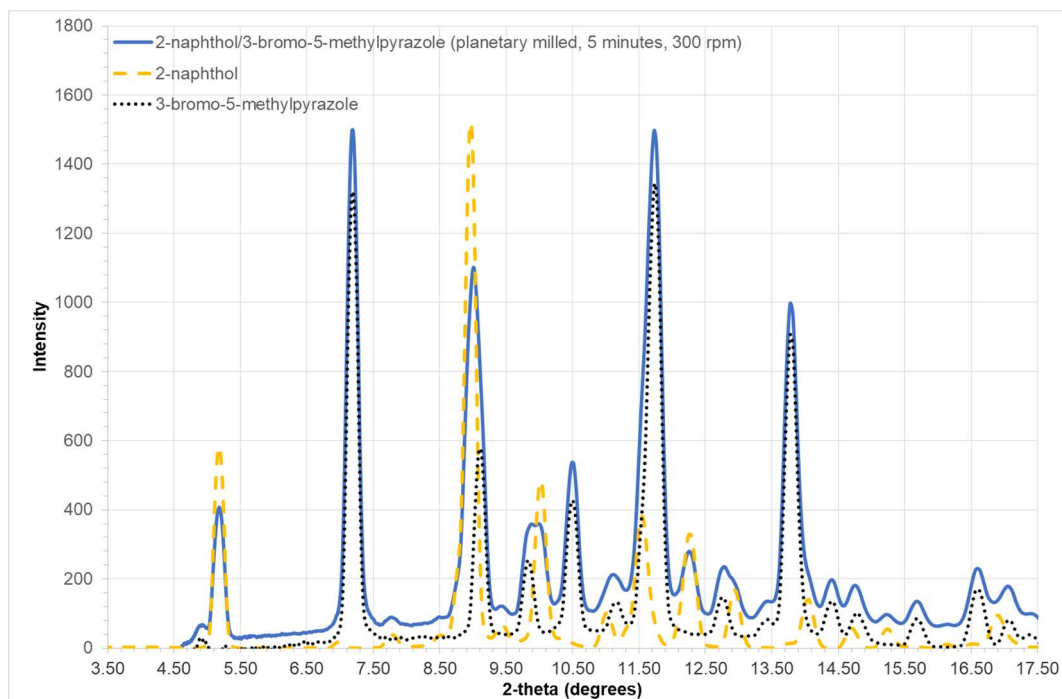


Figure B.47 – Powder x-ray pattern of 2-naphthol/3-bromo-5-methylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.28 2-naphthol/4-bromo-3,5-dimethylpyrazole

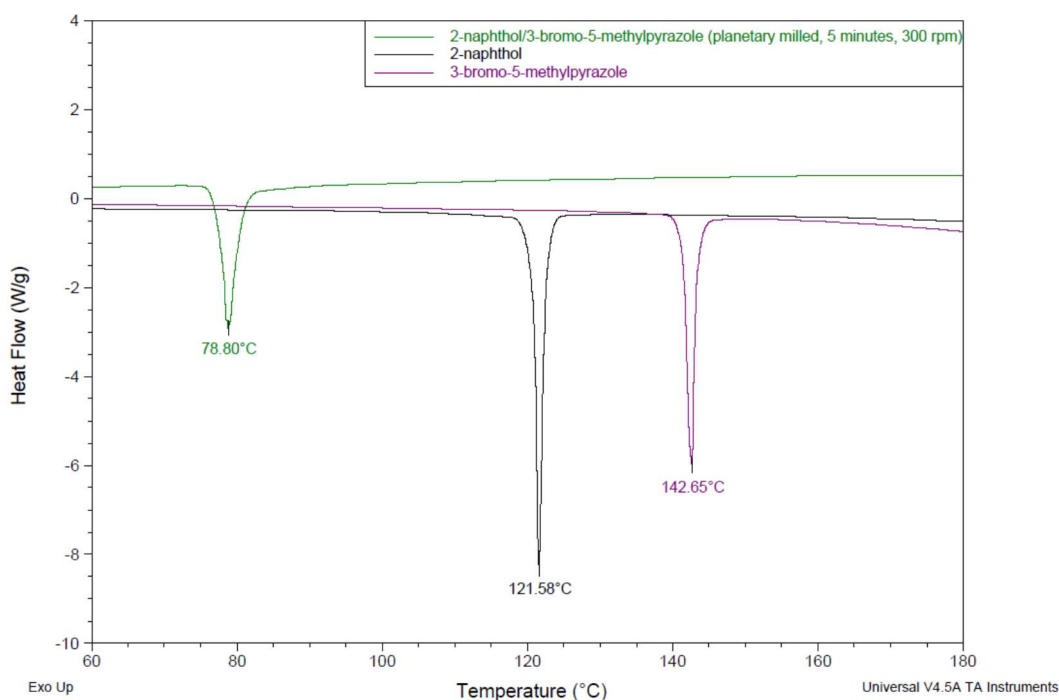


Figure B.48 - Thermal analysis of 2-naphthol/4-bromo-3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

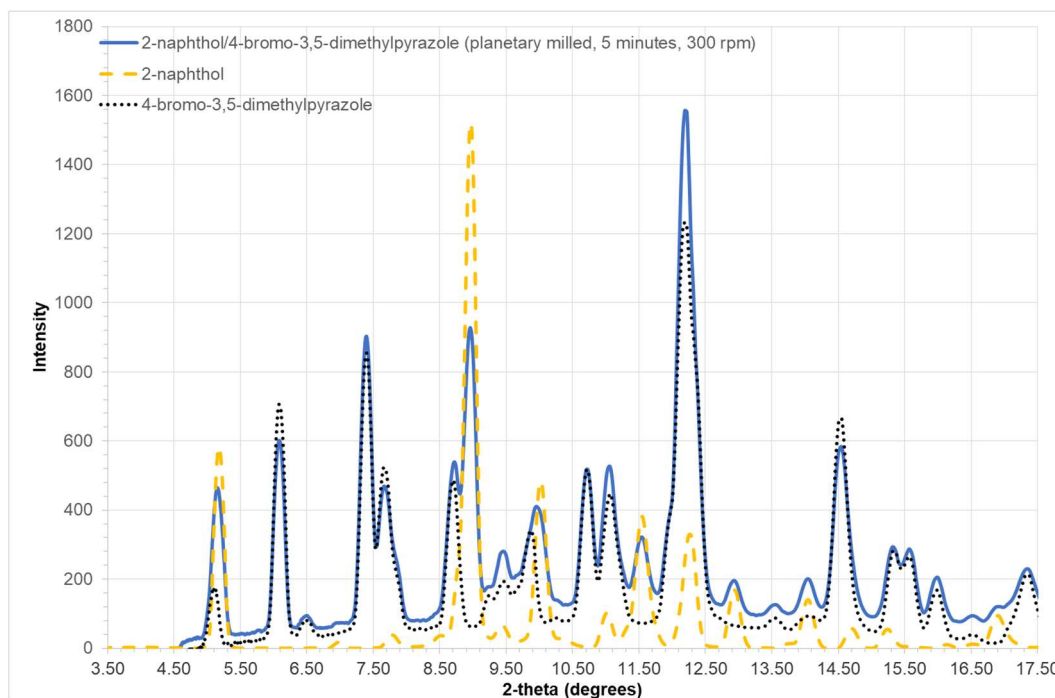


Figure B.49 – Powder x-ray pattern of 2-naphthol/4-bromo-3,5-dimethylpyrazole produced by planetary milling for 5 minutes at 300 rpm.

B.29 2-naphthol/imidazole

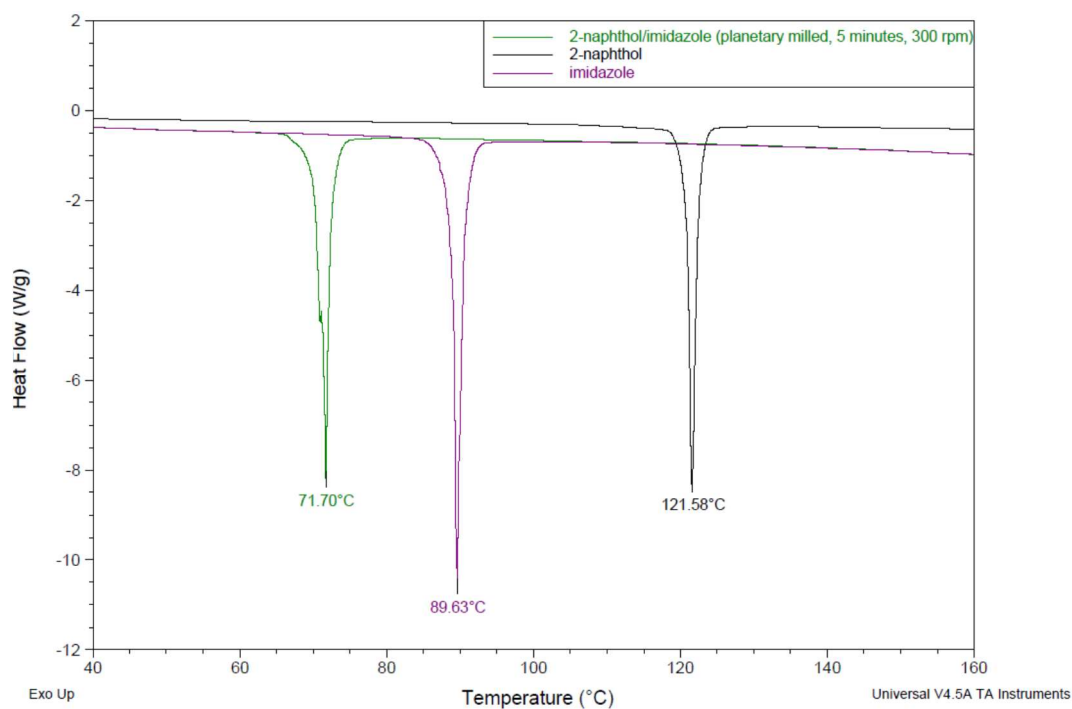


Figure B.50 - Thermal analysis of 2-naphthol/imidazole produced by planetary milling for 5 minutes at 300 rpm.

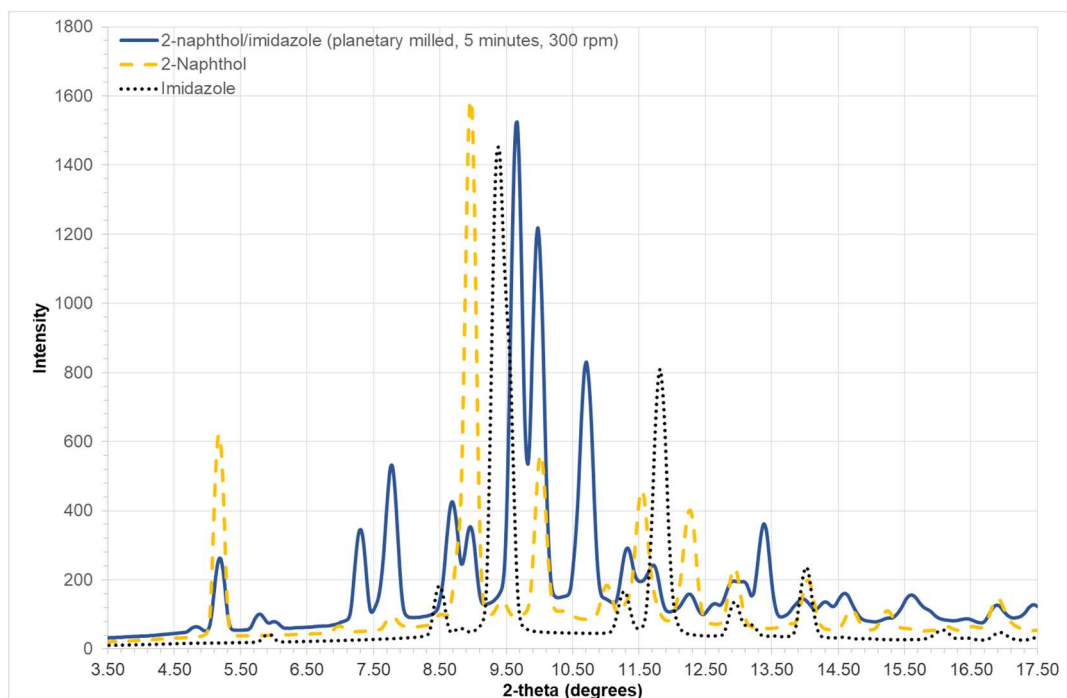


Figure B.51 – Powder x-ray pattern of 2-naphthol/imidazole produced by planetary milling for 5 minutes at 300 rpm.

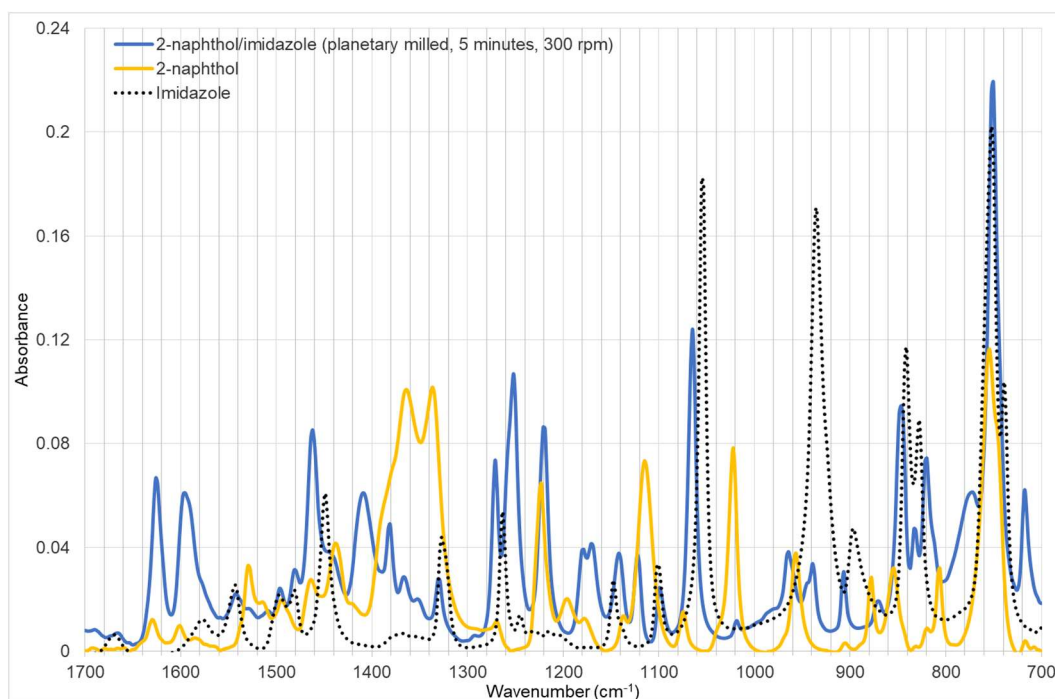


Figure B.52 – Infrared spectra of 2-naphthol/imidazole produced by planetary milling for 5 minutes at 300 rpm.

Table B.6 - Infrared spectra peak positions and heights of 2-naphthol/imidazole produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)	Peak Position (cm ⁻¹)	Peak Height (Absorbance)
3221.88	0.04	1179.11	0.04
3137.85	0.03	1170.38	0.04
1625.54	0.07	1141.8	0.04
1595.77	0.06	1122.32	0.04
1542.37	0.02	1099.17	0.02
1496.2	0.02	1064.84	0.12
1480.69	0.03	964.58	0.04
1462.14	0.09	939.27	0.03
1409.17	0.06	906.72	0.03
1381.48	0.05	870.54	0.02
1366.73	0.03	846.81	0.09
1352.43	0.02	832.61	0.05
1330.28	0.03	820.39	0.08
1271.07	0.07	772.25	0.06
1252.02	0.11	750.87	0.22
1220.22	0.09	717.46	0.06

B.30 2-naphthol/2-nitroimidazole

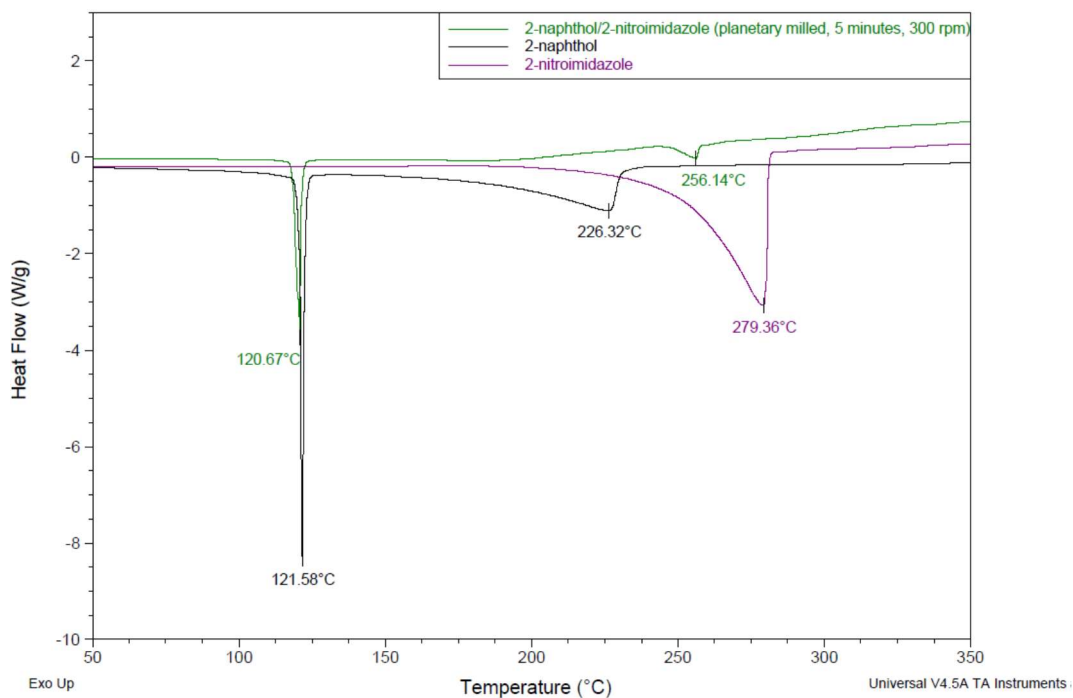


Figure B.53 - Thermal analysis of 2-naphthol/2-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

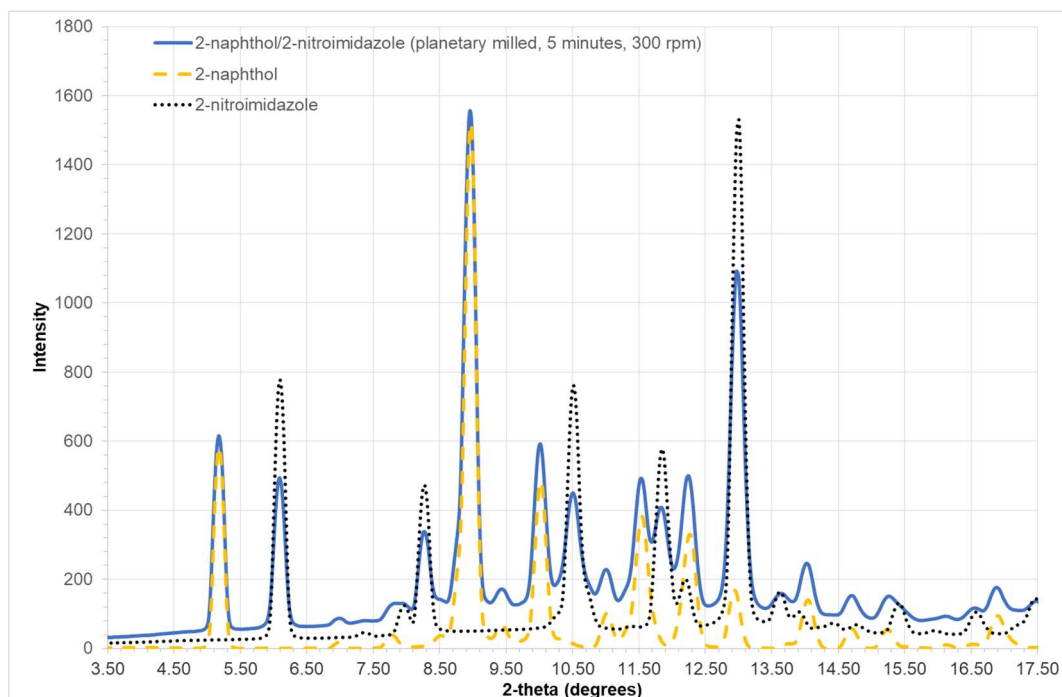


Figure B.54 – Powder x-ray pattern of 2-naphthol/2-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.31 2-naphthol/2-methylimidazole

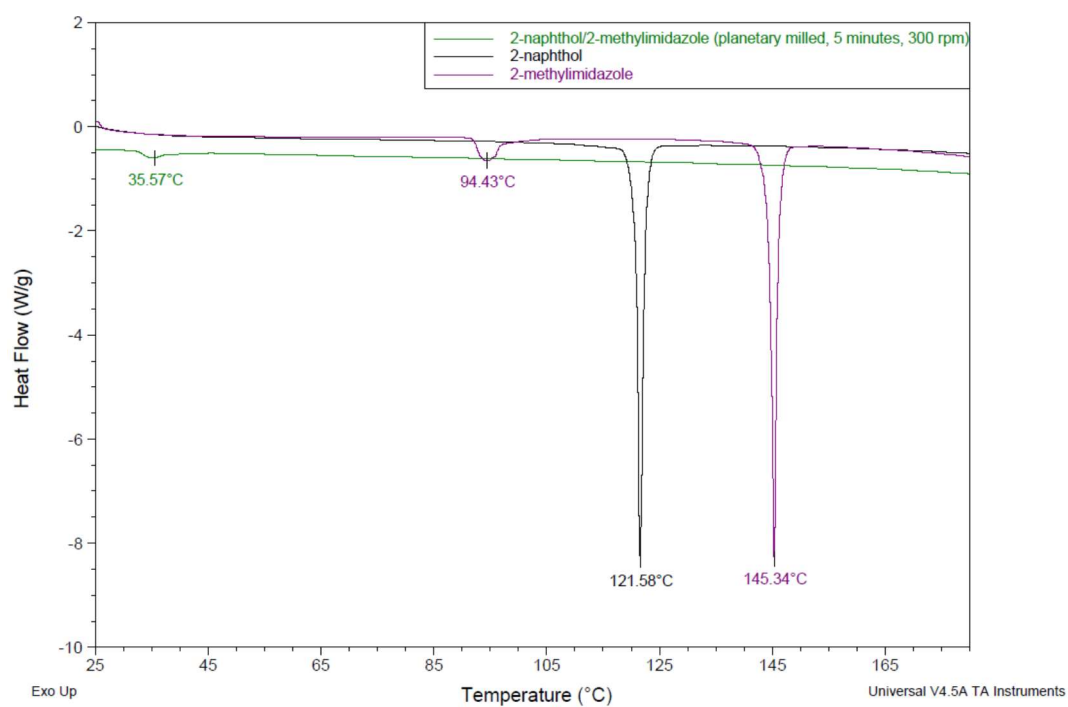


Figure B.55 - Thermal analysis of 2-naphthol/2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.32 2-naphthol/4-methylimidazole

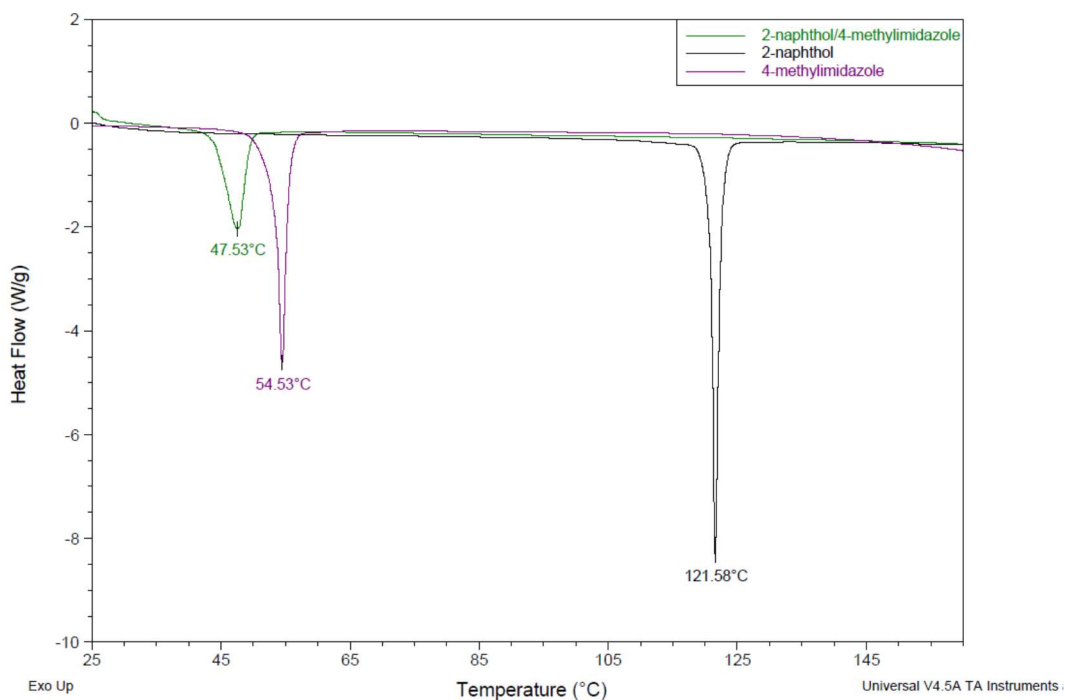


Figure B.56 - Thermal analysis of 2-naphthol/4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

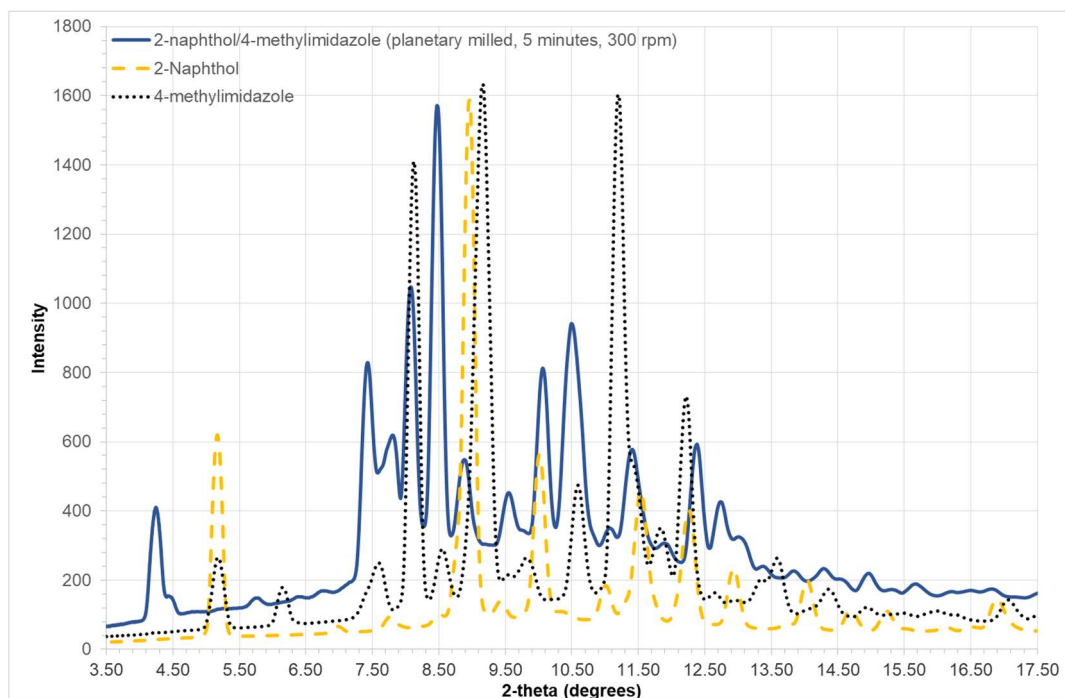


Figure B.57 – Powder x-ray pattern of 2-naphthol/4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

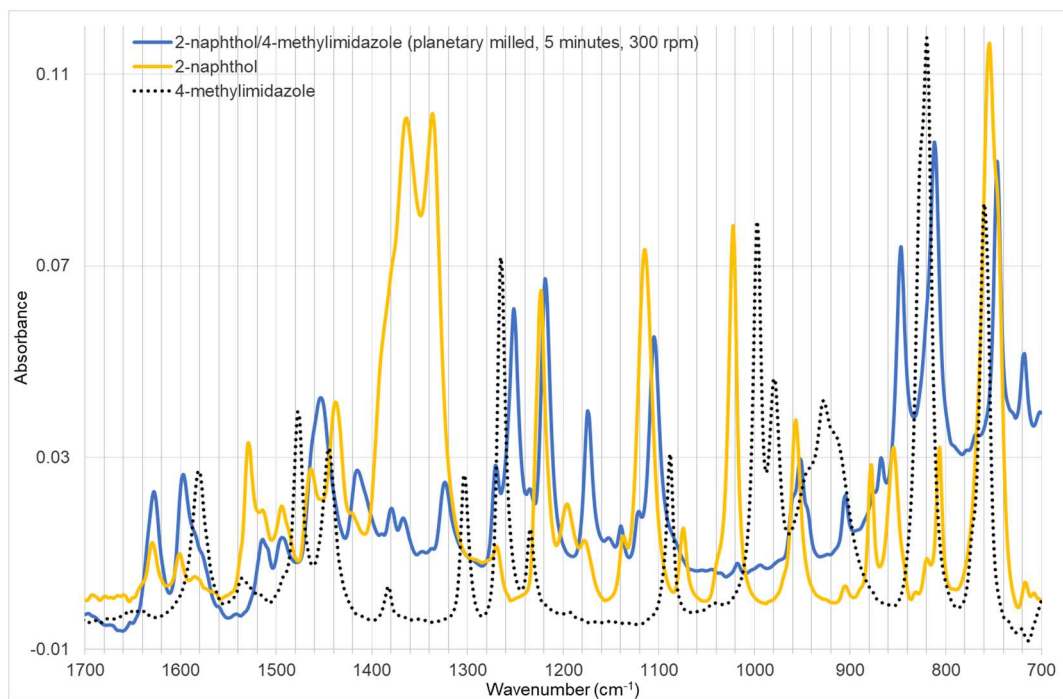


Figure B.58 – Infrared spectra of 2-naphthol/4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

Table B.7 - Infrared spectra peak positions and heights of 2-naphthol/4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)	Peak Position (cm ⁻¹)	Peak Height (Absorbance)
1627.94	0.02	1152.91	0.01
1597.27	0.03	1139.75	0.02
1514.18	0.01	1120.9	0.02
1493.59	0.01	1104.92	0.06
1453.65	0.04	952.31	0.03
1415.38	0.03	904.98	0.02
1389.27	0.01	875.23	0.02
1379.47	0.02	867.6	0.03
1367.43	0.02	846.89	0.07
1336.65	0.01	811.78	0.1
1323.58	0.02	776.83	0.03
1270.56	0.03	767.84	0.03
1251.63	0.06	746.28	0.09
1234.97	0.02	718.08	0.05
1218.76	0.07	701.56	0.04
1174.2	0.04		

B.33 2-naphthol/imidazol-2-amine

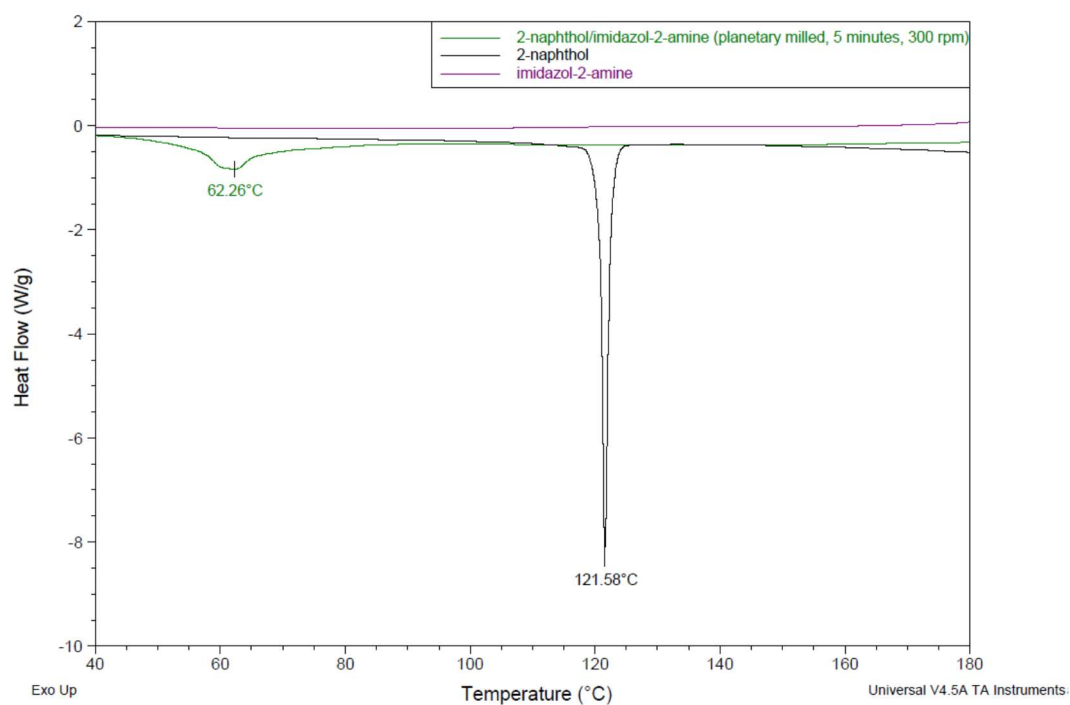


Figure B.59 - Thermal analysis of 2-naphthol/imidazol-2-amine produced by planetary milling for 5 minutes at 300 rpm. Imidazol-2-amine is a liquid and did not display a melt.

B.34 2-naphthol/2-bromoimidazole

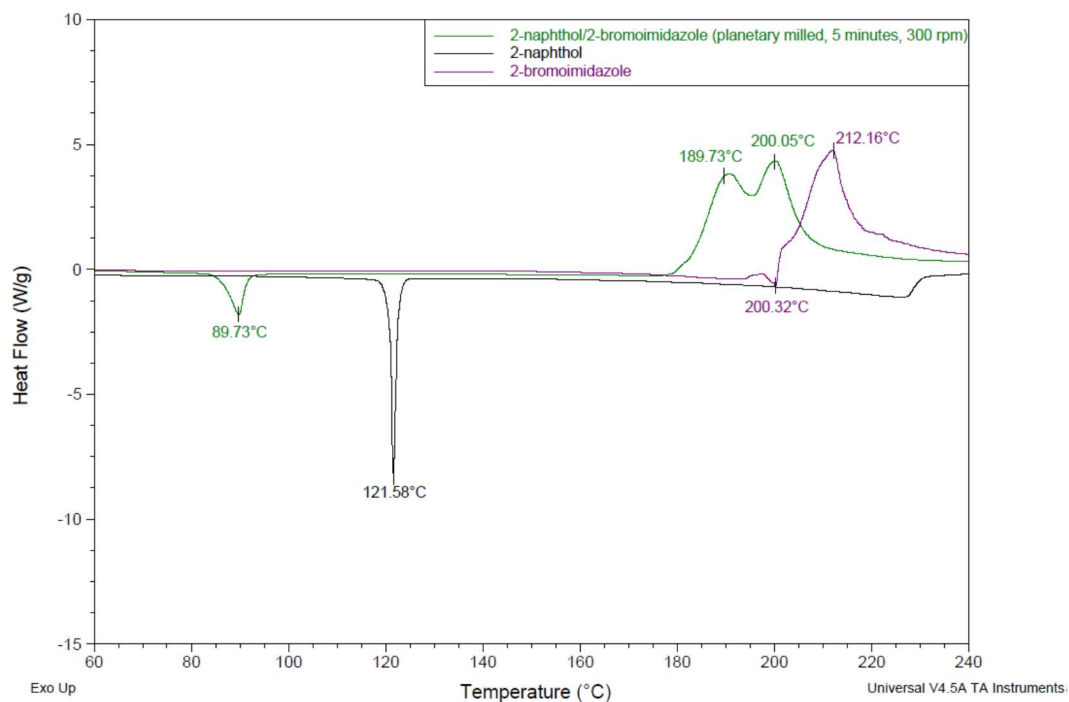


Figure B.60 - Thermal analysis of 2-naphthol/2-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

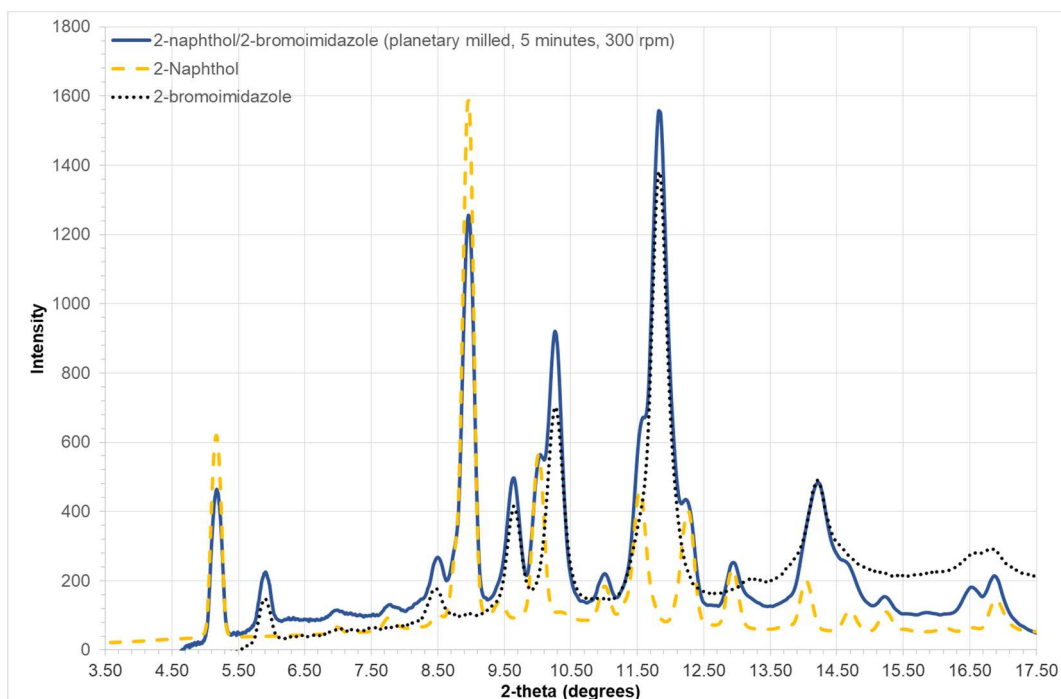


Figure B.61 – Powder x-ray pattern of 2-naphthol/2-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.35 2-naphthol/4-bromoimidazole

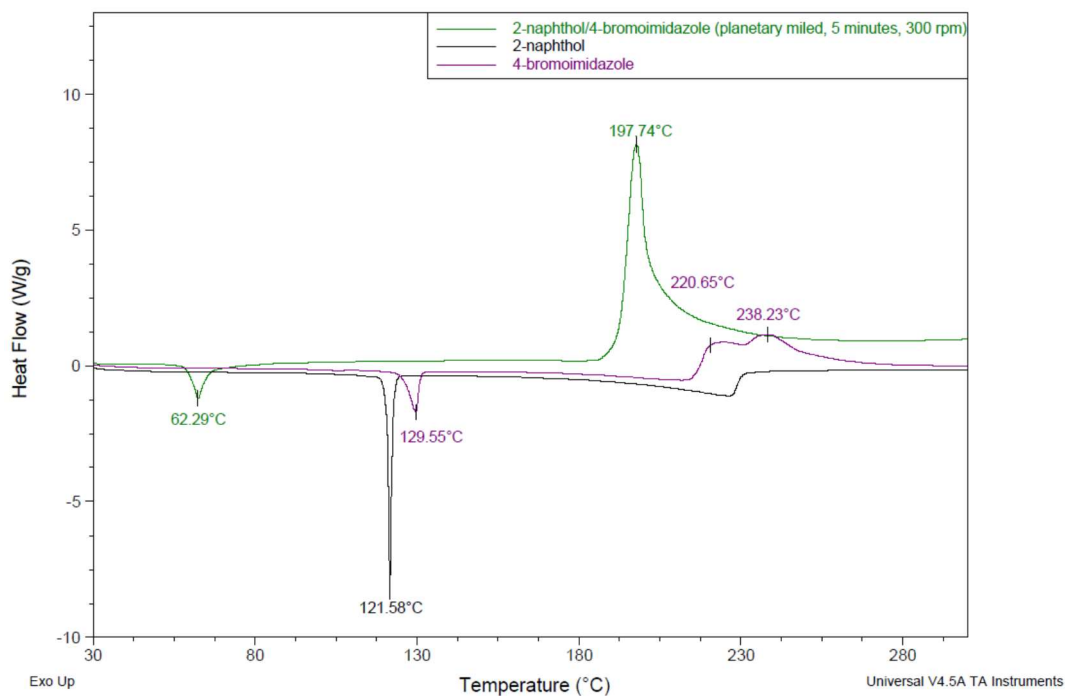


Figure B.62 - Thermal analysis of 2-naphthol/4-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

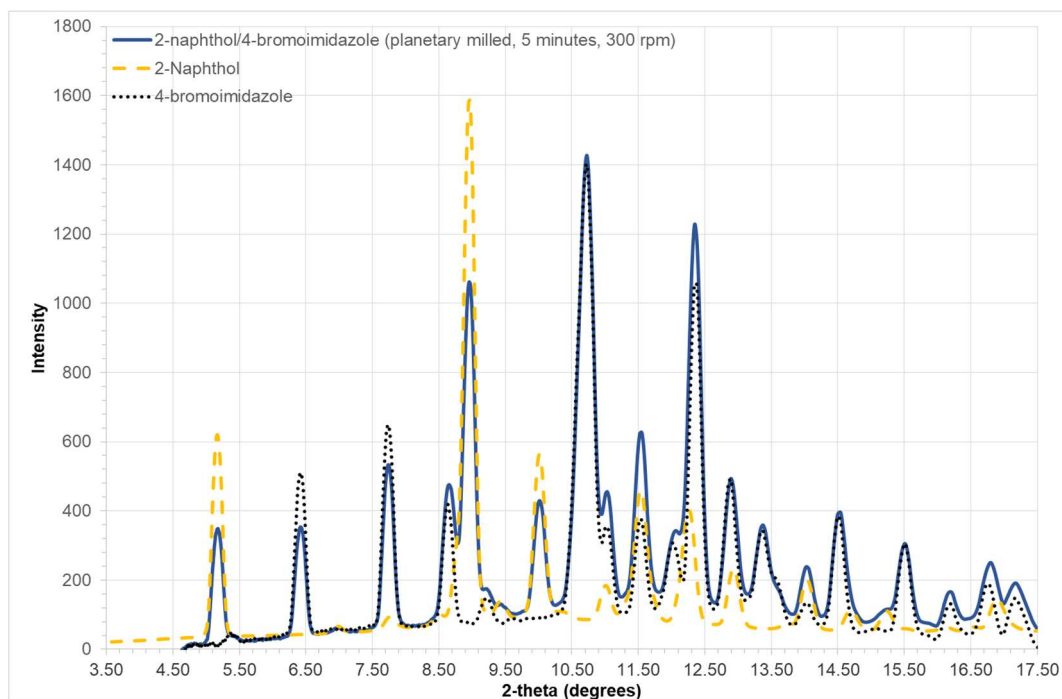


Figure B.63 – Powder x-ray pattern of 2-naphthol/4-bromoimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.36 2-naphthol/2,4-dimethylimidazole

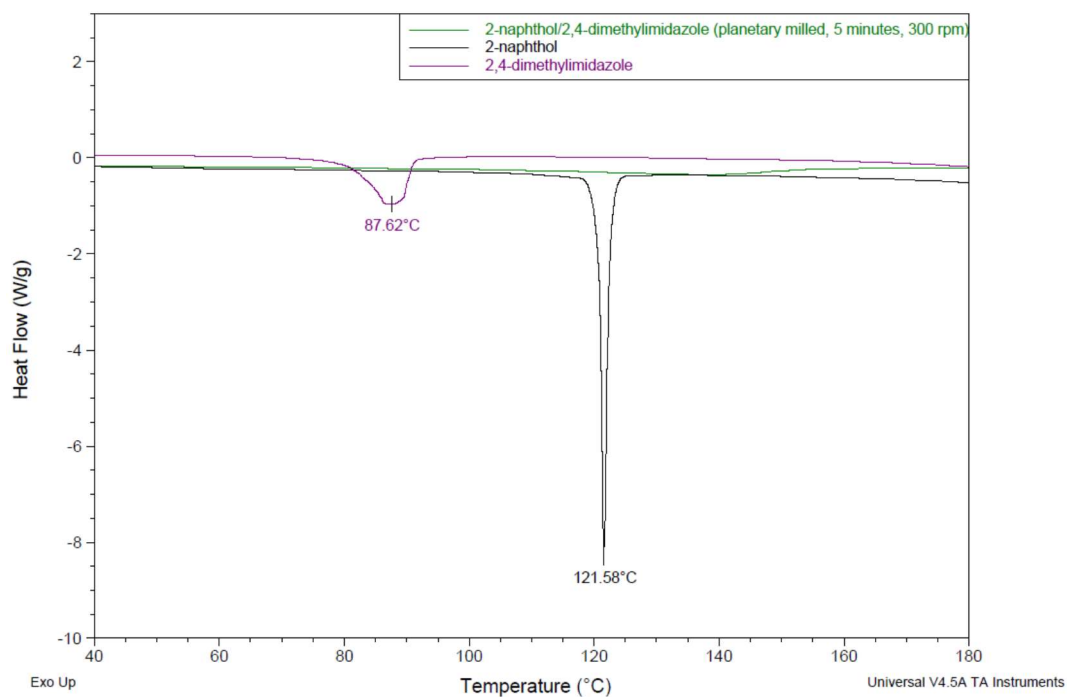


Figure B.64 - Thermal analysis of 2-naphthol/2,4-dimethylimidazole produced by planetary milling for 5 minutes at 300 rpm. The mixed system is a liquid and did not display a melt.

B.37 2-naphthol/4,5-dinitroimidazole

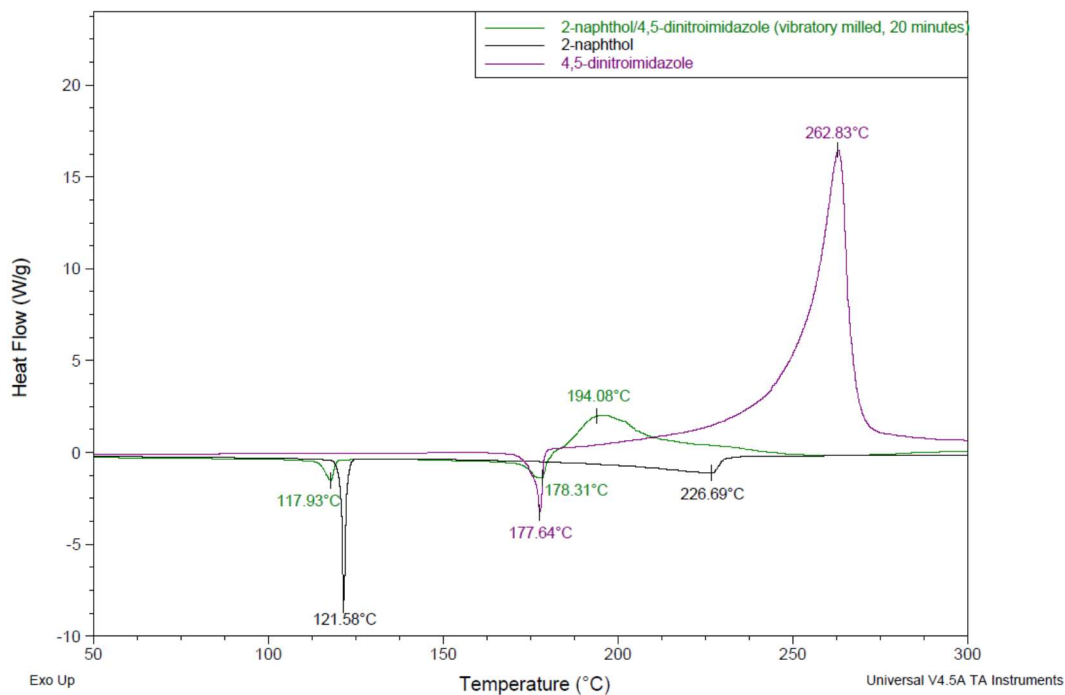


Figure B.65 - Thermal analysis of 2-naphthol/4,5-dinitroimidazole produced by vibratory milling for 20 minutes.

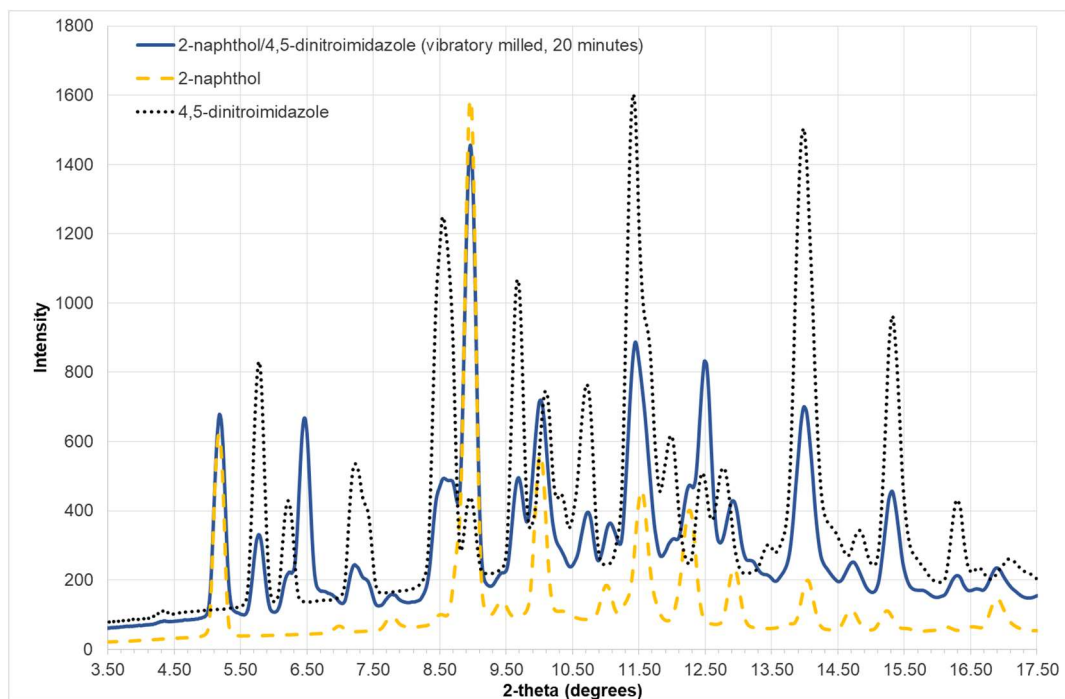


Figure B.66 – Powder x-ray pattern of 2-naphthol/4,5-dinitroimidazole produced by vibratory milling for 20 minutes.

B.38 2-naphthol/4,5-dichlororimidazole

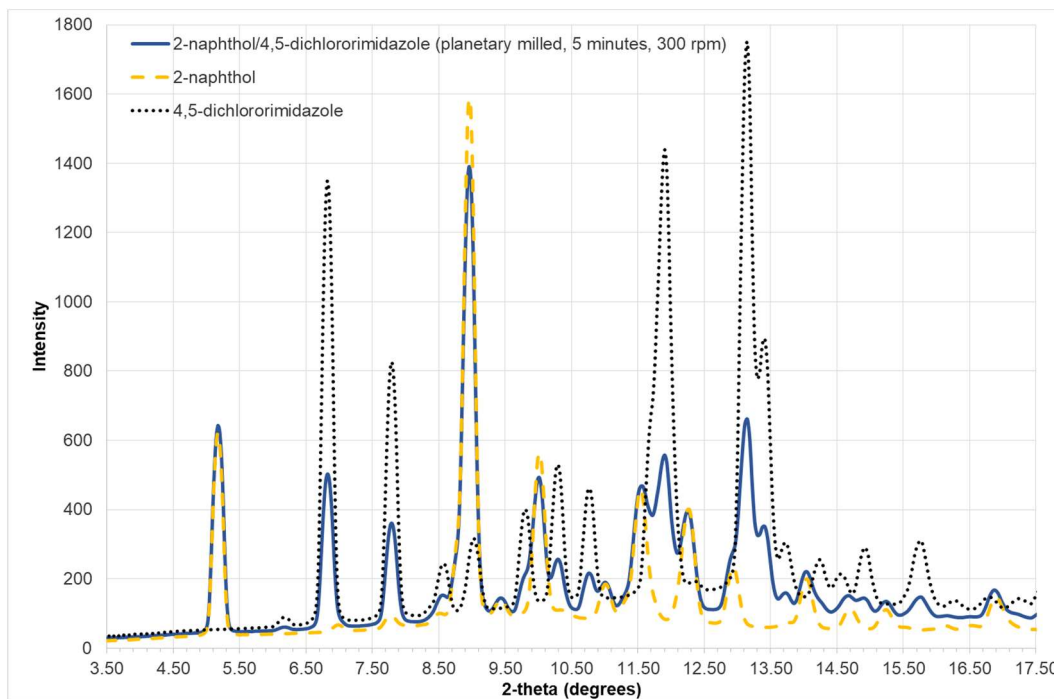


Figure B.67 - Powder x-ray pattern of 2-naphthol/4,5-dichlororimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.39 2-naphthol/2,4,5-tribromoimidazole

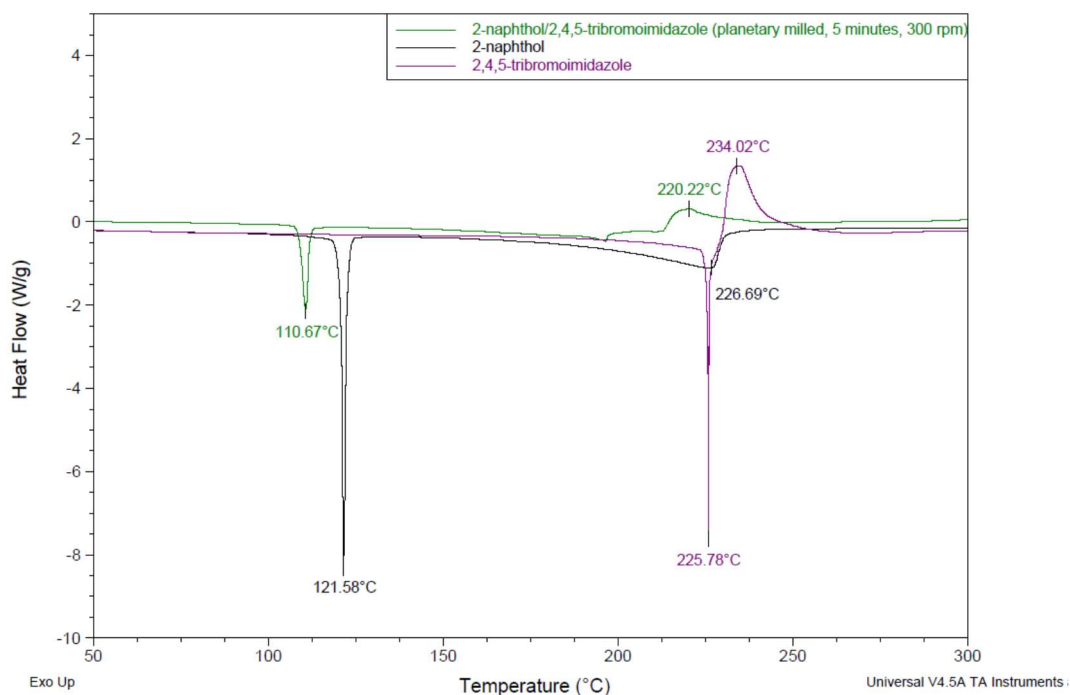


Figure B.68 – Thermal analysis of 2-naphthol/2,4,5-tribromolimidazole produced by planetary milling for 5 minutes at 300 rpm.

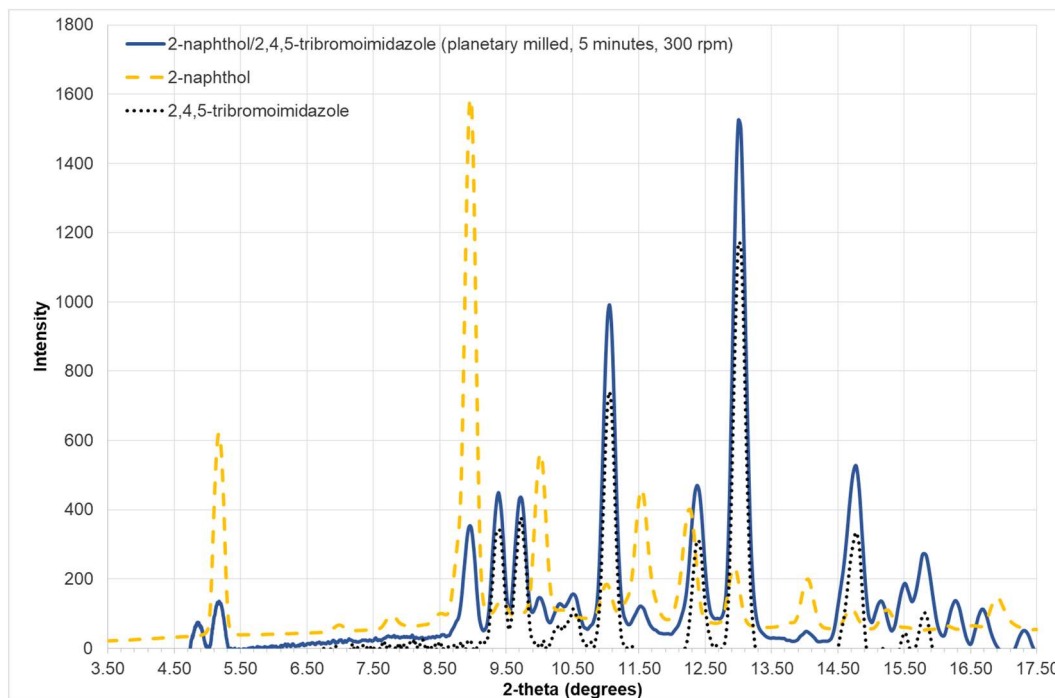


Figure B.69 - Powder x-ray pattern of 2-naphthol/2,4,5-tribromolimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.40 2-naphthol/2-methyl-5-nitroimidazole

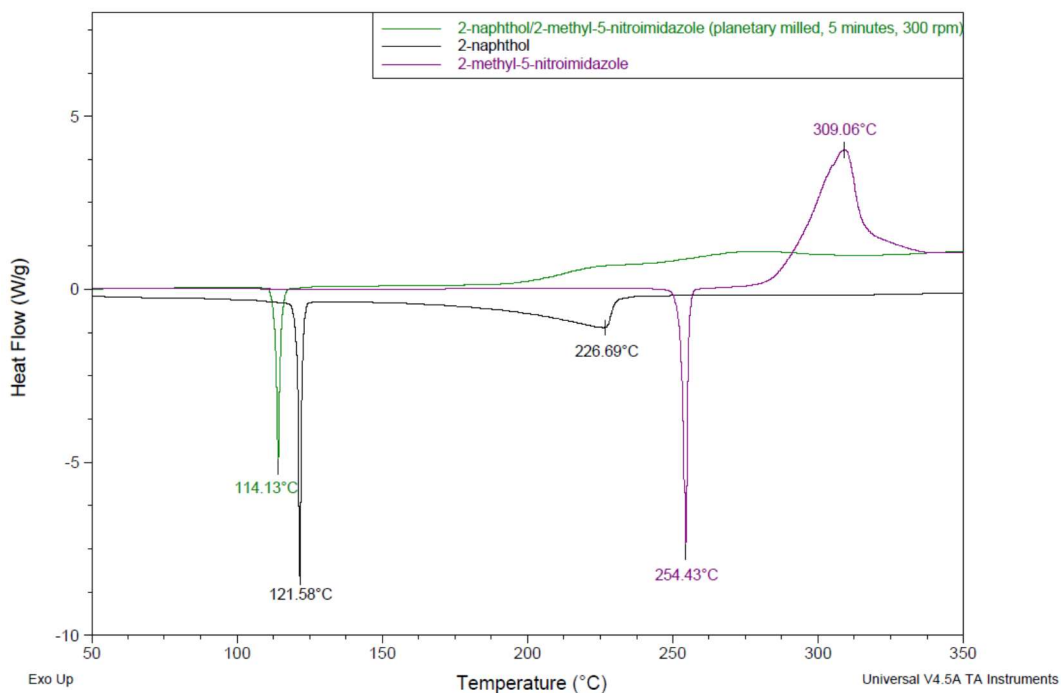


Figure B.70 - Thermal analysis of 2-naphthol/2-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

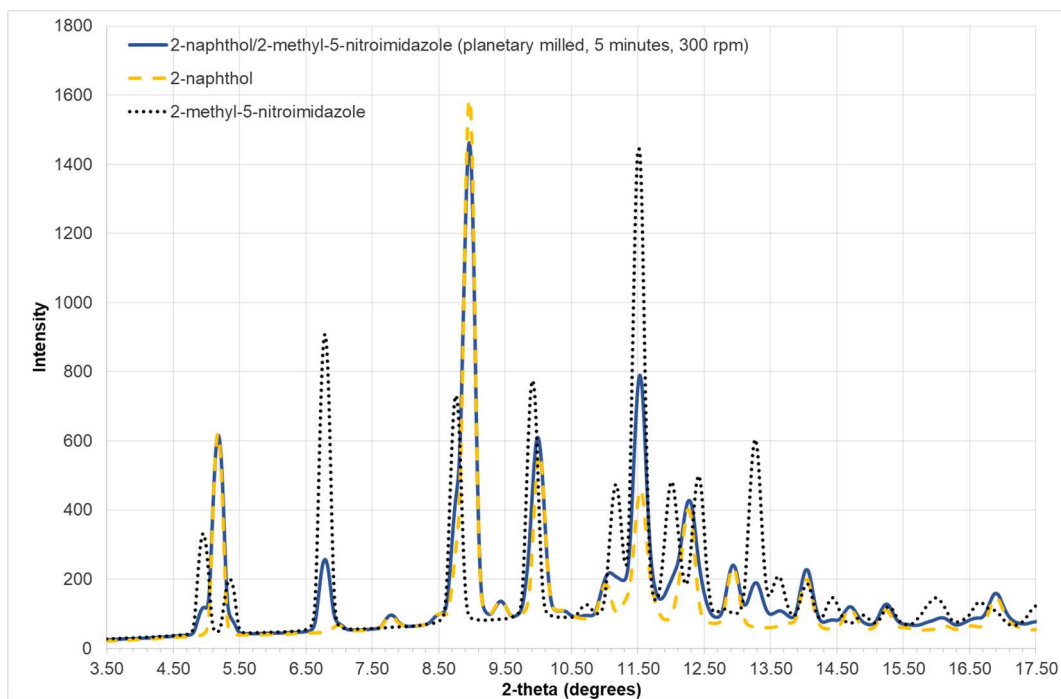


Figure B.71 – Powder x-ray pattern of 2-naphthol/2-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.41 2-naphthol/4-methyl-5-nitroimidazole

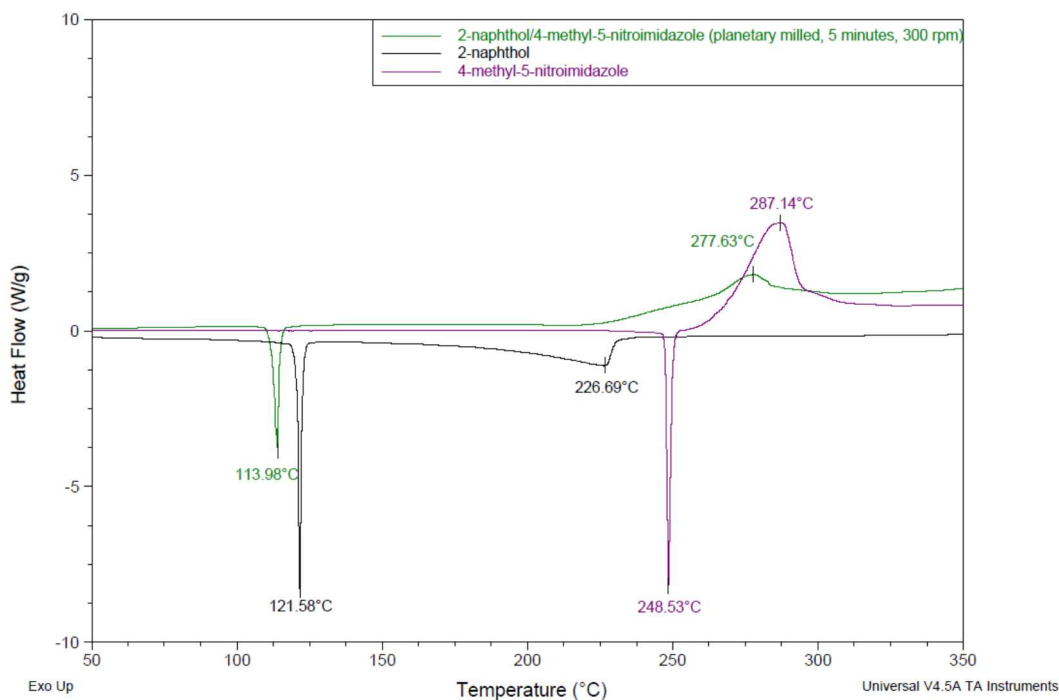


Figure B.72 - Thermal analysis of 2-naphthol/4-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

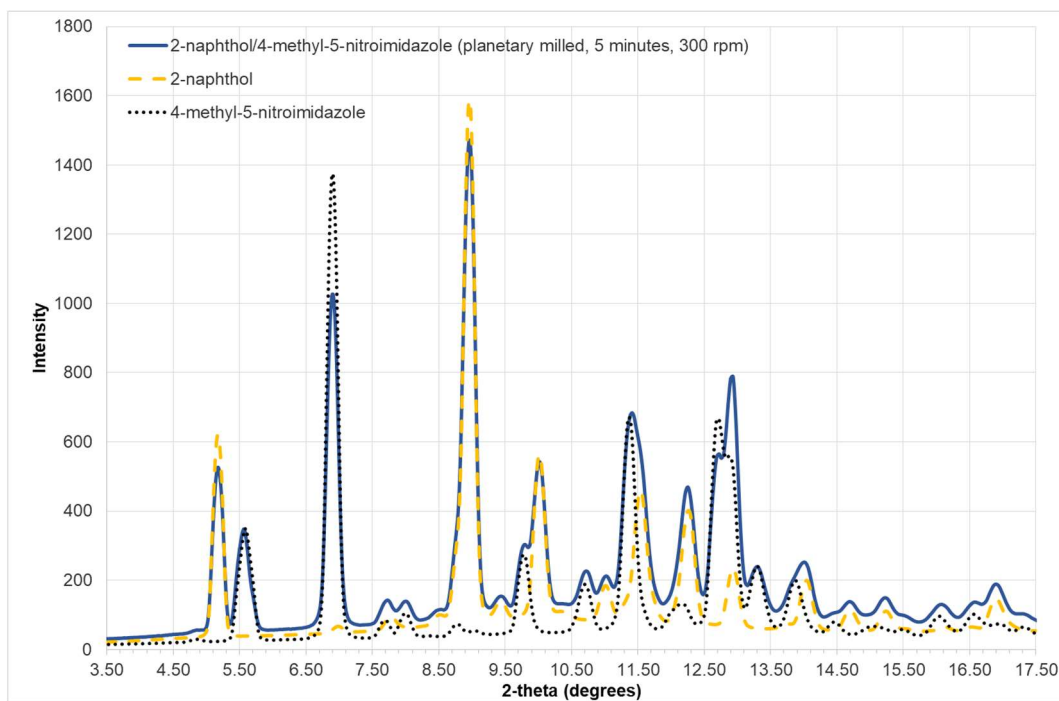


Figure B.73 – Powder x-ray pattern of 2-naphthol/4-methyl-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.42 2-naphthol/2-bromo-5-nitroimidazole

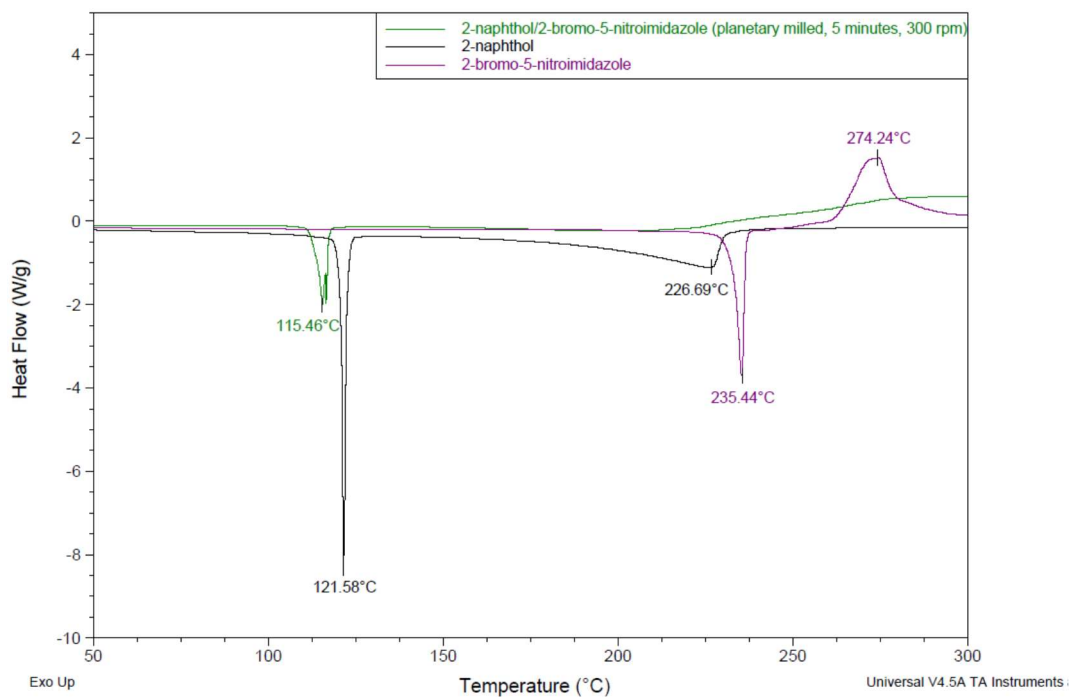


Figure B.74 - Thermal analysis of 2-naphthol/2-bromo-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

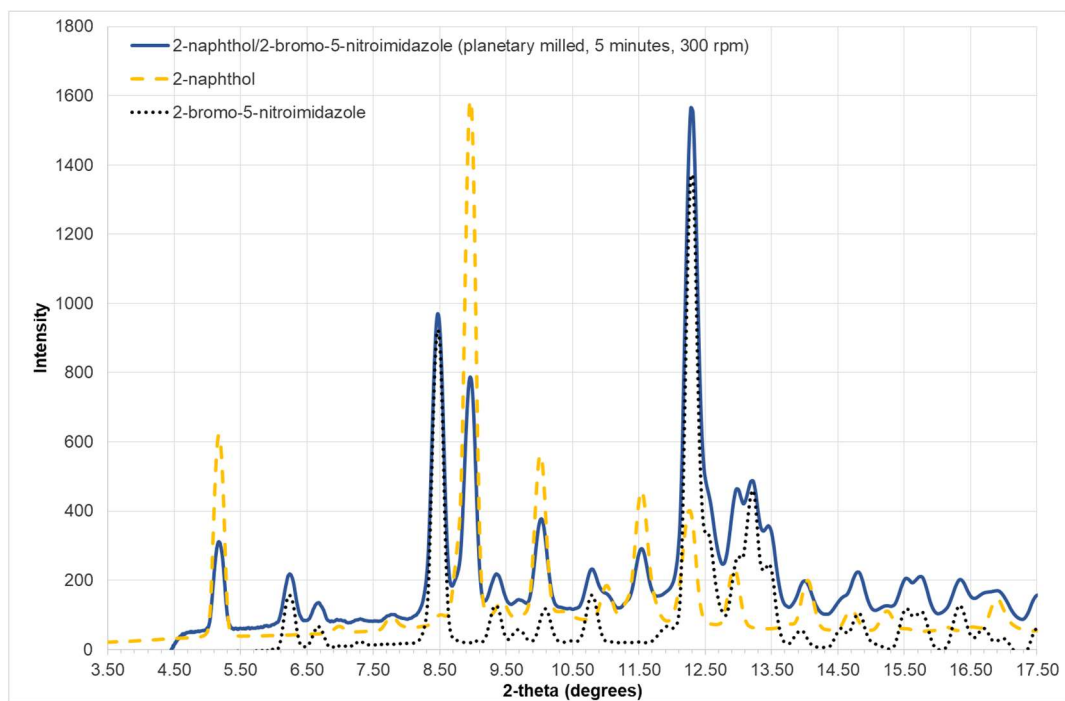


Figure B.75 – Powder x-ray pattern of 2-naphthol/2-bromo-5-nitroimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.43 2-naphthol/4-bromo-2-methylimidazole

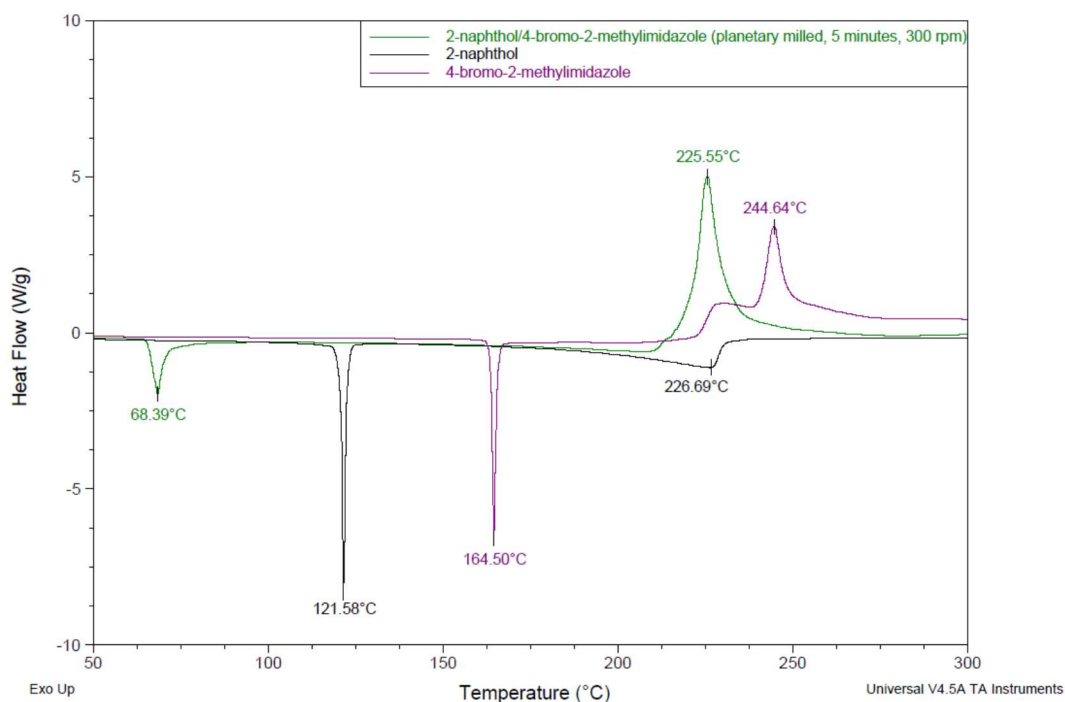


Figure B.76 – Thermal analysis of 2-naphthol/4-bromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

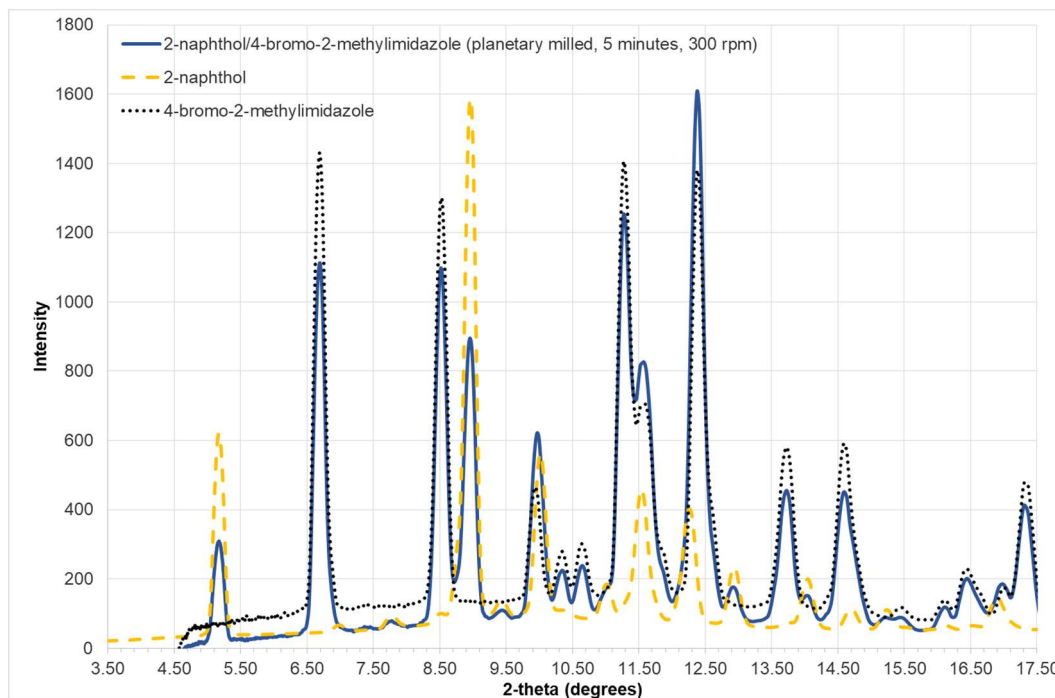


Figure B.77 - Powder x-ray pattern of 2-naphthol/4-bromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.44 2-naphthol/5-bromo-4-methylimidazole

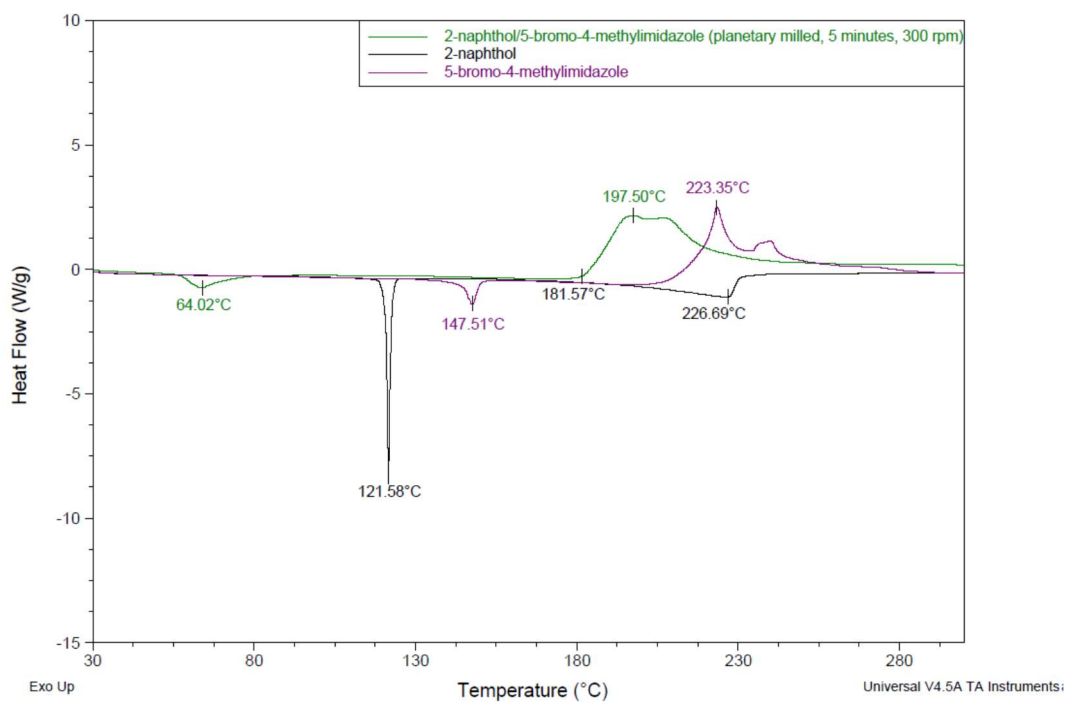


Figure B.78 - Thermal analysis of 2-naphthol/5-bromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

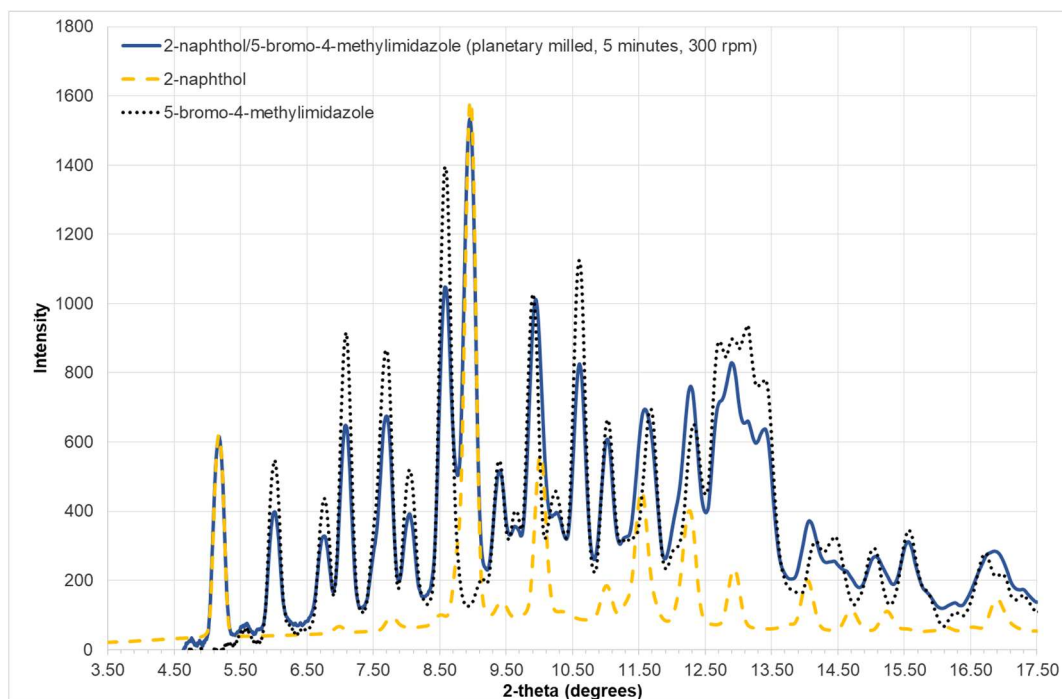


Figure B.79 – Powder x-ray pattern of 2-naphthol/5-bromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

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

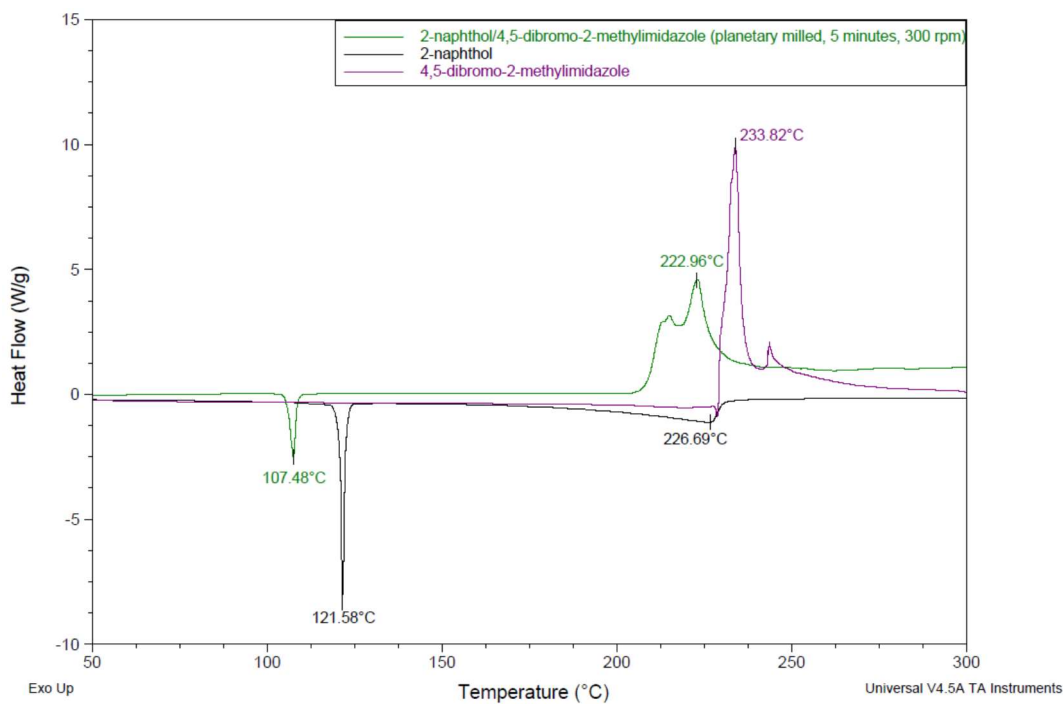


Figure B.80 - Thermal analysis of 2-naphthol/4,5-dibromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

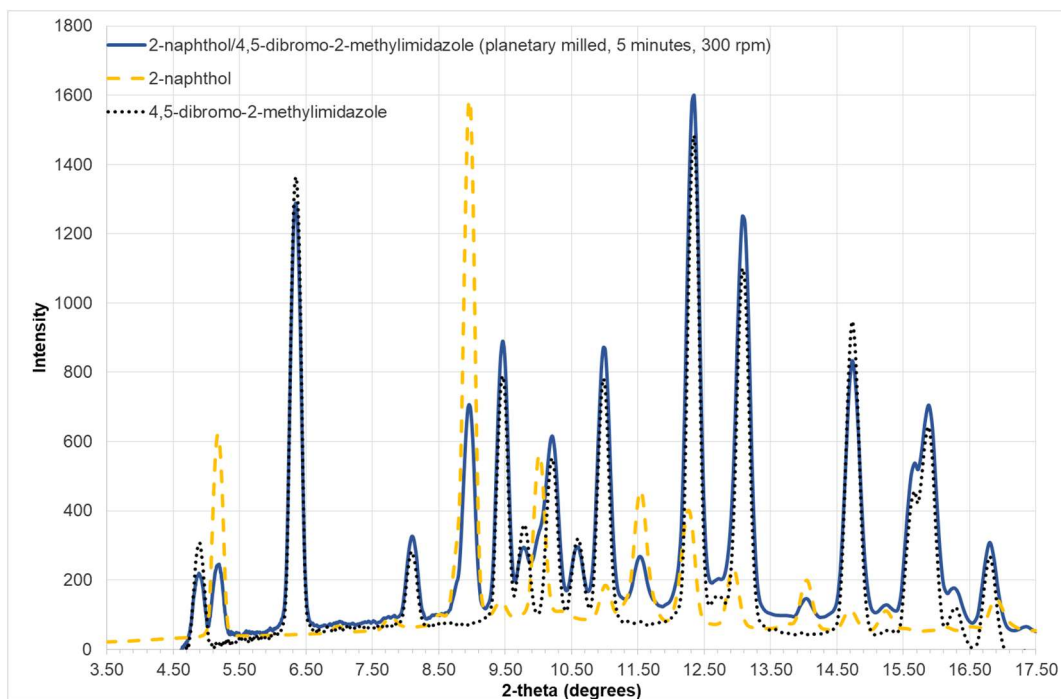


Figure B.81 – Powder x-ray pattern of 2-naphthol/4,5-dibromo-2-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.46 2-naphthol/2,5-dibromo-4-methylimidazole

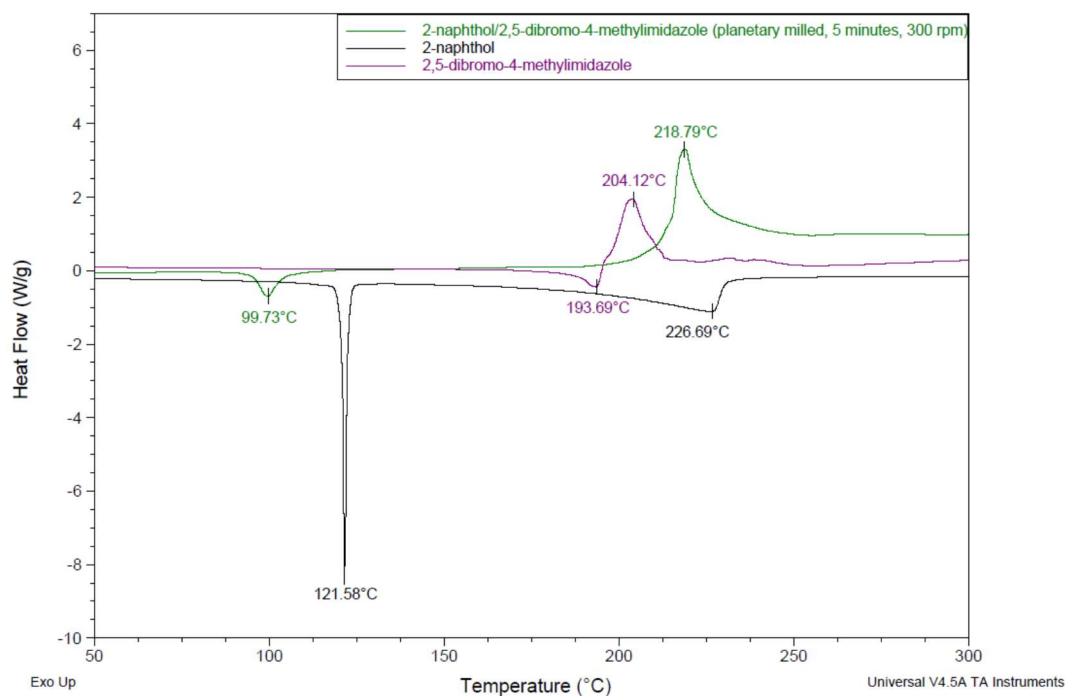


Figure B.82 - Thermal analysis of 2-naphthol/2,5-dibromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

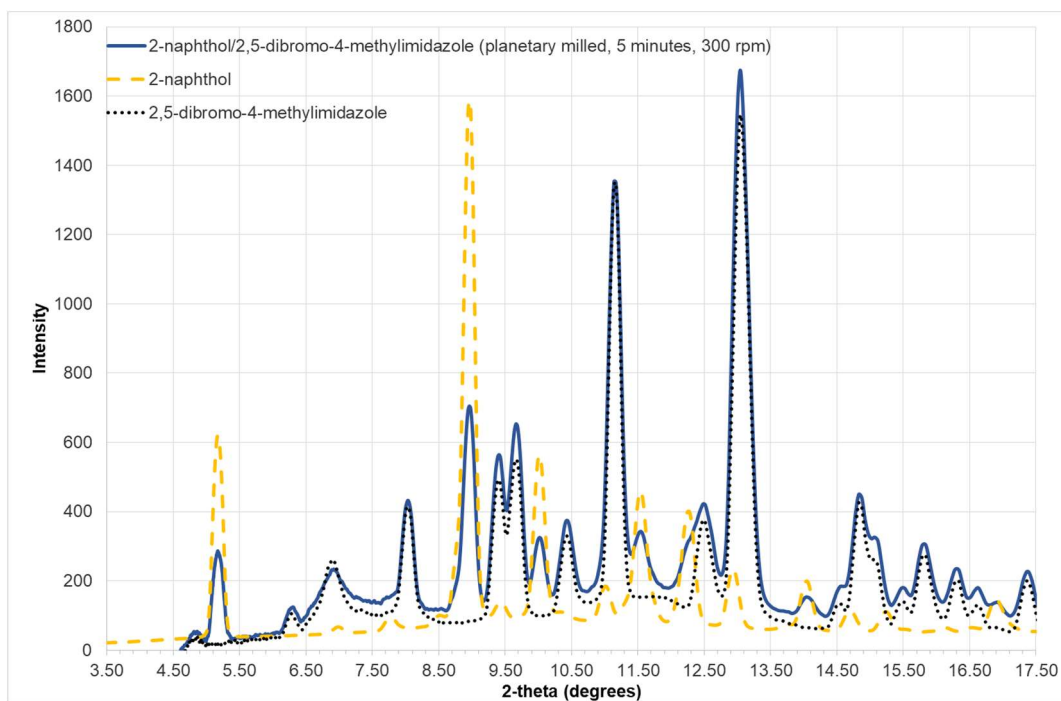


Figure B.83 – Powder x-ray pattern of 2-naphthol/2,5-dibromo-4-methylimidazole produced by planetary milling for 5 minutes at 300 rpm.

B.47 2-naphthol/1,2,3-triazole

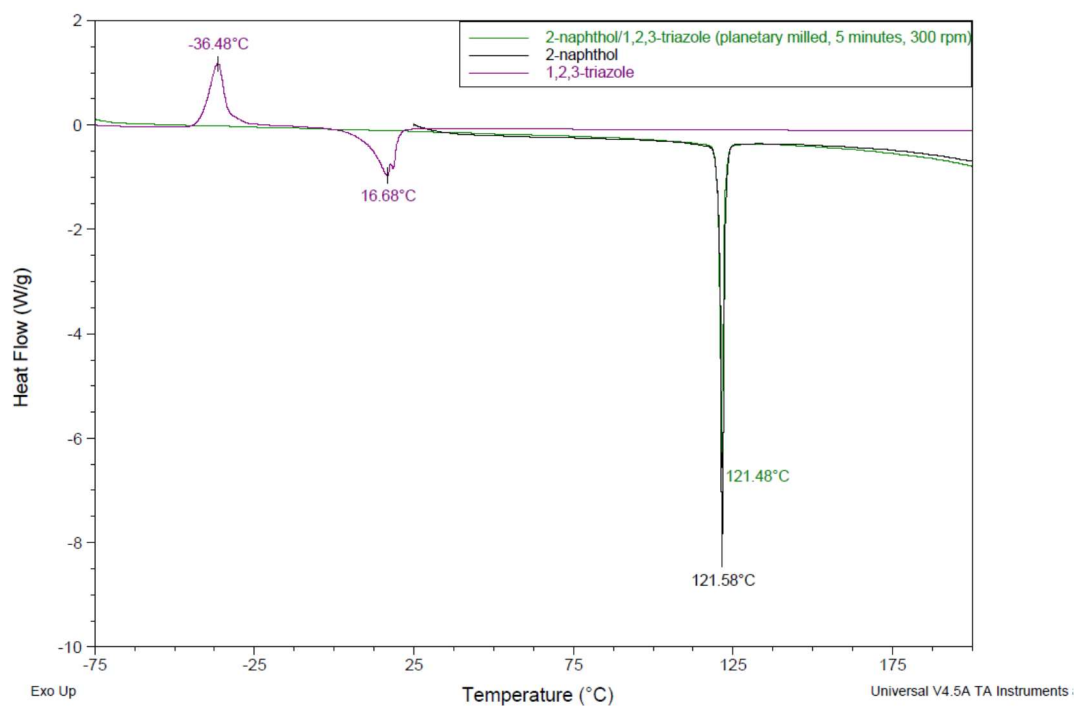


Figure B.84 - Thermal analysis of 2-naphthol/1,2,3-triazole produced by planetary milling for 5 minutes at 300 rpm.

B.48 2-naphthol/5-nitro-1,2,3-triazole

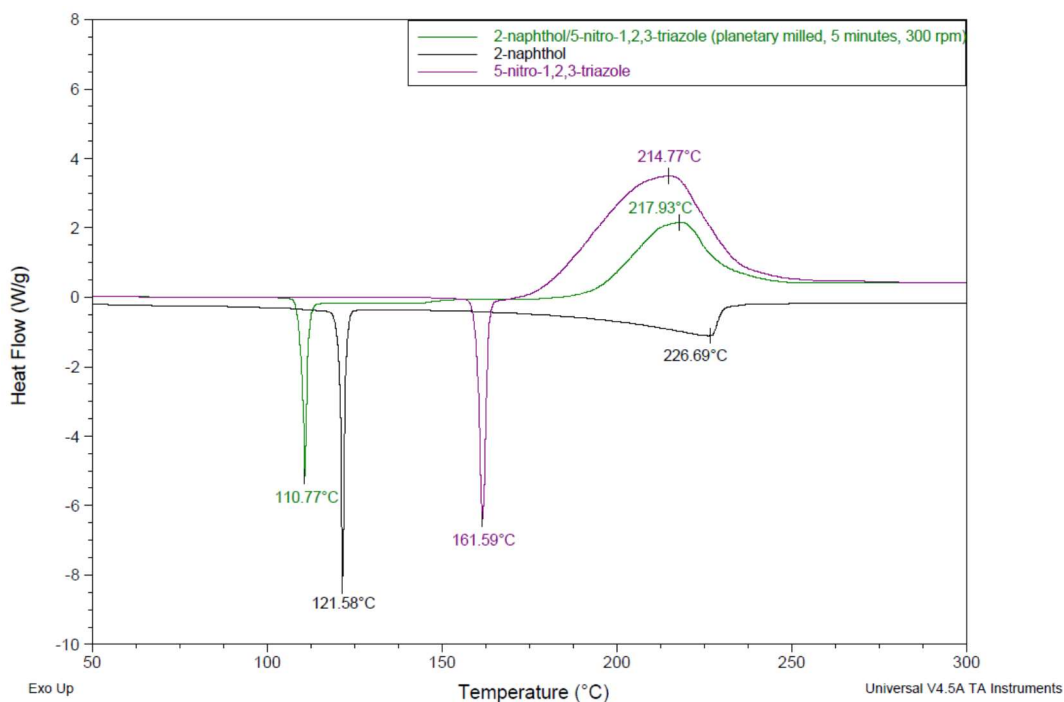


Figure B.85 - Thermal analysis of 2-naphthol/5-nitro-1,2,3-triazole produced by planetary milling for 5 minutes at 300 rpm.

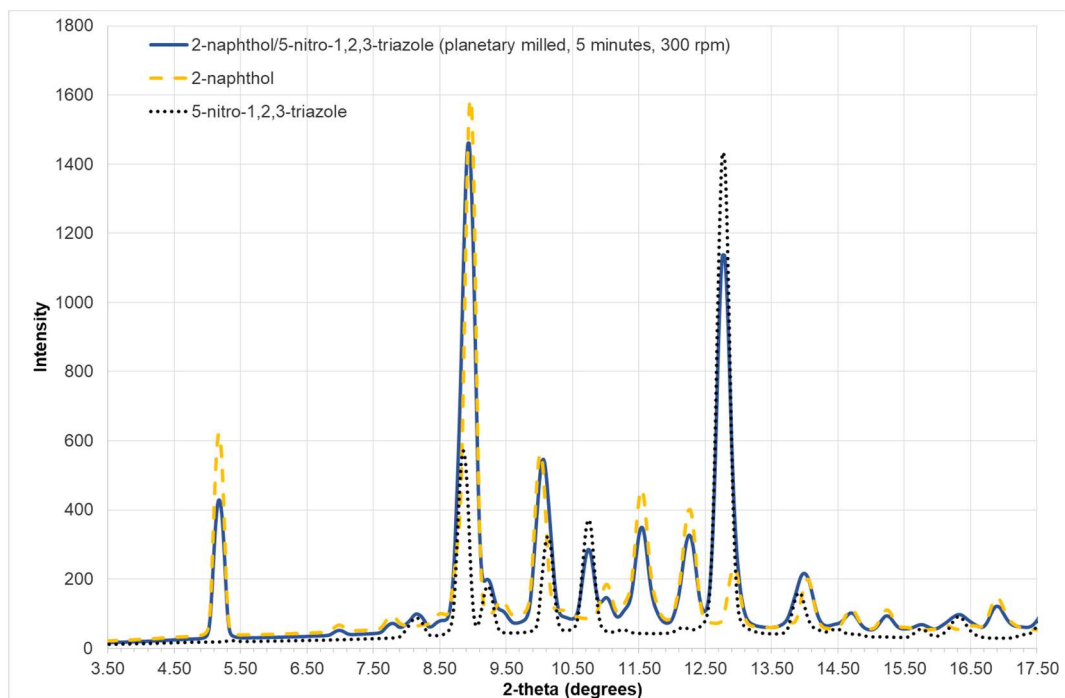


Figure B.86 – Powder x-ray pattern of 2-naphthol/5-nitro-1,2,3-triazole produced by planetary milling for 5 minutes at 300 rpm.

B.49 2-naphthol/1,2,4-triazole

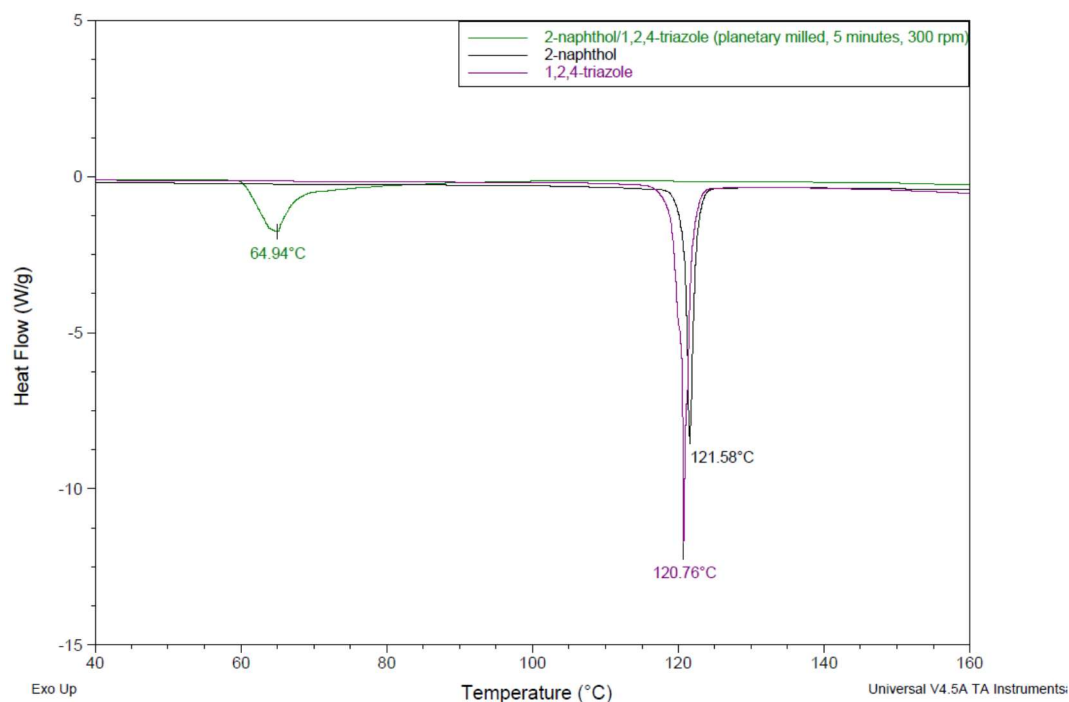


Figure B.87 - Thermal analysis of 2-naphthol/1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

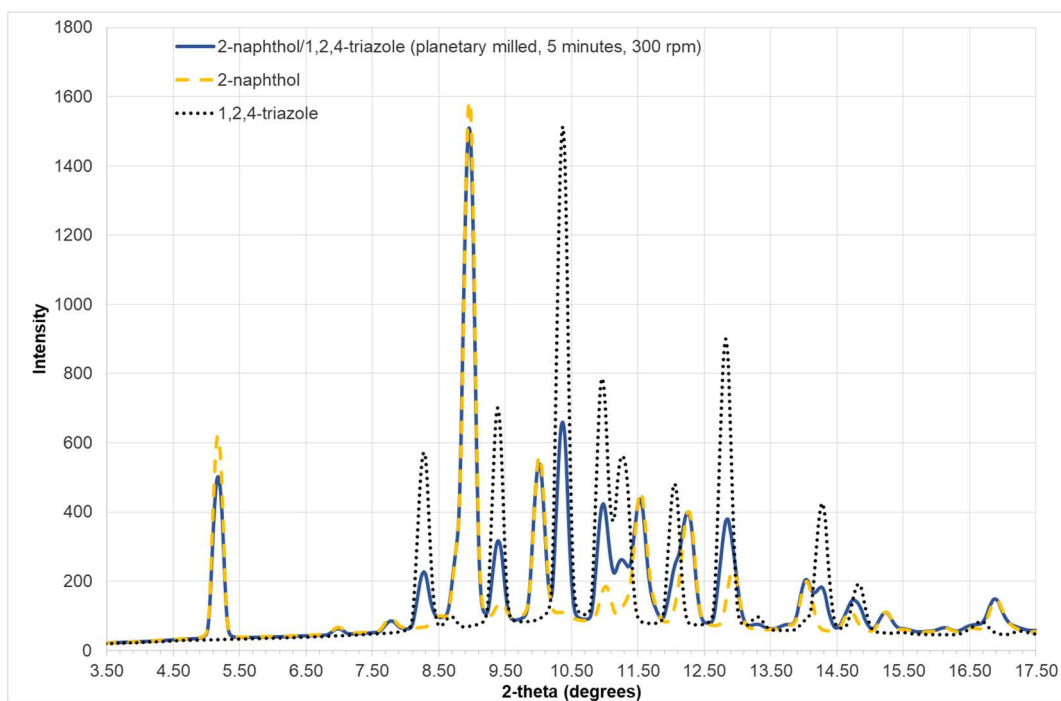


Figure B.88 – Powder x-ray pattern of 2-naphthol/1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

B.50 2-naphthol/3-methyl-1,2,4-triazole

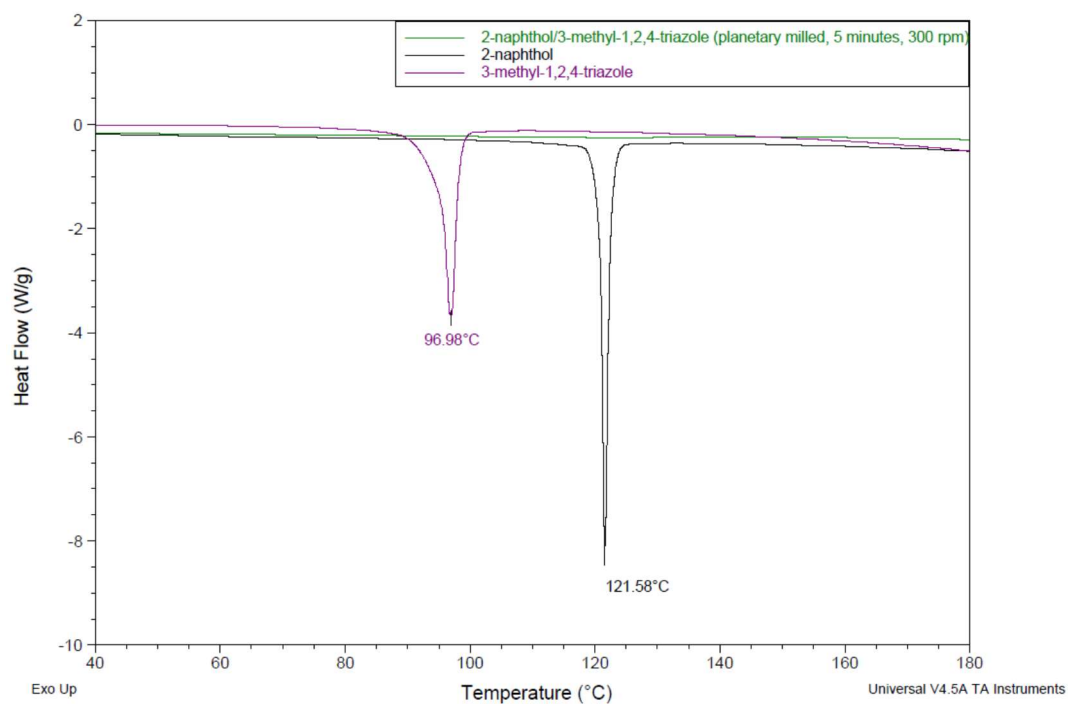


Figure B.89 - Thermal analysis of 2-naphthol/3-methyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

B.51 2-naphthol/1,2,4-triazol-3-amine

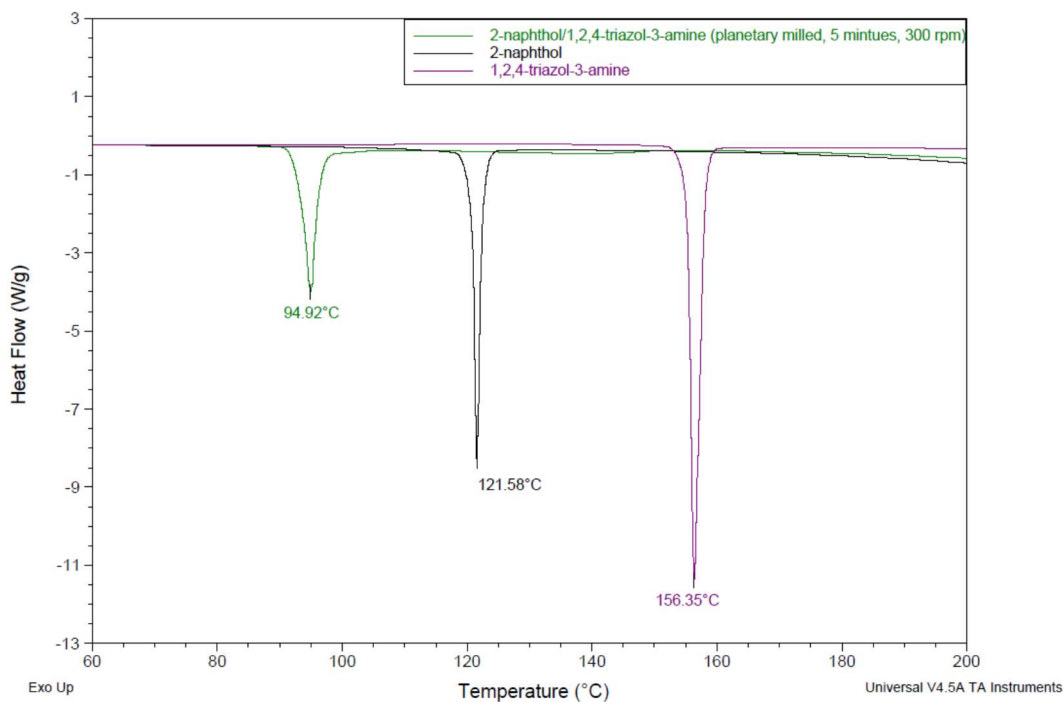


Figure B.90 - Thermal analysis of 2-naphthol/1,2,4-triazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

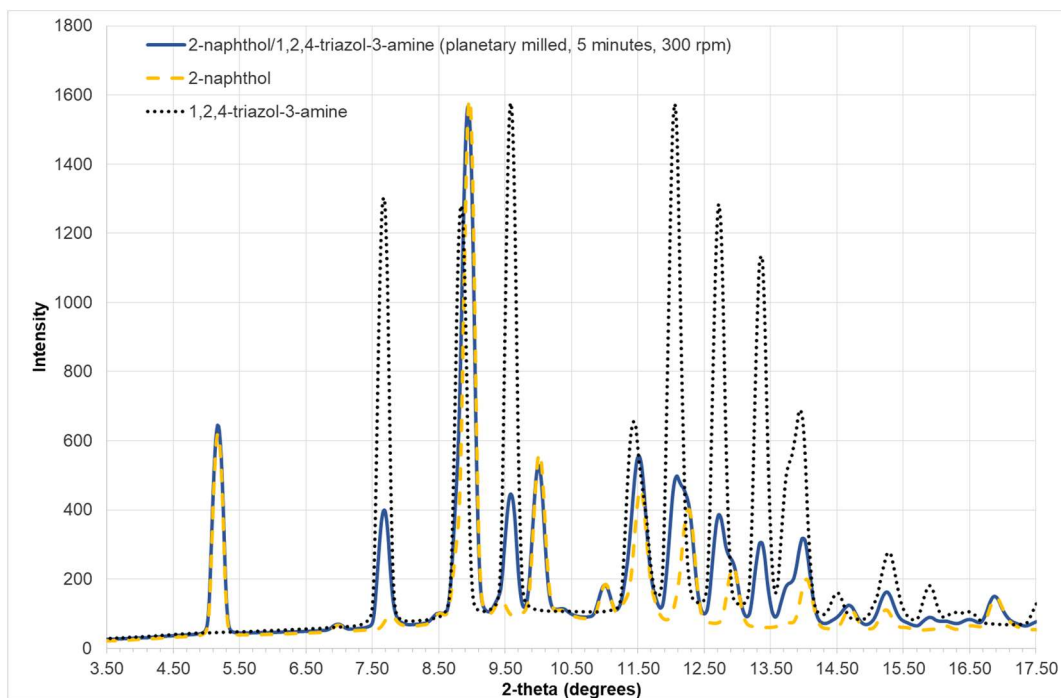


Figure B.91 – Powder x-ray pattern of 2-naphthol/1,2,4-triazol-3-amine produced by planetary milling for 5 minutes at 300 rpm.

B.52 2-naphthol/5-bromo-1,2,4-triazole

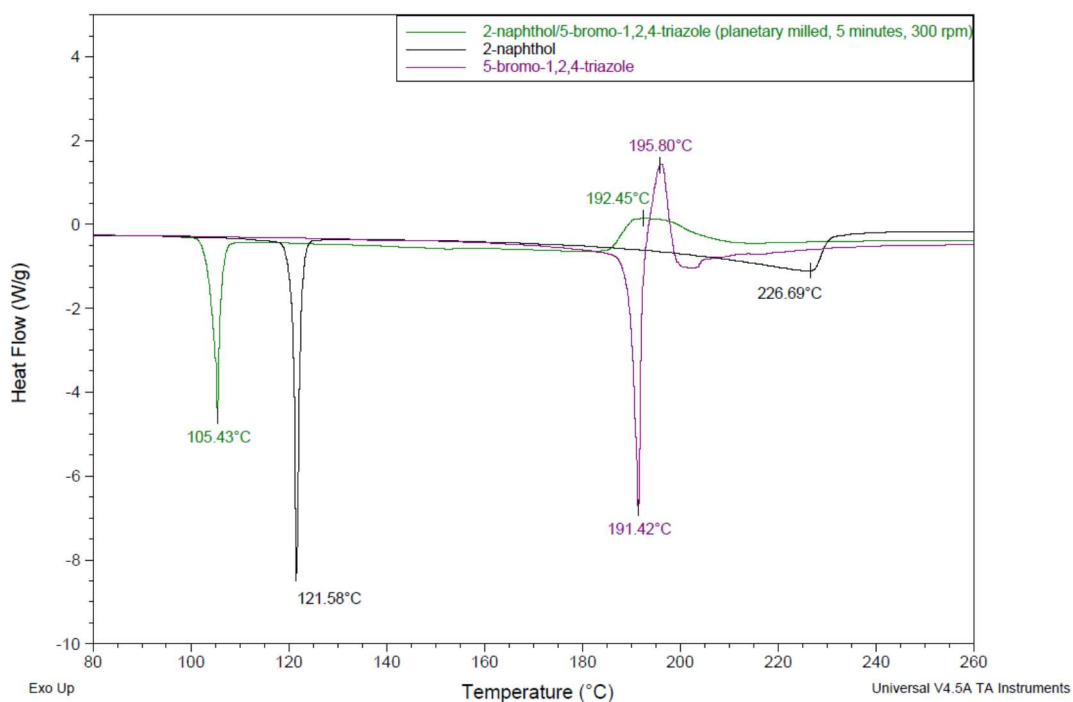


Figure B.92 - Thermal analysis of 2-naphthol/5-bromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

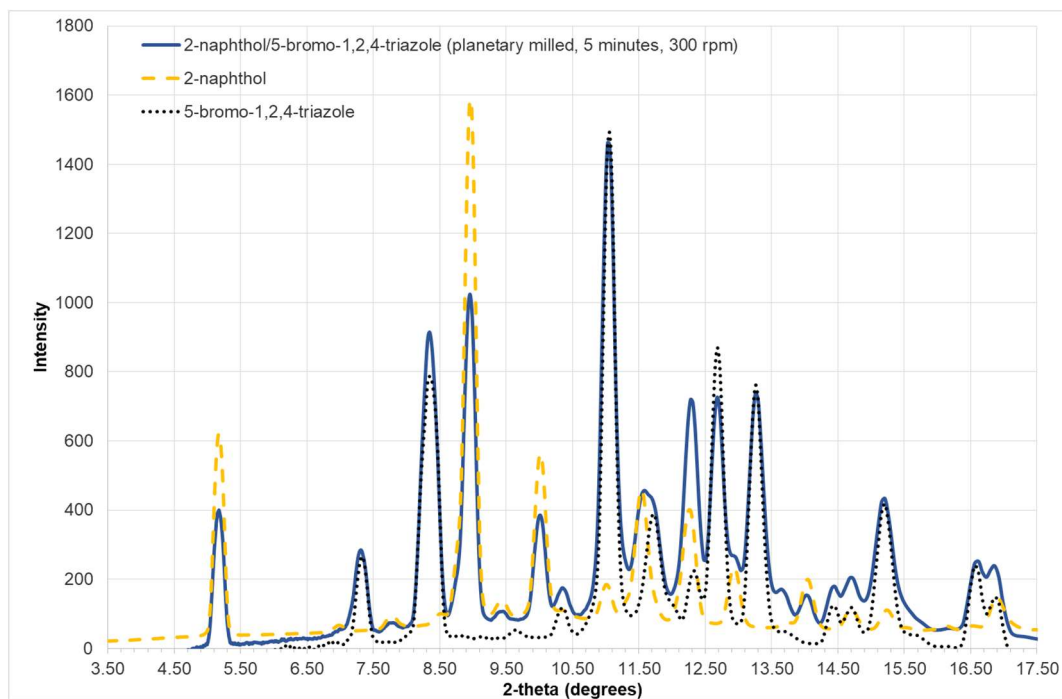


Figure B.93 – Powder x-ray pattern of 2-naphthol/5-bromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

B.53 2-naphthol/1,2,4-triazol-3,5-diamine

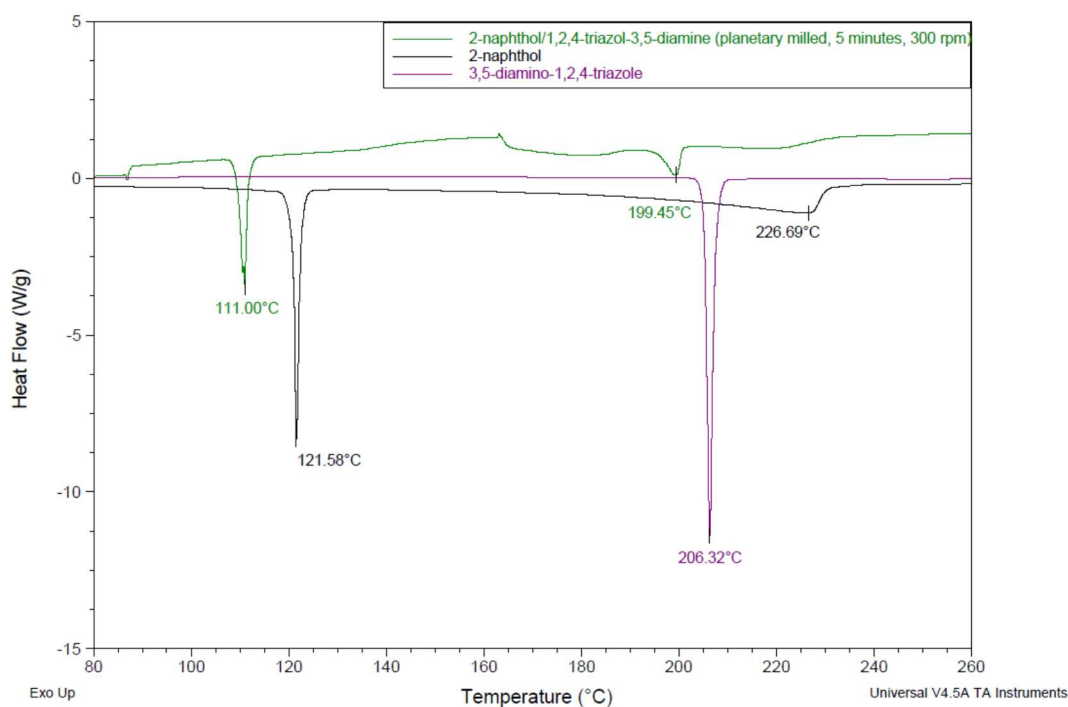


Figure B.94 - Thermal analysis of 2-naphthol/1,2,4-triazol-3,5-diamine produced by planetary milling for 5 minutes at 300 rpm.

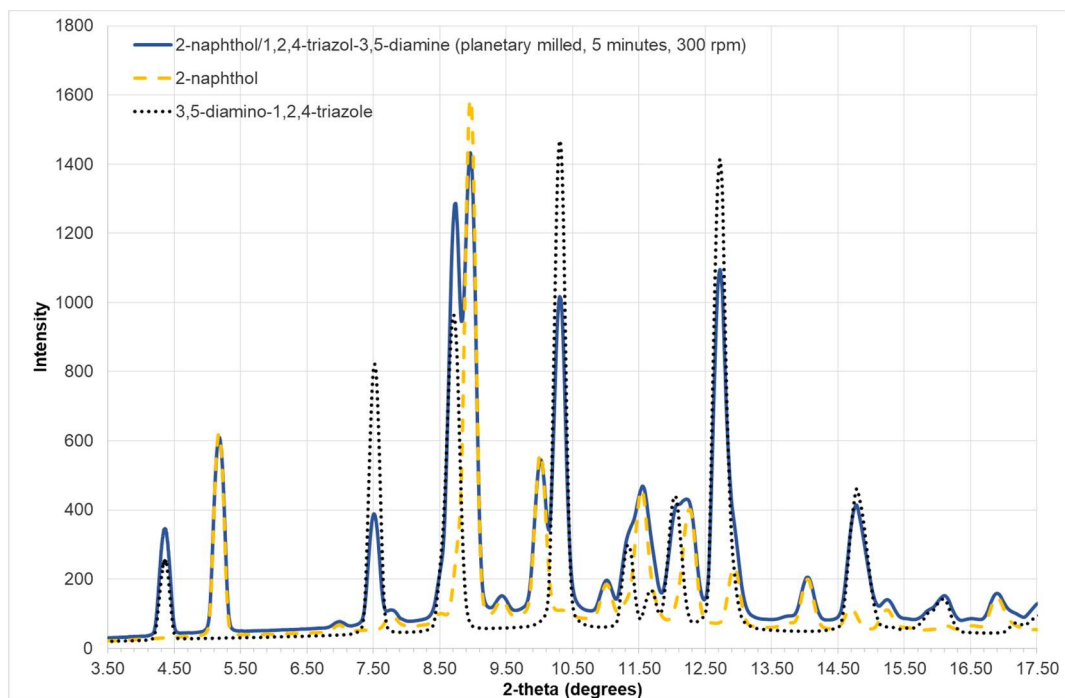


Figure B.95 – Powder x-ray pattern of 2-naphthol/1,2,4-triazol-3,5-diamine produced by planetary milling for 5 minutes at 300 rpm.

B.54 2-naphthol/3,5-dimethyl-1,2,4-triazole

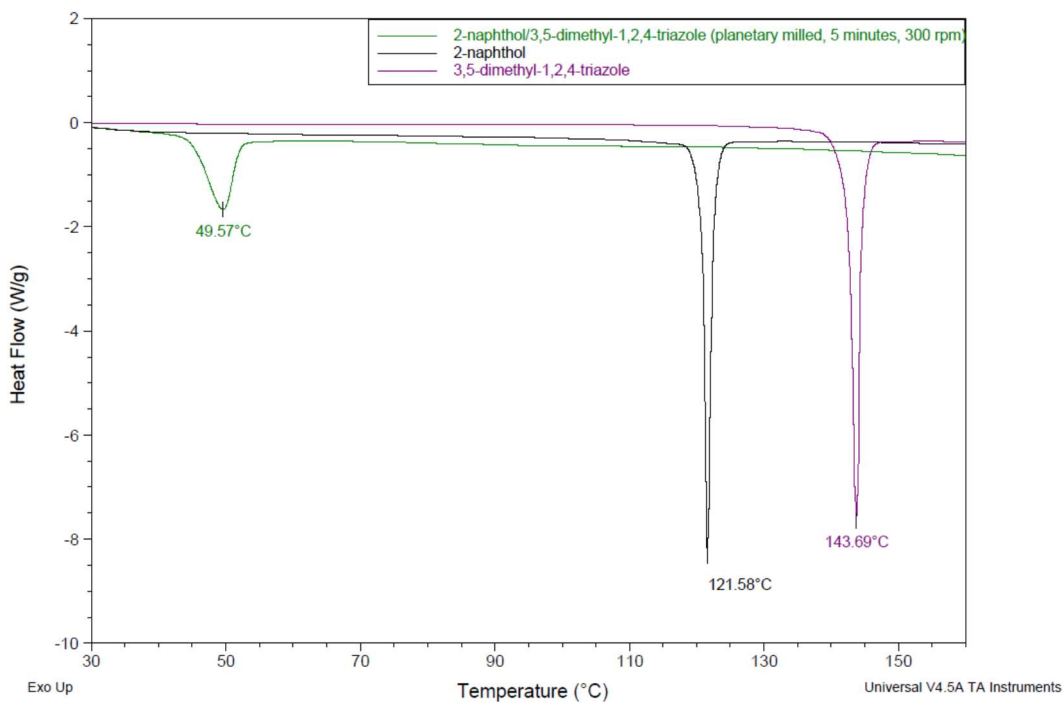


Figure B.96 - Thermal analysis of 2-naphthol/3,5-dimethyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

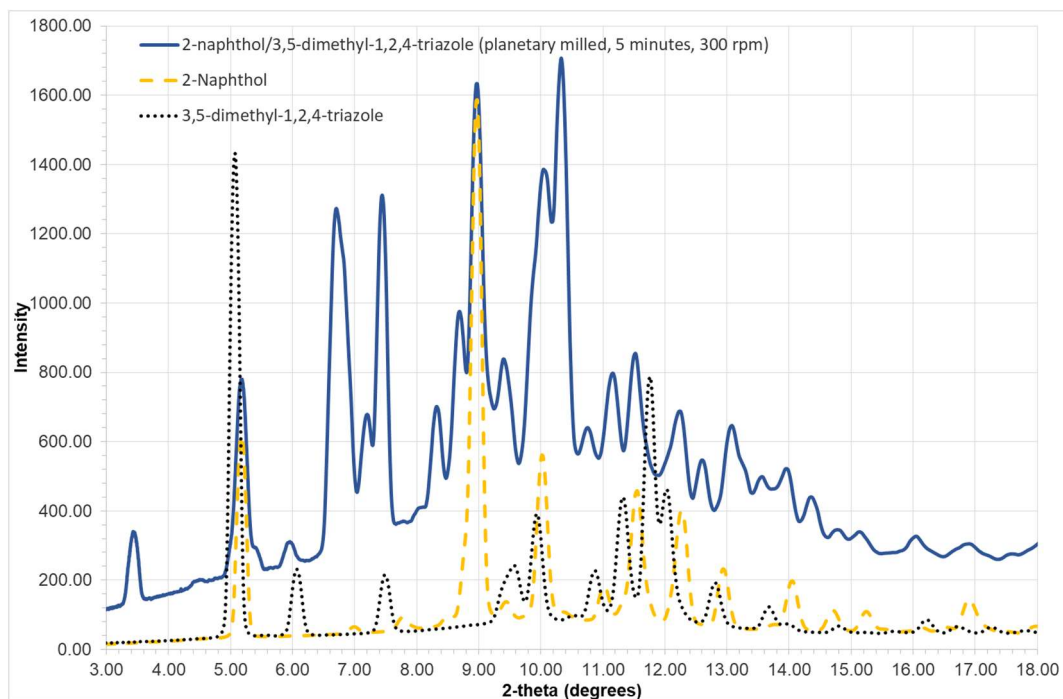


Figure B.97 – Powder x-ray pattern of 2-naphthol/3,5-dimethyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

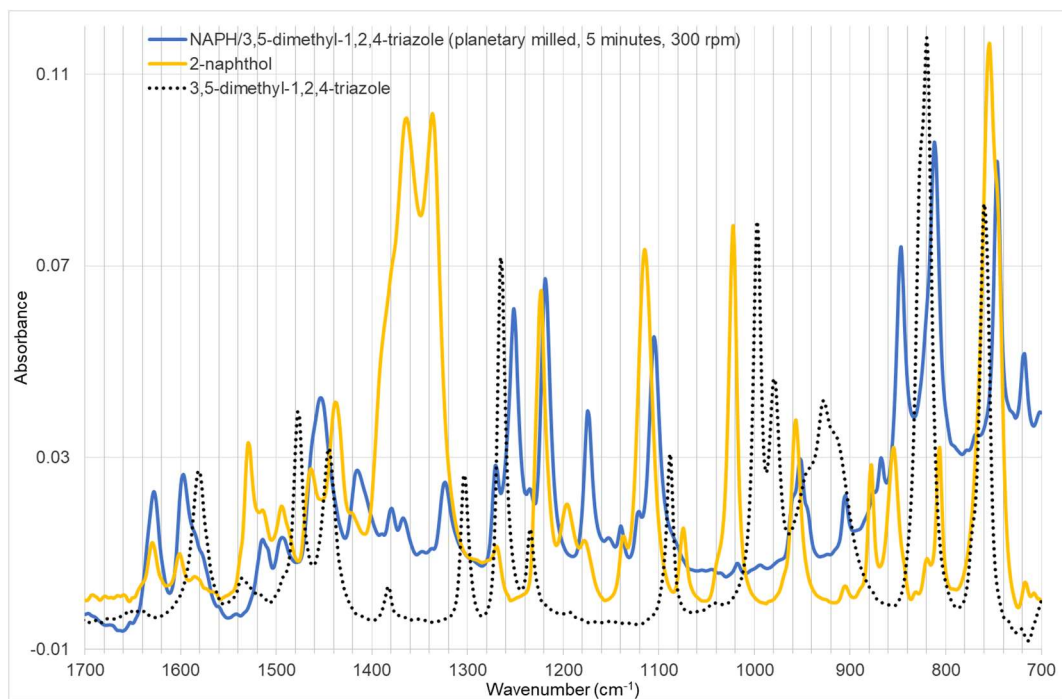


Figure B.98 – Infrared spectra of 2-naphthol/3,5-dimethyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

Table B.8 - Infrared spectra peak positions and heights of 2-naphthol/3,5-dimethyl-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm, with a 1:1 stoichiometry.

Peak Position (cm ⁻¹)	Peak Height (Absorbance)	Peak Position (cm ⁻¹)	Peak Height (Absorbance)
2769.14	0.01	1241.63	0.03
2764.09	0.01	1218.64	0.05
2758.97	0.01	1176.13	0.02
2700.52	0.01	1119.32	0.01
2661.94	0.01	1063.34	0.04
2604.43	0.01	1043.24	0.03
2552.35	0.01	1018.01	0.01
1629.64	0.03	960.14	0.02
1601.01	0.02	937.66	0.01
1589.25	0.02	906.06	0.02
1512.17	0.03	872.04	0.02
1457.43	0.02	852.05	0.08
1431.12	0.01	817.99	0.04
1409.91	0.03	796.78	0.03
1400.15	0.03	749.1	0.09
1381.64	0.02	729.07	0.02
1366.81	0.01	718.16	0.03
1305.91	0.05	702.62	0.02
1275.71	0.01		

B.55 2-naphthol/3,5-dibromo-1,2,4-triazole

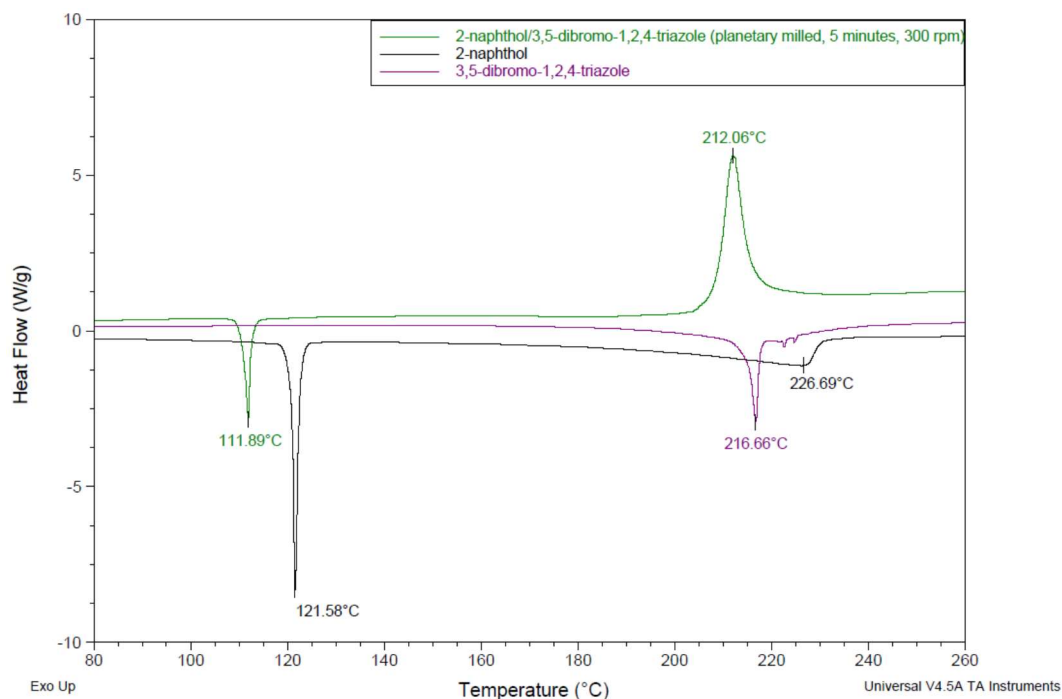


Figure B.99 - Thermal analysis of 2-naphthol/3,5-dibromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

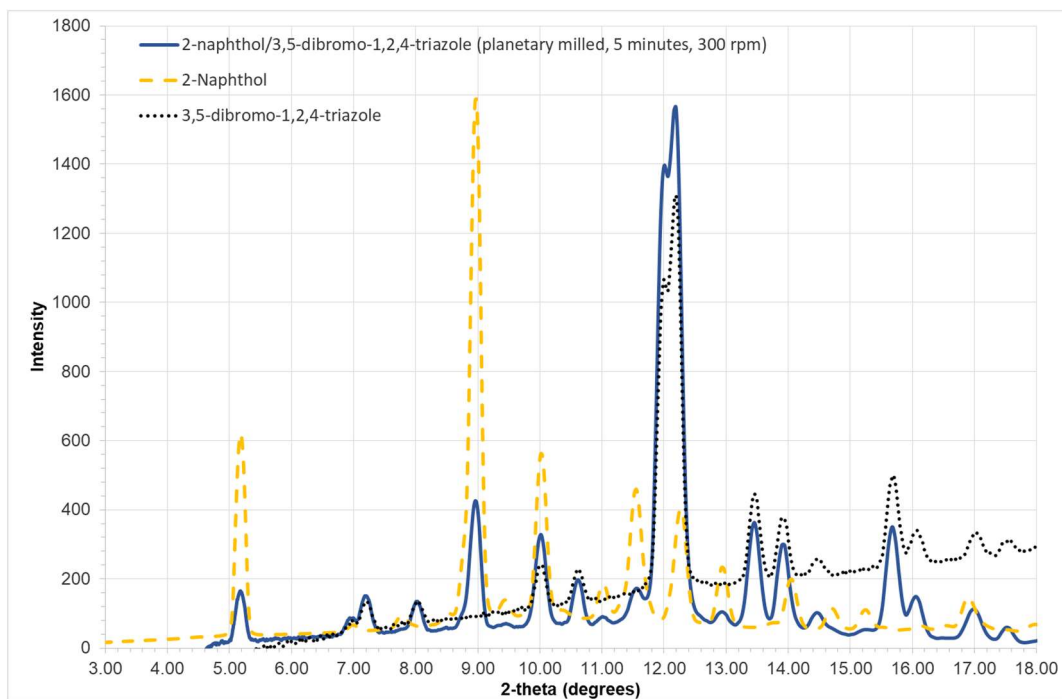


Figure B.100 – Powder x-ray analysis of 2-naphthol/3,5-dibromo-1,2,4-triazole produced by planetary milling for 5 minutes at 300 rpm.

B.56 2-naphthol/1,2,3,4-tetrazole

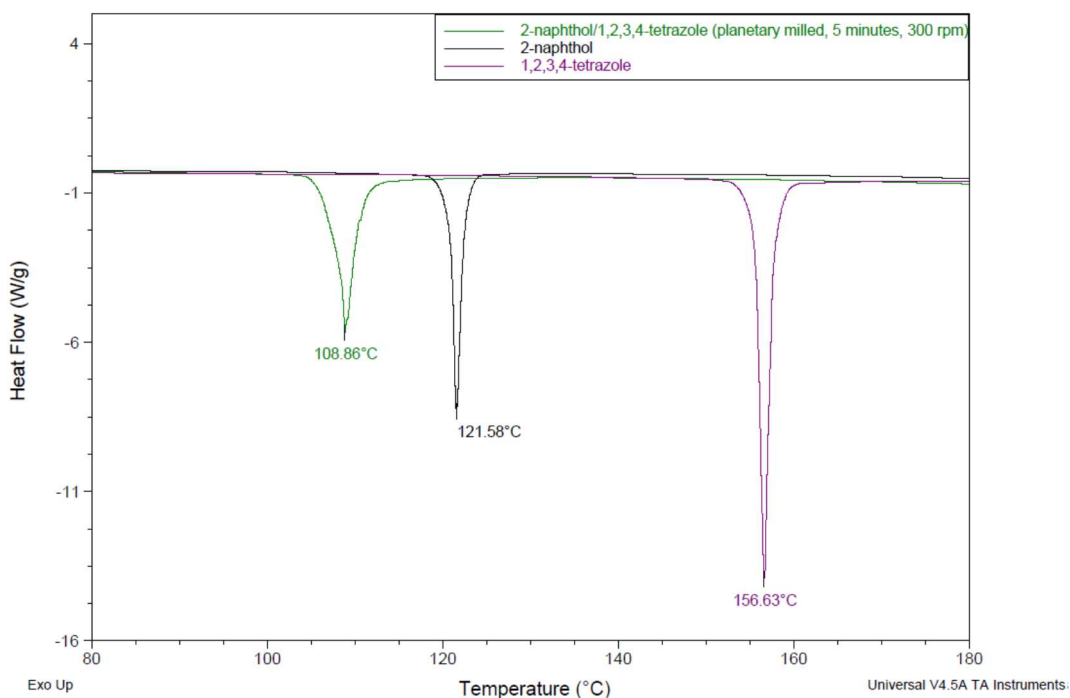


Figure B.101 - Thermal analysis of 2-naphthol/1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

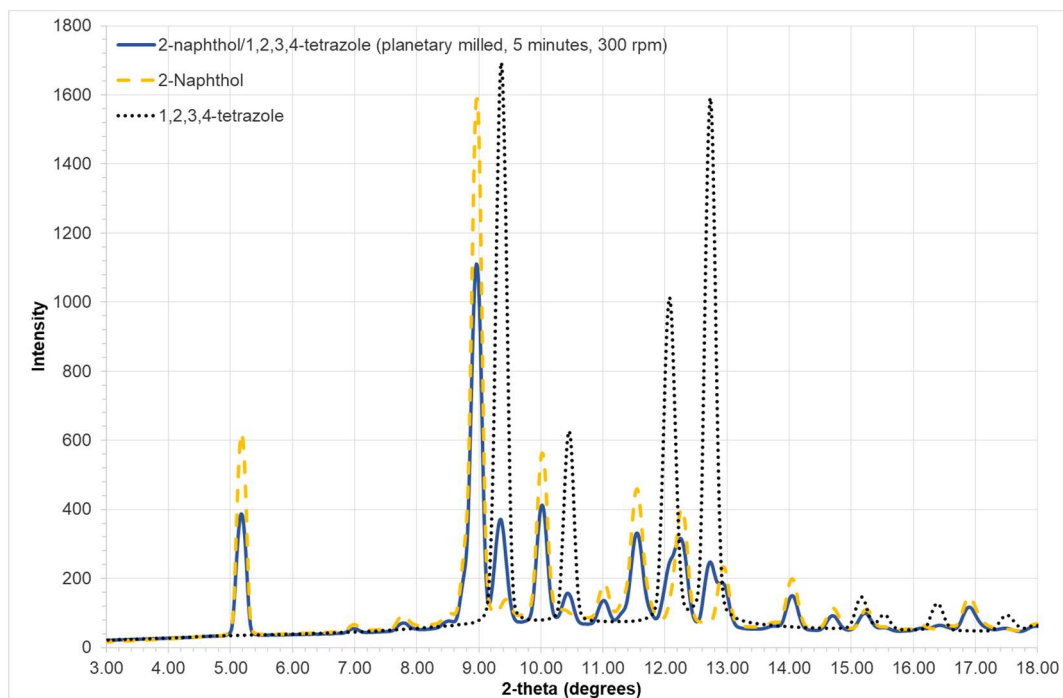


Figure B.102 – Powder x-ray pattern of 2-naphthol/1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

B.57 2-naphthol/1,2,3,4-tetrazol-5-amine

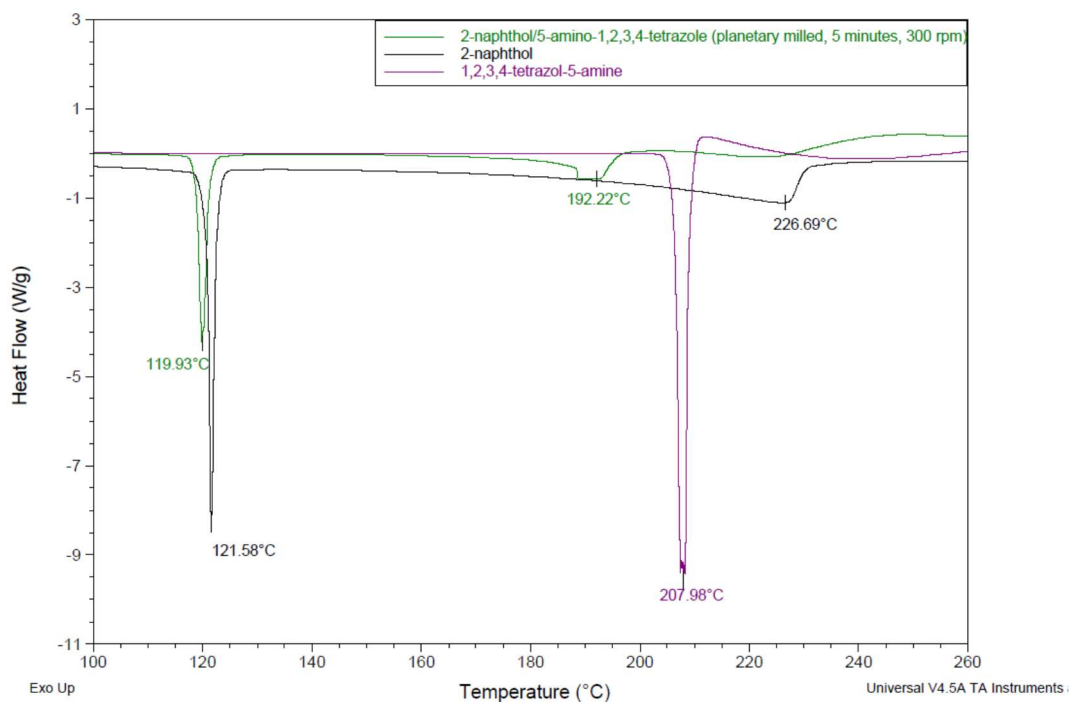


Figure B.103 - Thermal analysis of 2-naphthol/1,2,3,4-tetrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

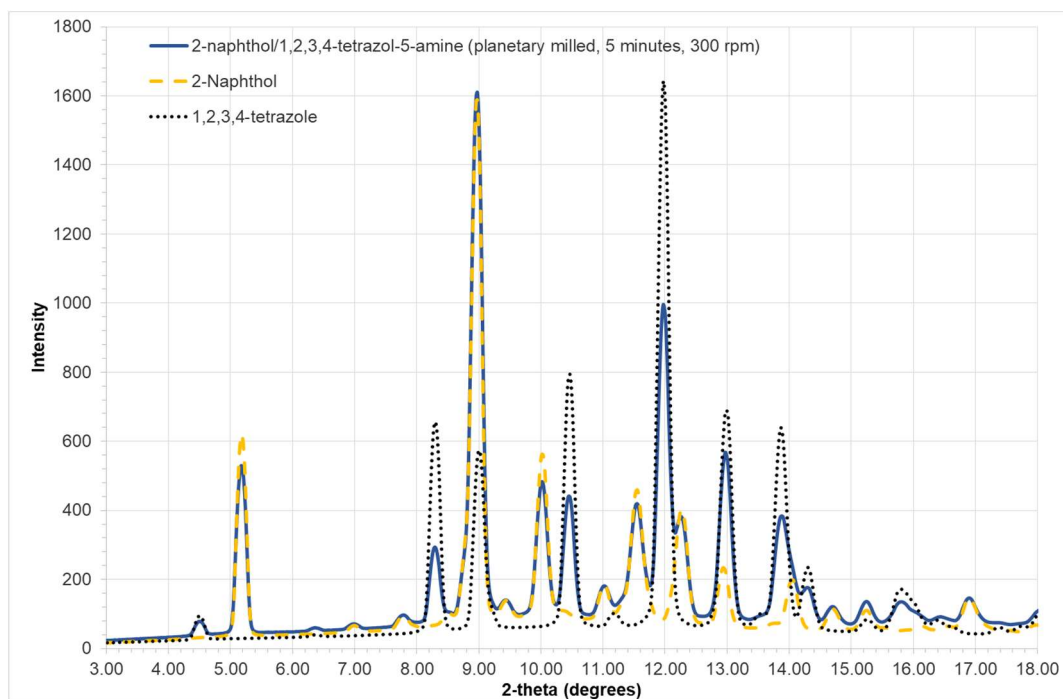


Figure B.104 – Powder x-ray pattern of 2-naphthol/1,2,3,4-tetrazol-5-amine produced by planetary milling for 5 minutes at 300 rpm.

B.58 2-naphthol/5-methyl-1,2,3,4-tetrazole

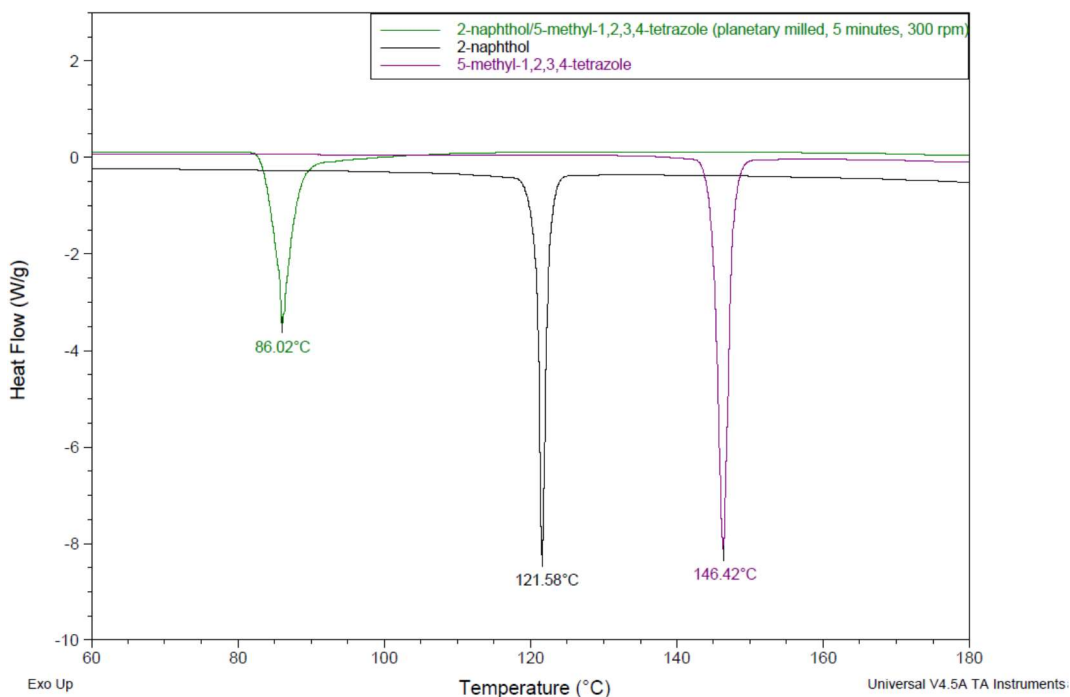


Figure B.105 - Thermal analysis of 2-naphthol/5-methyl-1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

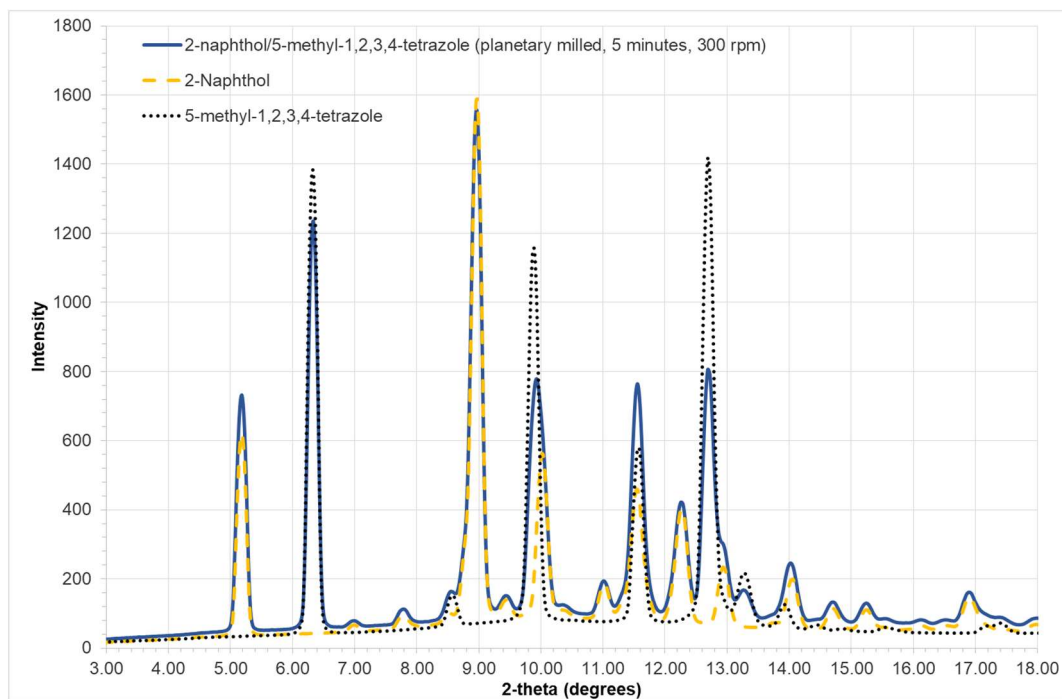


Figure B.106 – Powder x-ray pattern of 2-naphthol/5-methyl-1,2,3,4-tetrazole produced by planetary milling for 5 minutes at 300 rpm.

B.59 2-naphthol/3-nitro-1,2,4-triazol-5-one

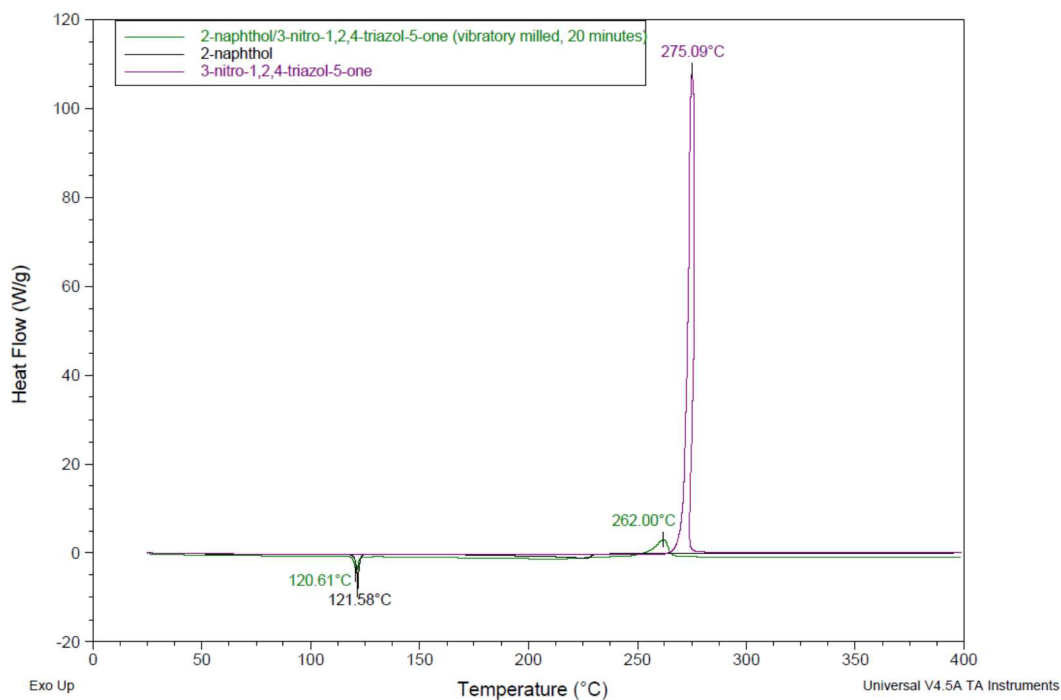


Figure B.107 - Thermal analysis of 2-naphthol/3-nitro-1,2,4-triazol-5-one produced by planetary milling for 5 minutes at 300 rpm.

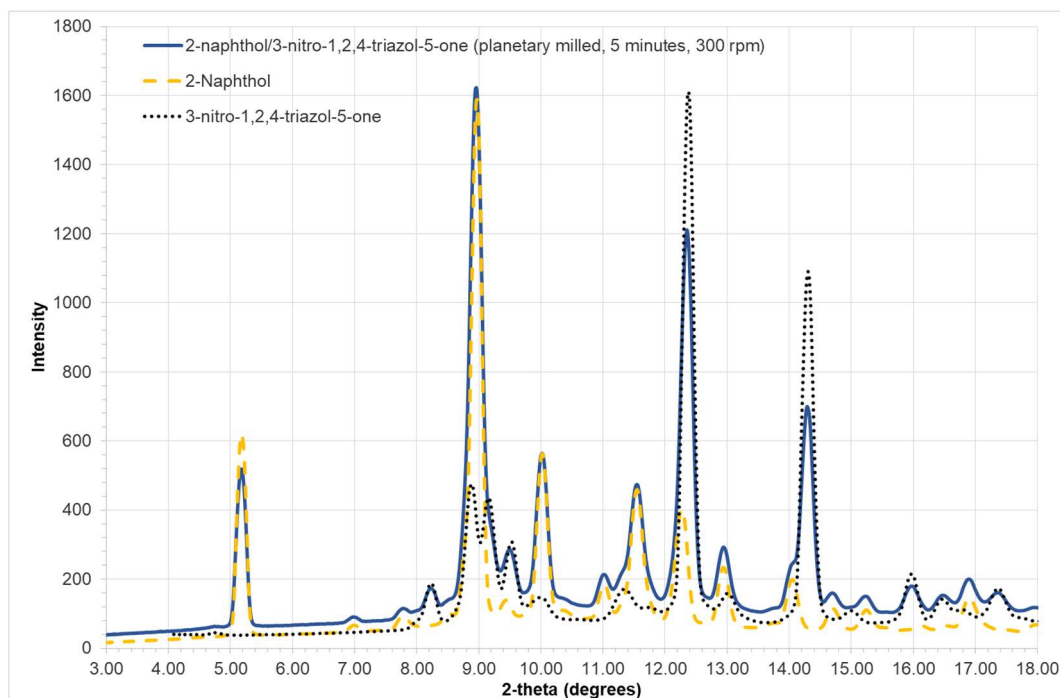


Figure B.108 – Powder x-ray analysis of 2-naphthol/3-nitro-1,2,4-triazol-5-one produced by planetary milling for 5 minutes at 300 rpm.

B.60 Molecular Electrostatic Potentials

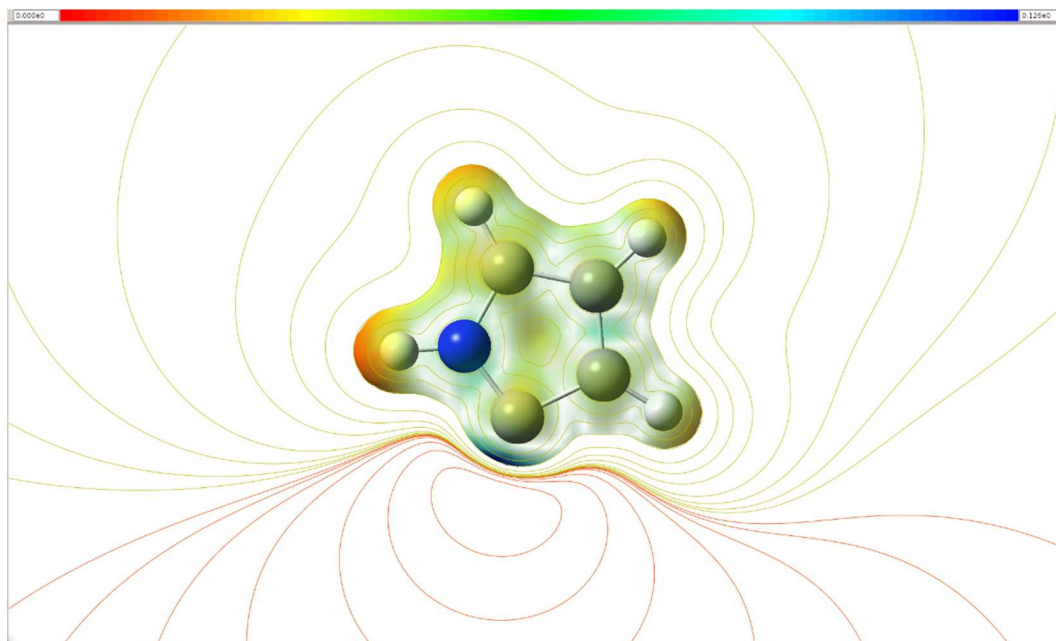


Figure B.109 - Molecular electrostatic potential map of pyrrolidine.

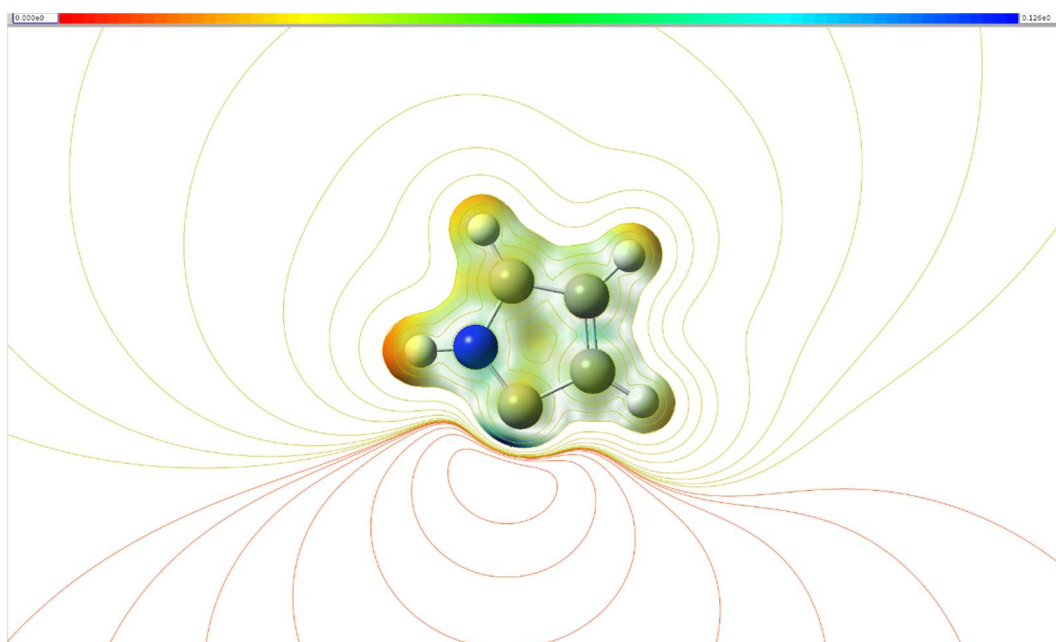


Figure B.110 - Molecular electrostatic potential map of 3-pyrroline.

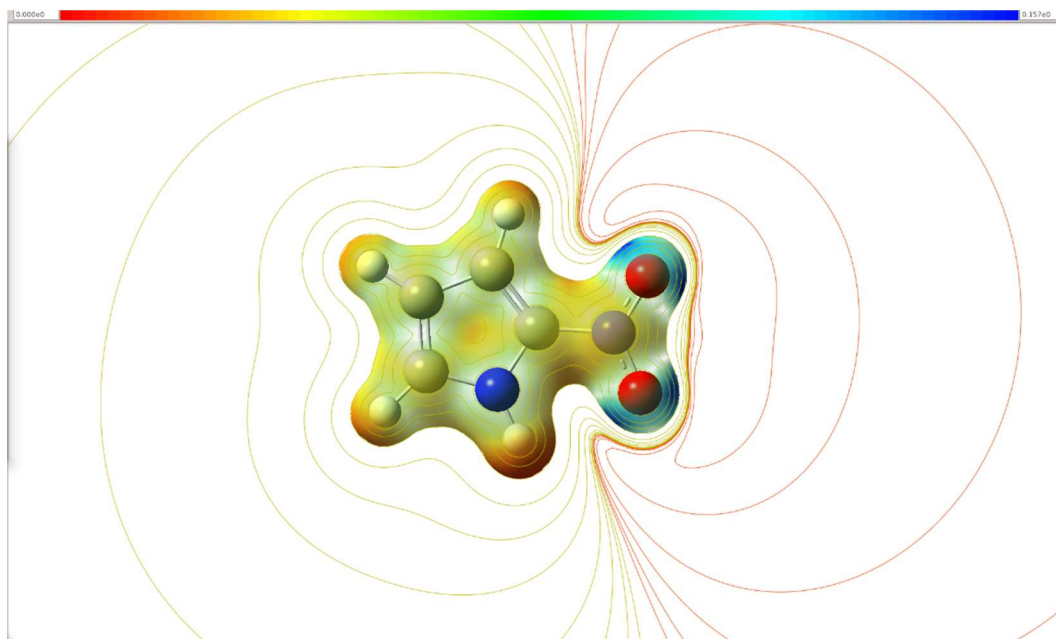


Figure B.111 - Molecular electrostatic potential map of 2-nitropyrrole.

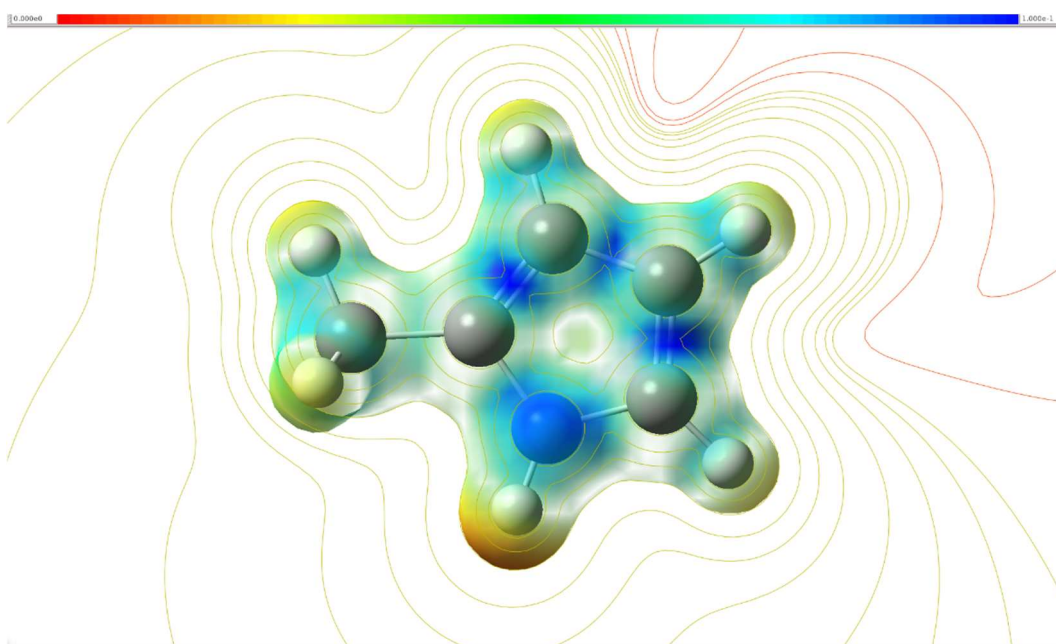


Figure B.112 - Molecular electrostatic potential map of 2-methylpyrrole.

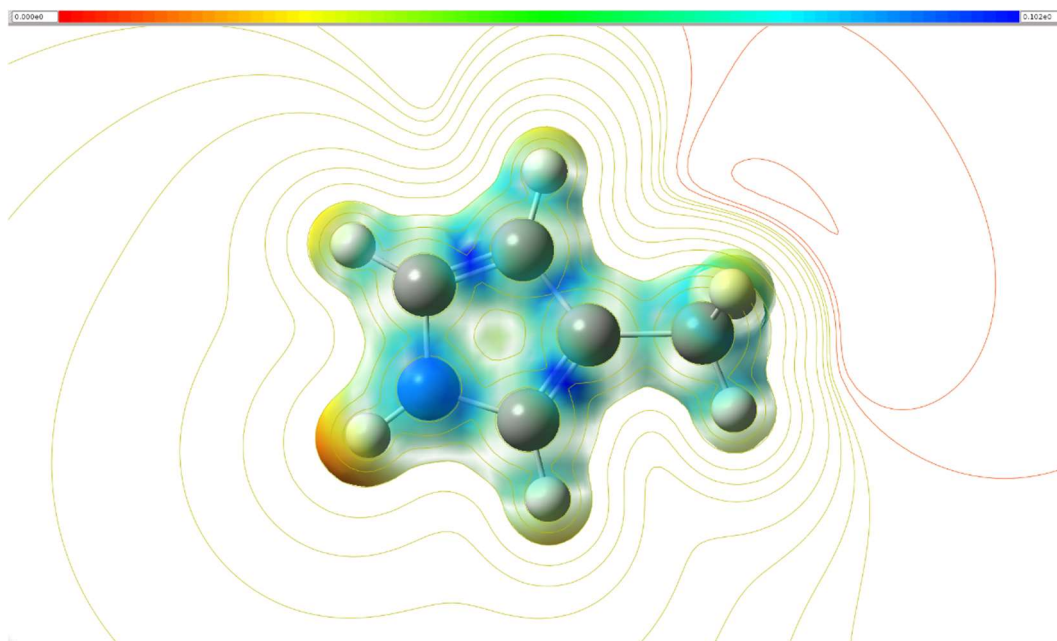


Figure B.113 - Molecular electrostatic potential map of 3-methylpyrrole.

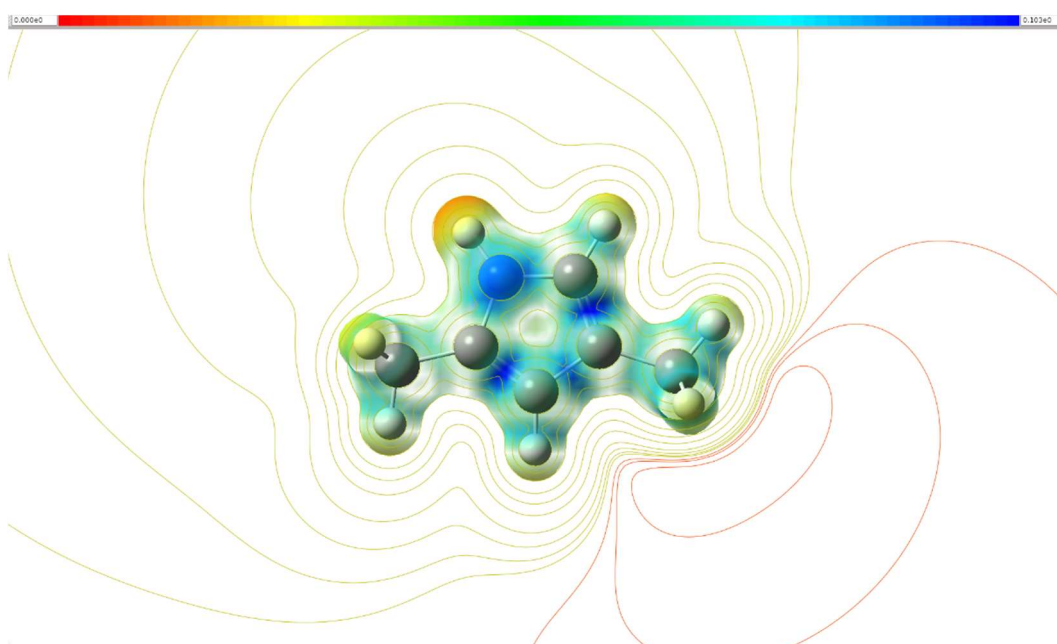


Figure B.114 - Molecular electrostatic potential map of 2,4-dimethylpyrrole.

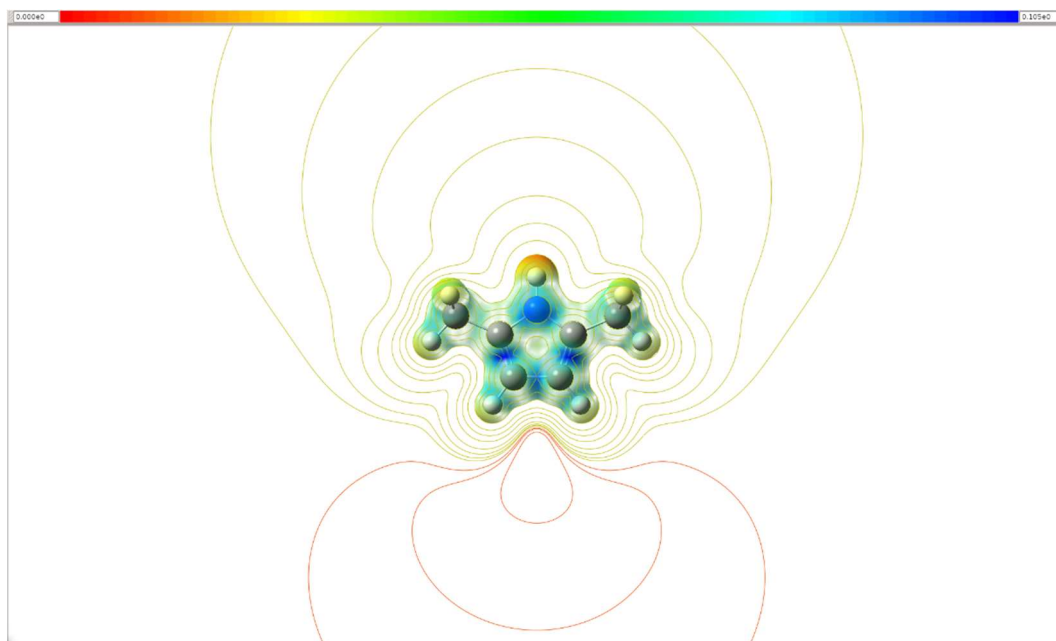


Figure B.115 - Molecular electrostatic potential map of 2,5-dimethylpyrrole.

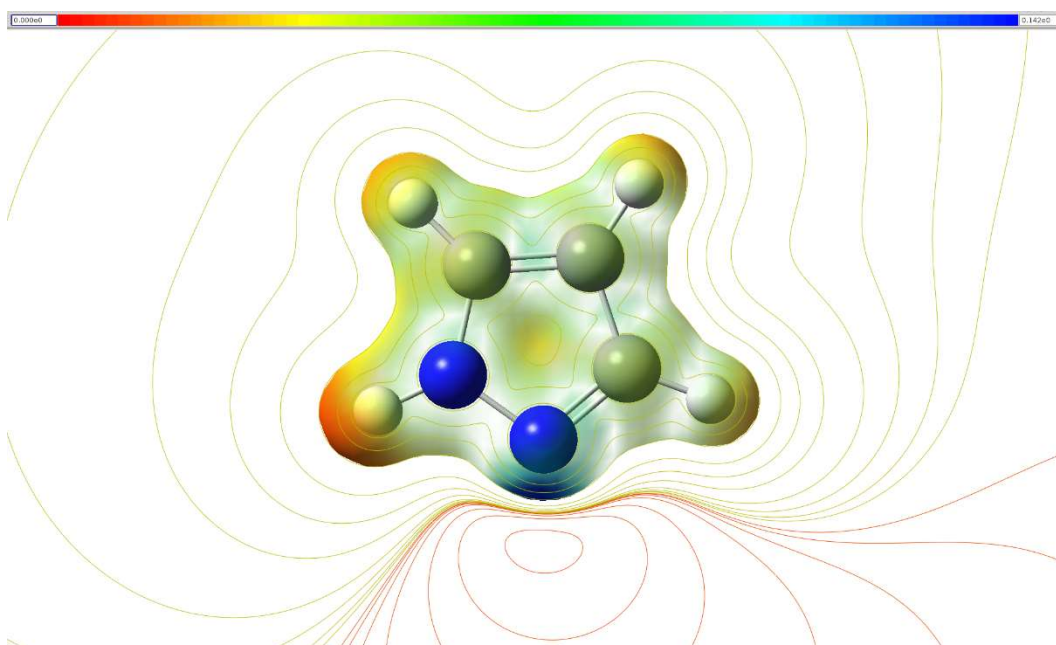


Figure B.116 - Molecular electrostatic potential map of pyrazole.

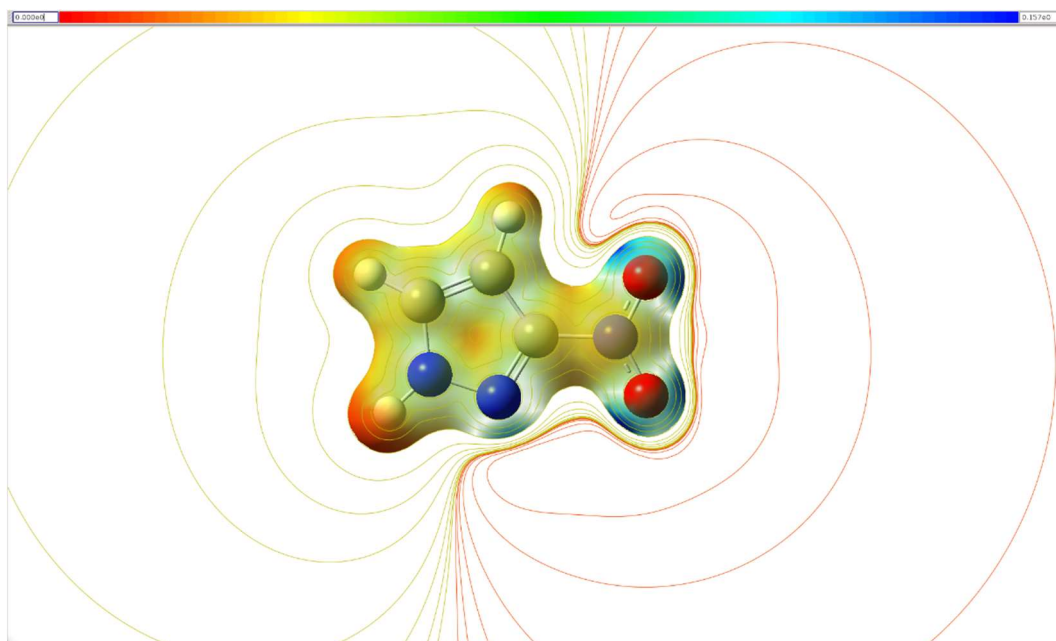


Figure B.117 - Molecular electrostatic potential map of 3-nitropyrazole.

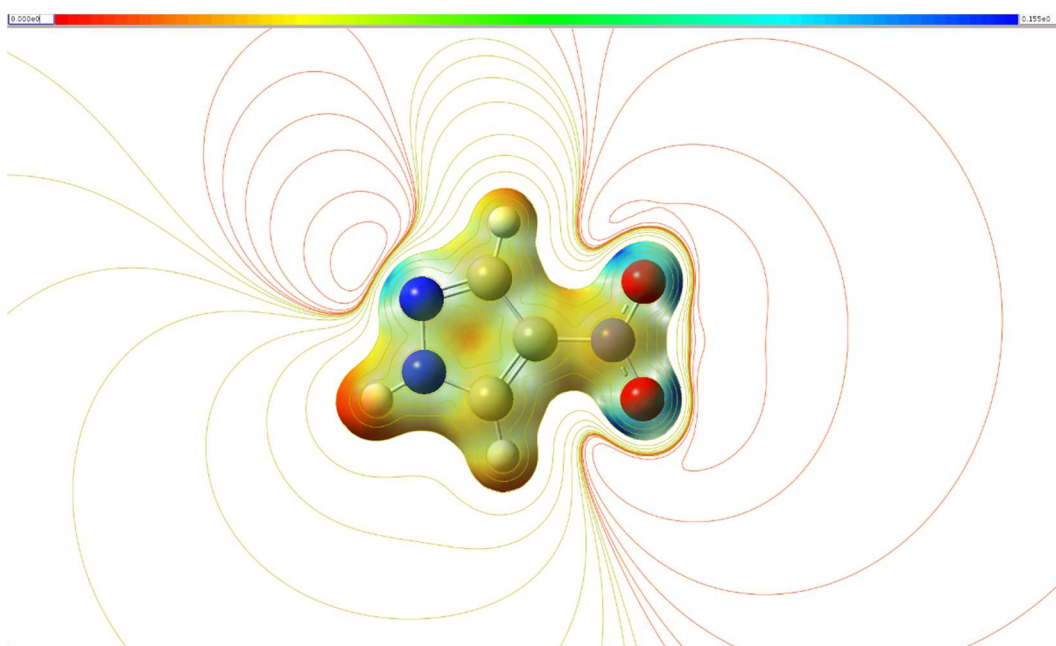


Figure B.118 - Molecular electrostatic potential map of 4-nitropyrazole.

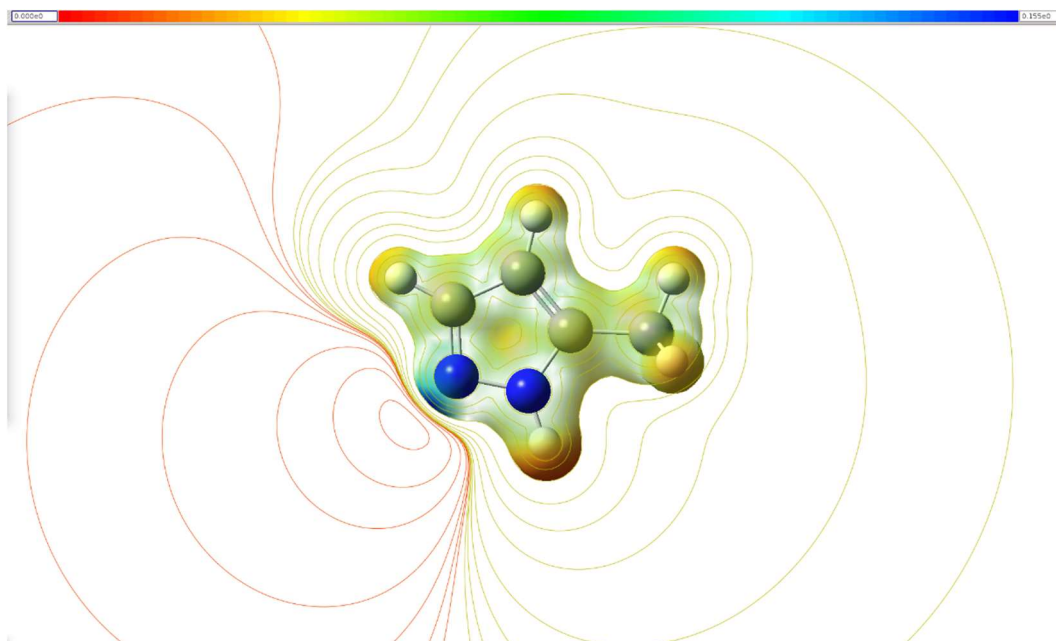


Figure B.119 - Molecular electrostatic potential map of 5-methylpyrazole.

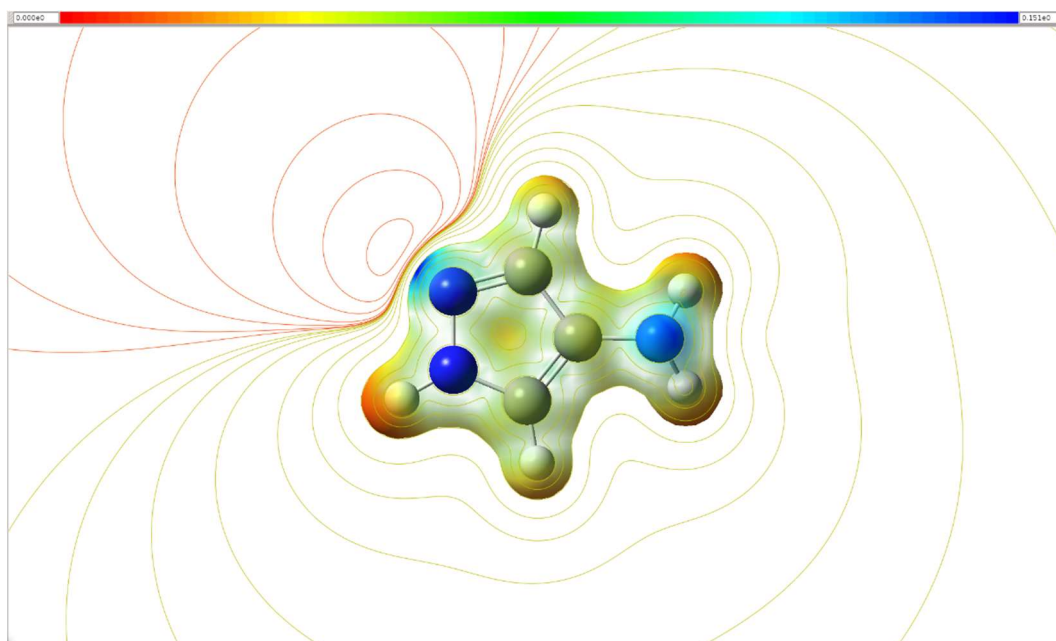


Figure B.120 - Molecular electrostatic potential map of pyrazol-4-amine.

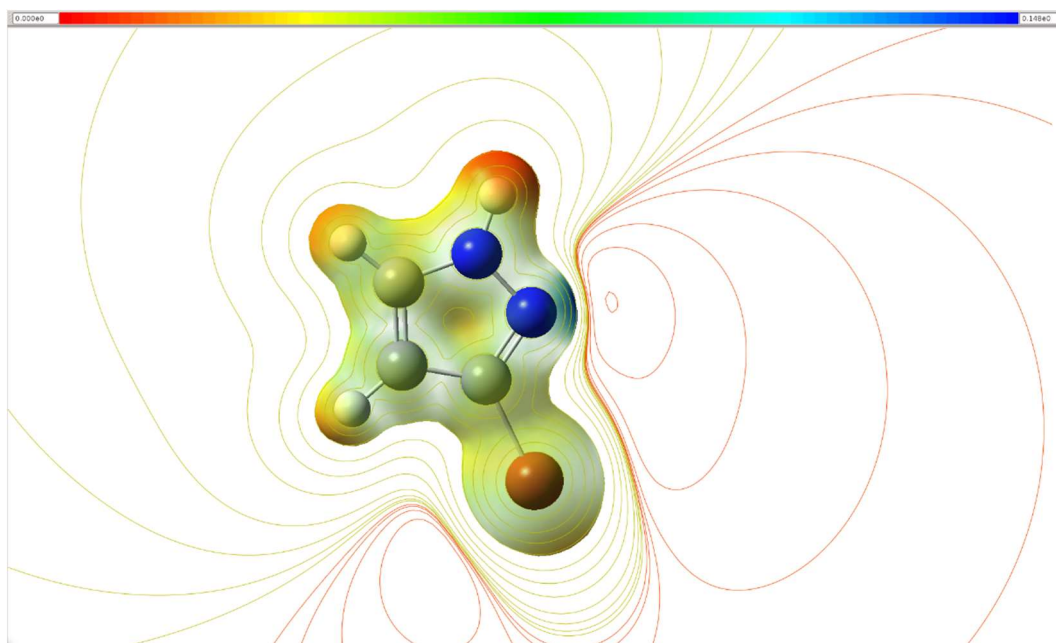


Figure B.121 - Molecular electrostatic potential map of 3-bromopyrazole.

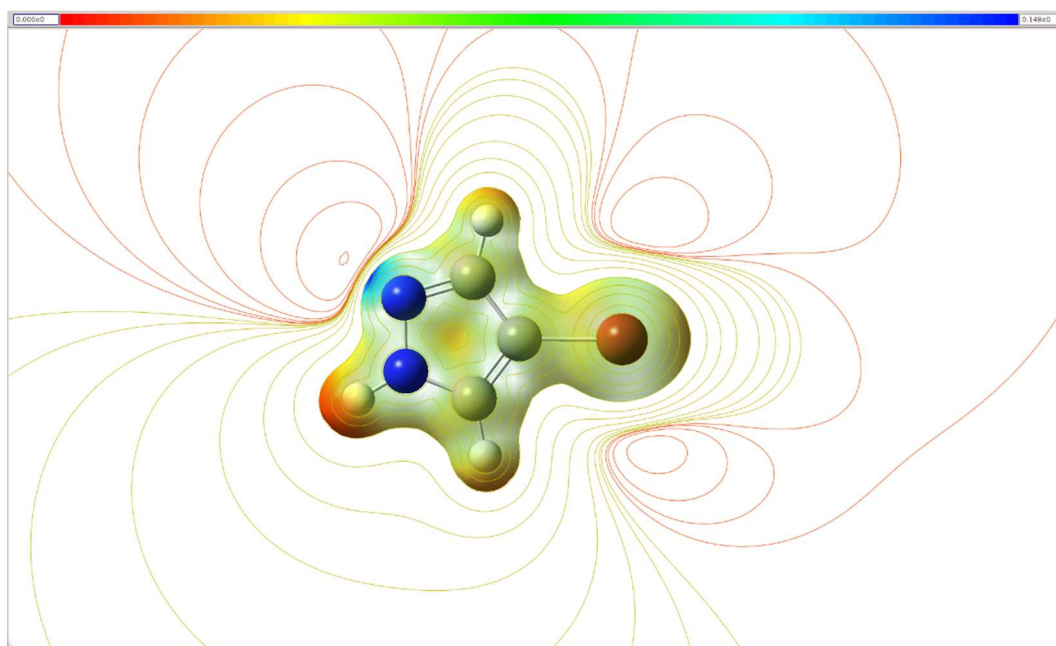


Figure B.122 - Molecular electrostatic potential map of 4-bromopyrazole.

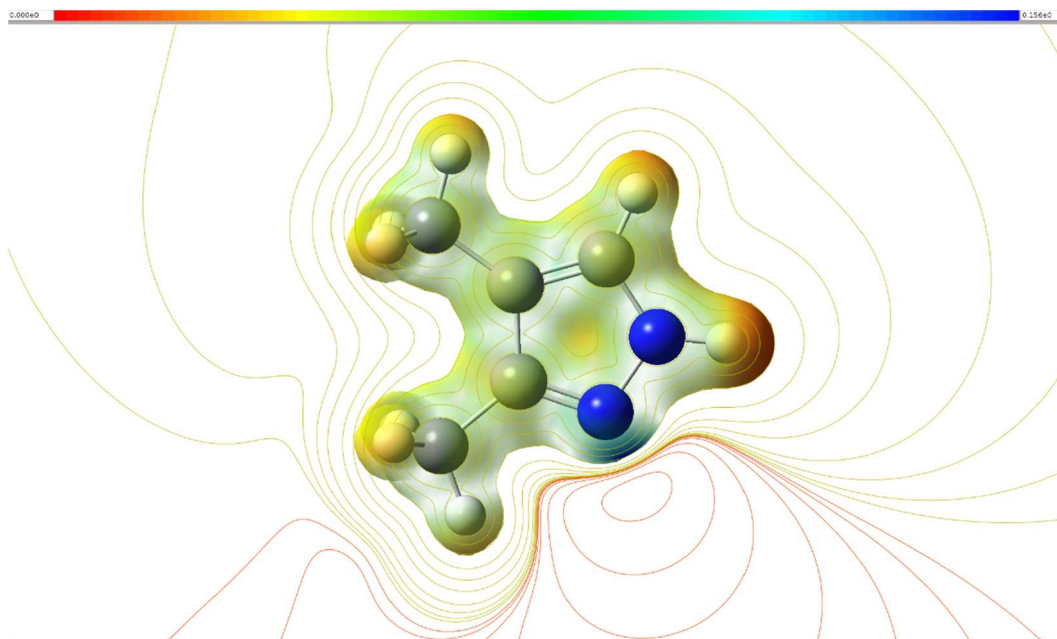


Figure B.123 - Molecular electrostatic potential map of 3,4-dimethylpyrazole.

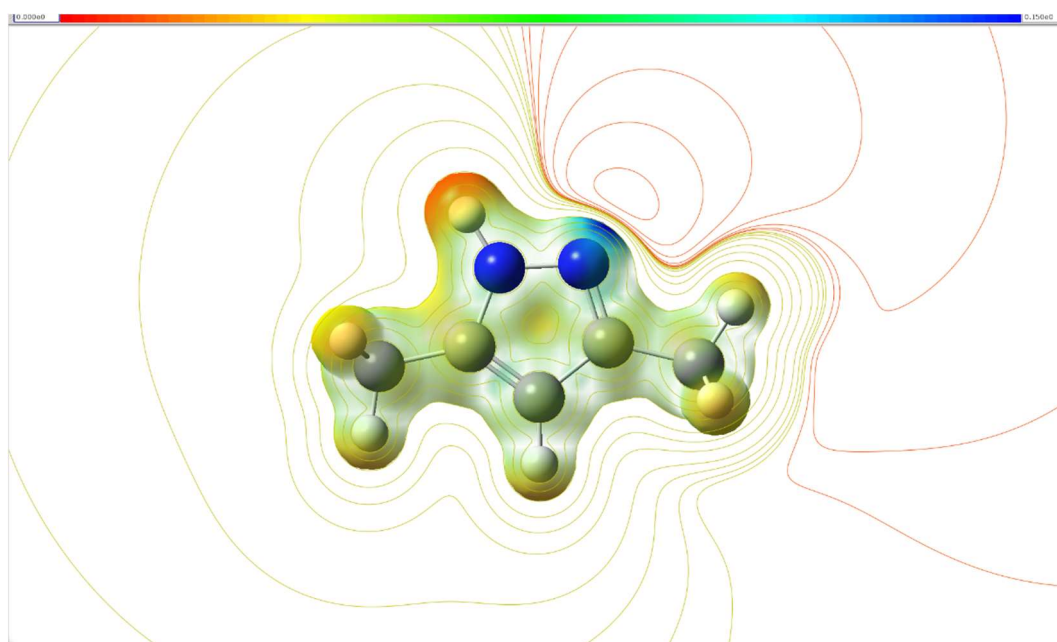


Figure B.124 - Molecular electrostatic potential map of 3,4-dimethylpyrazole.

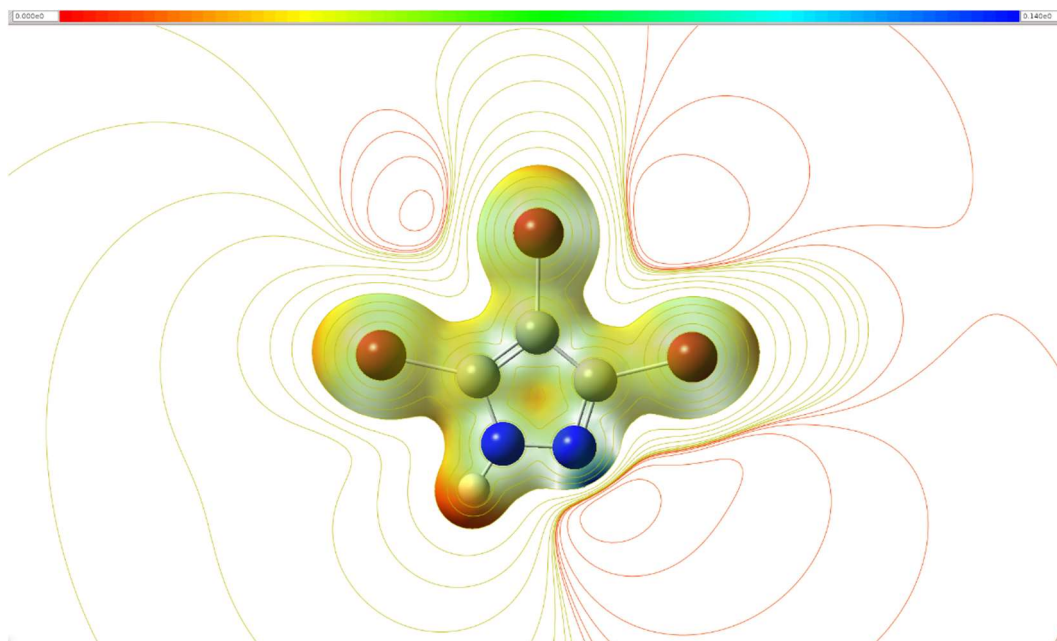


Figure B.125 - Molecular electrostatic potential map of 3,4,5-tribromopyrazole.

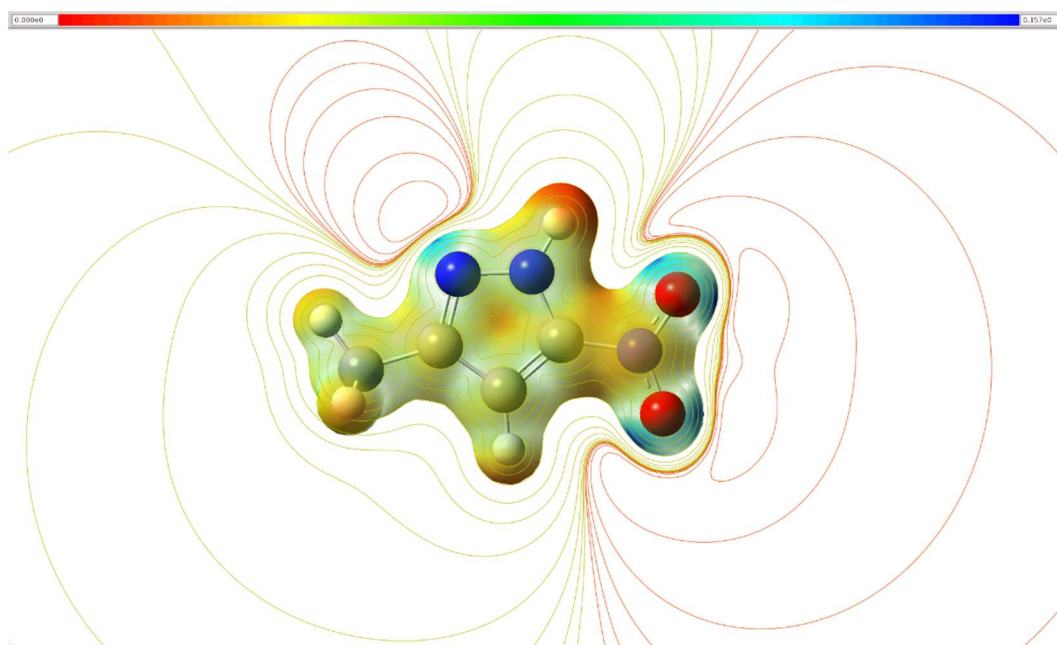


Figure B.126 - Molecular electrostatic potential map of 3-methyl-5-nitropyrazole.

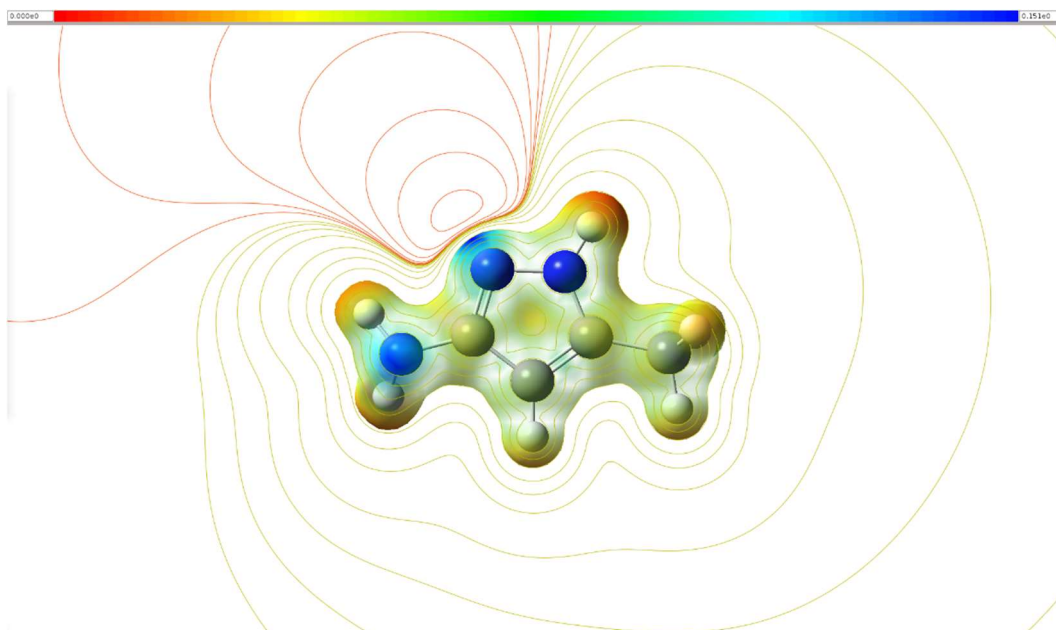


Figure B.127 - Molecular electrostatic potential map of 5-methylpyrazol-3-amine.

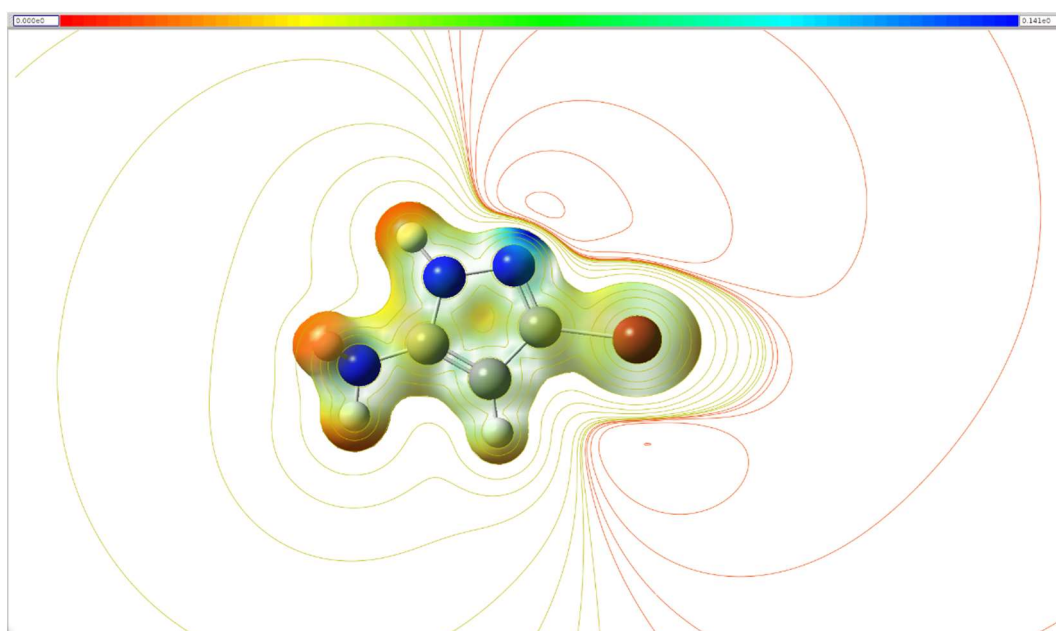


Figure B.128 - Molecular electrostatic potential map of 3-bromopyrazol-5-amine.

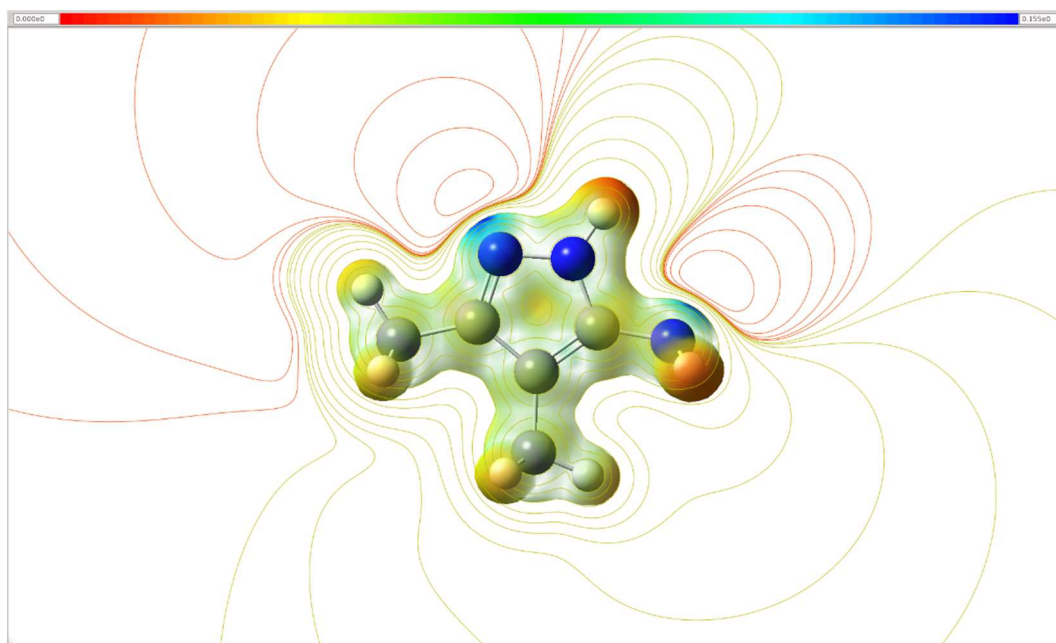


Figure B.129 - Molecular electrostatic potential map of 3,4-dimethylpyrazol-5-amine.

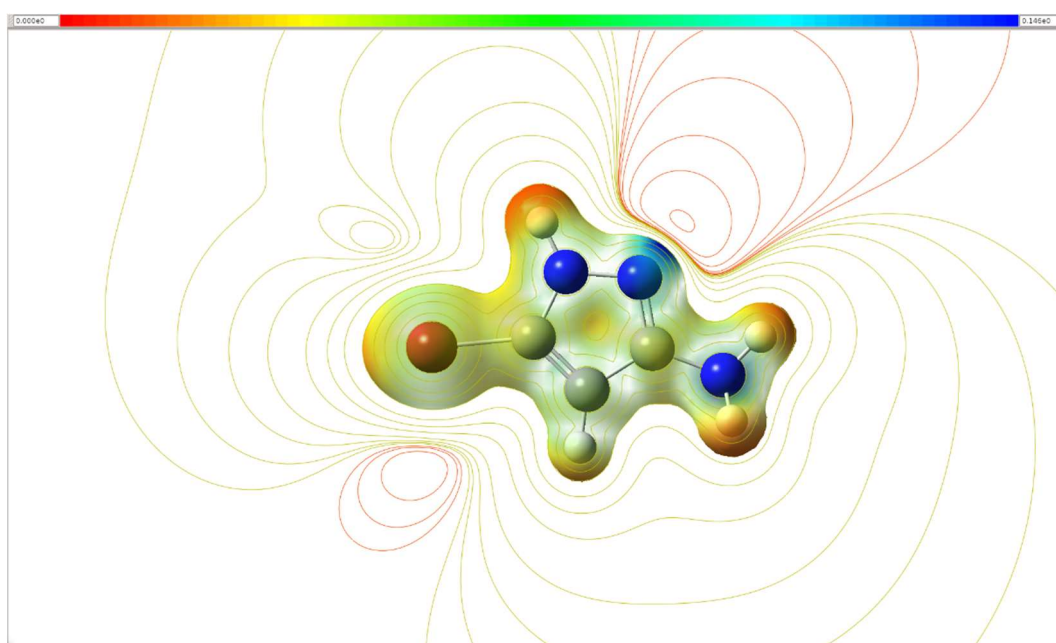


Figure B.130 - Molecular electrostatic potential map of 3-methyl-4-bromopyrazole.

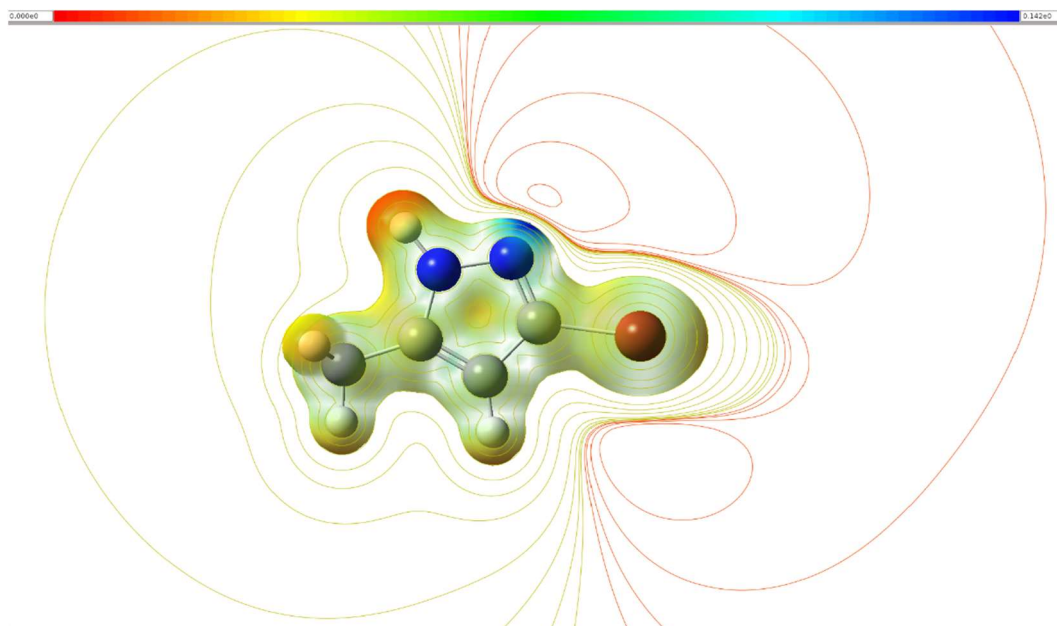


Figure B.131 - Molecular electrostatic potential map of 3-bromo-5-methylpyrazole.

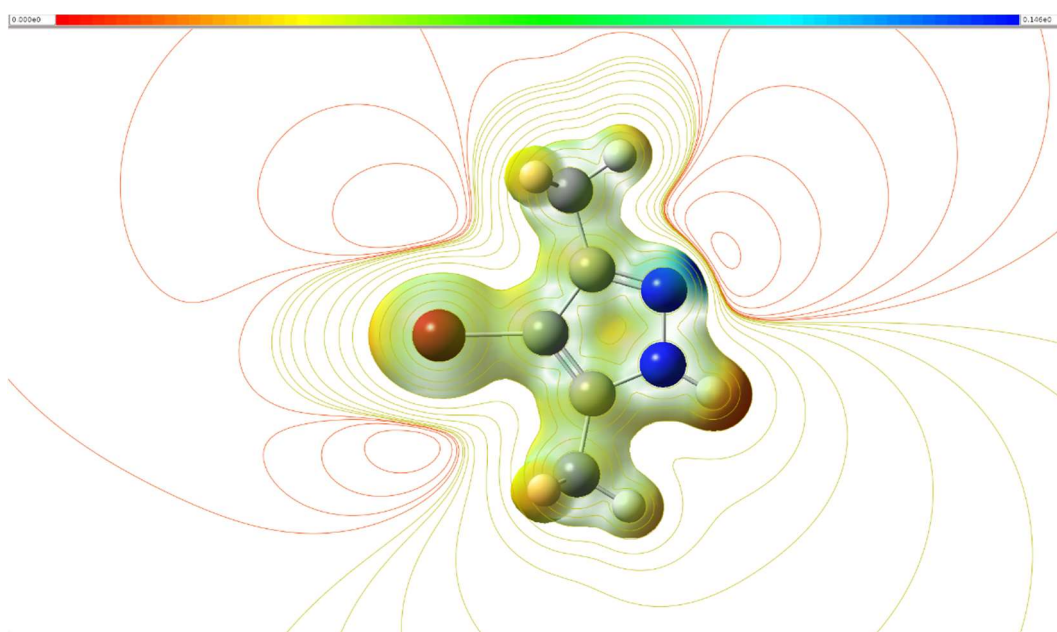


Figure B.132 - Molecular electrostatic potential map of 4-bromo-3,5-dimethylpyrazole.

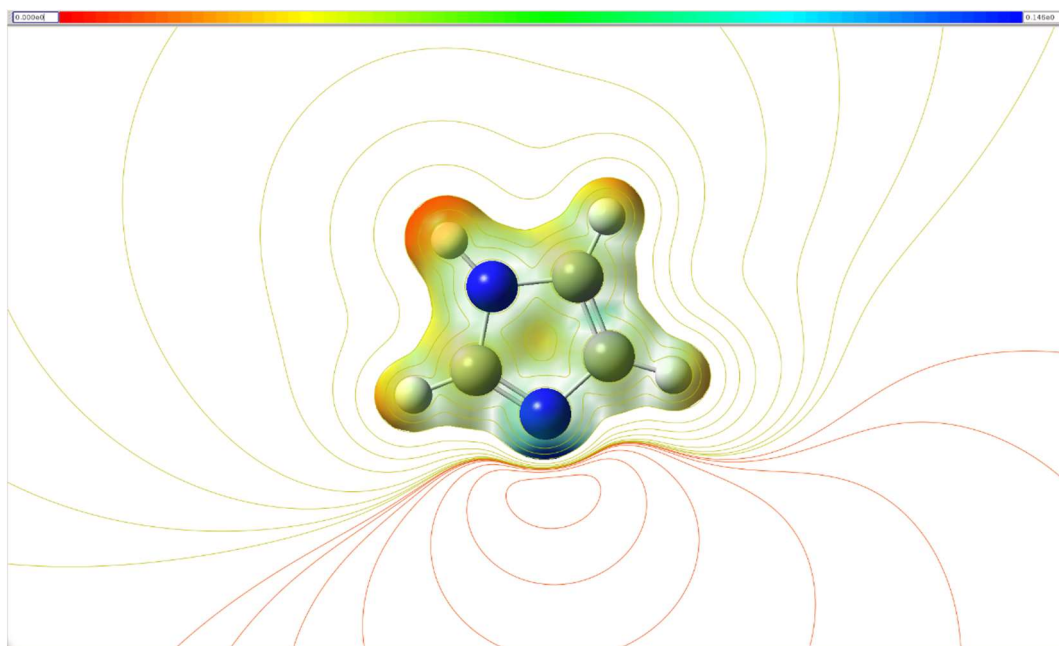


Figure B.133 - Molecular electrostatic potential map of imidazole.

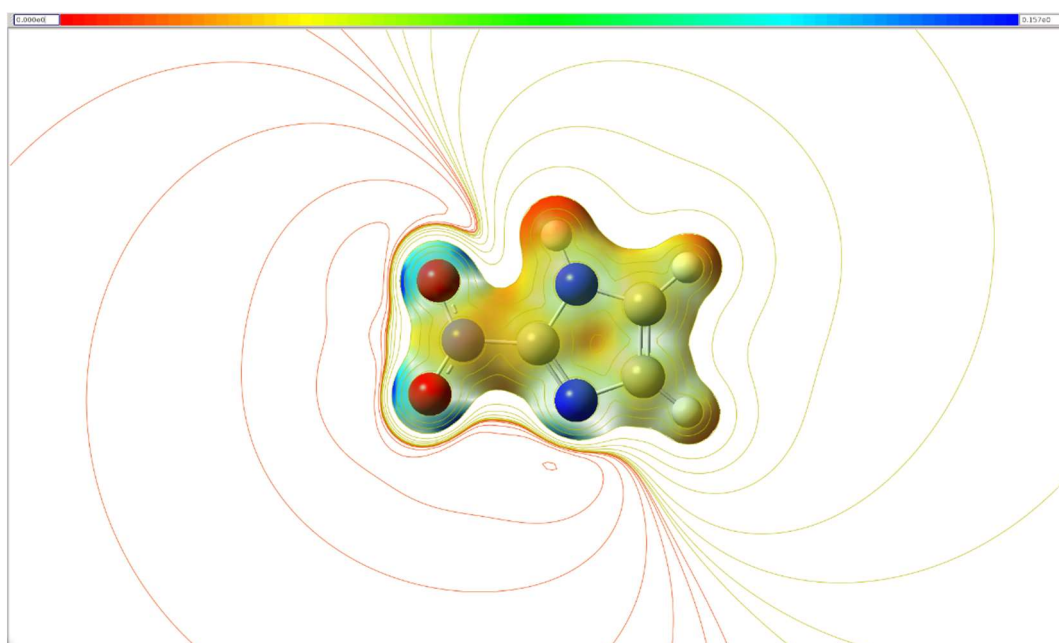


Figure B.134 - Molecular electrostatic potential map of 2-nitroimidazole.

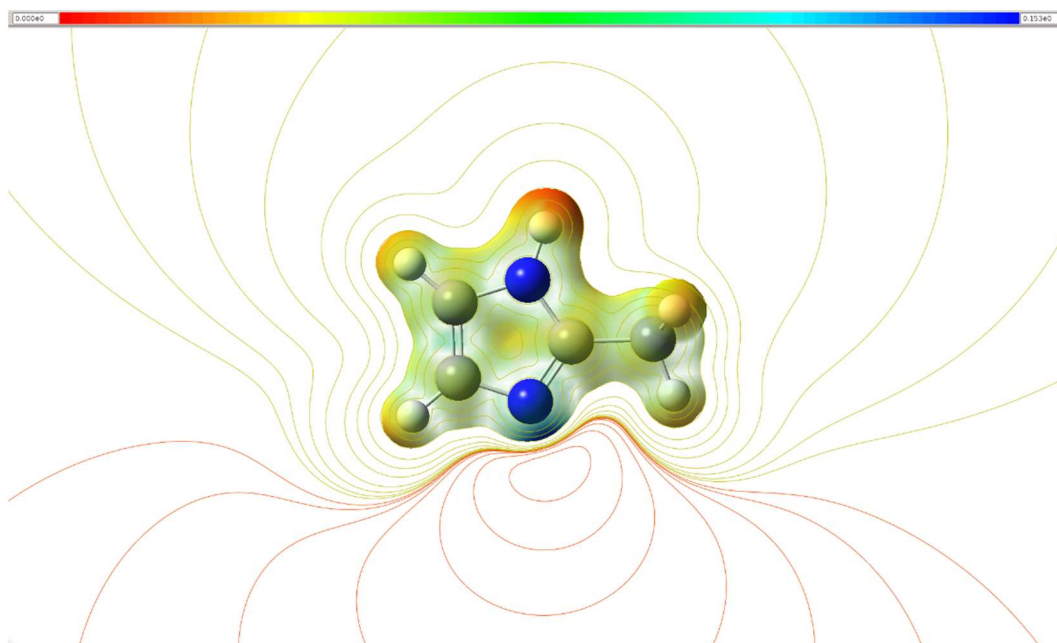


Figure B.135 - Molecular electrostatic potential map of 2-methylimidazole.

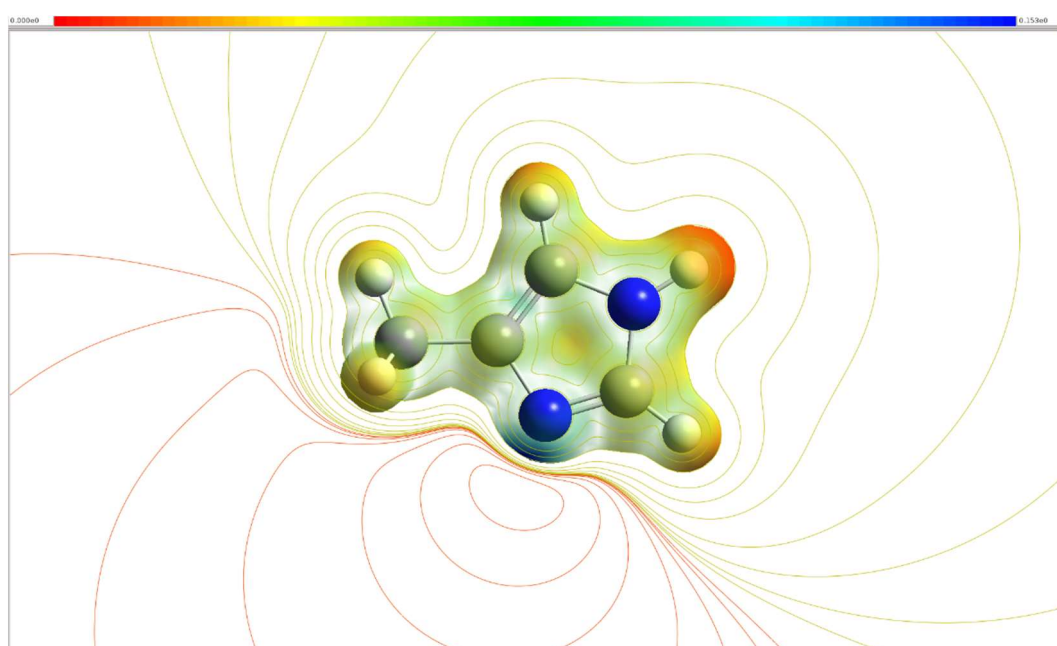


Figure B.136 - Molecular electrostatic potential map of 4-methylimidazole.

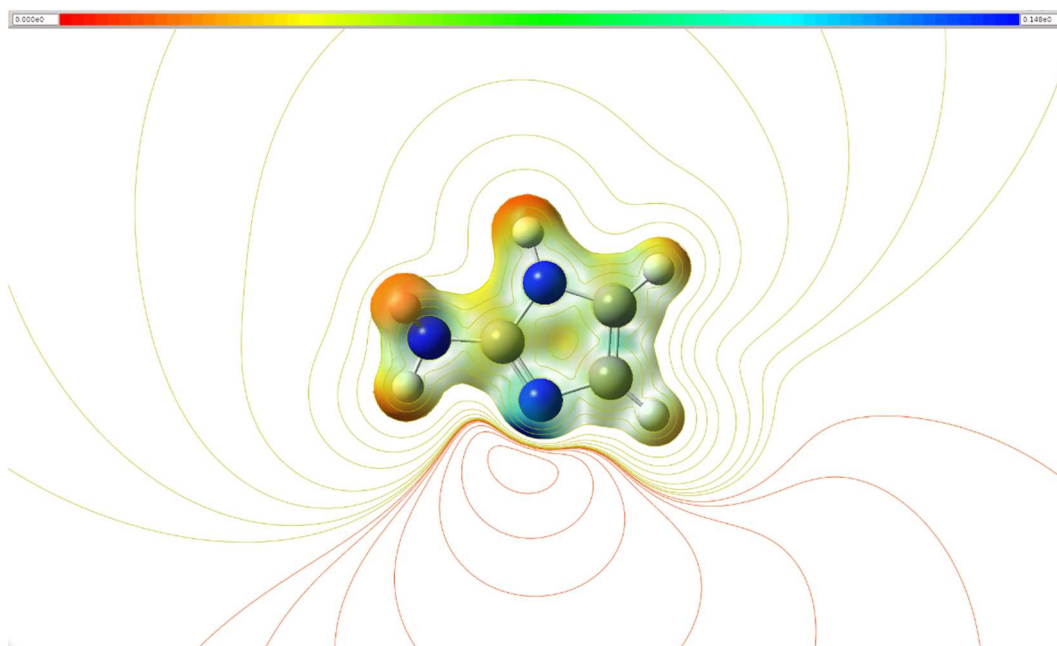


Figure B.137 - Molecular electrostatic potential map of imidazol-2-amine.

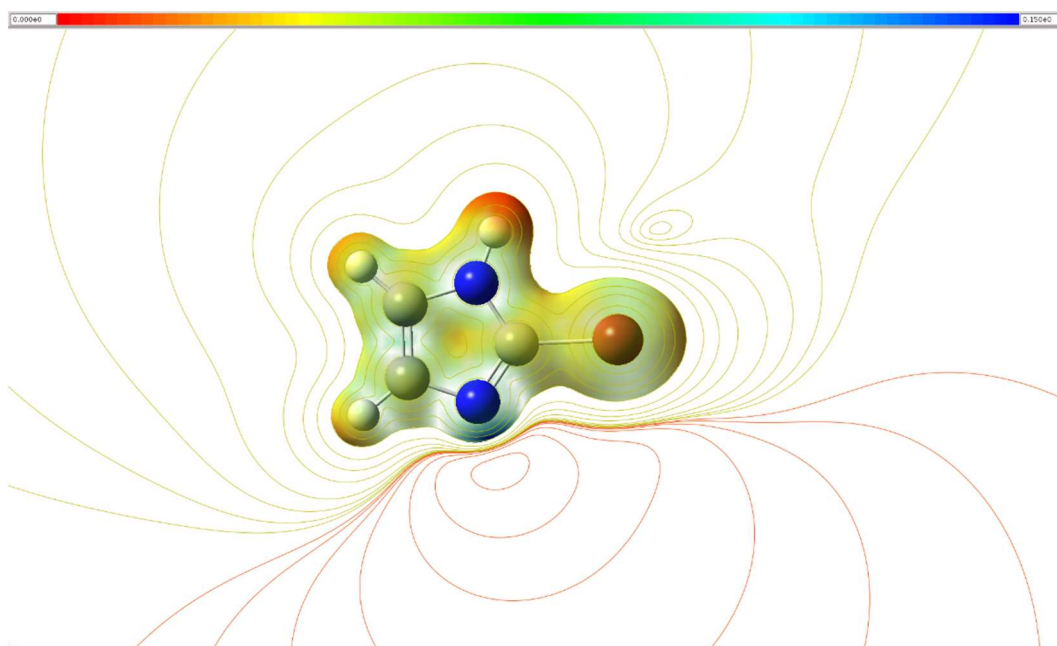


Figure B.138 - Molecular electrostatic potential map of 2-bromoimidazole.

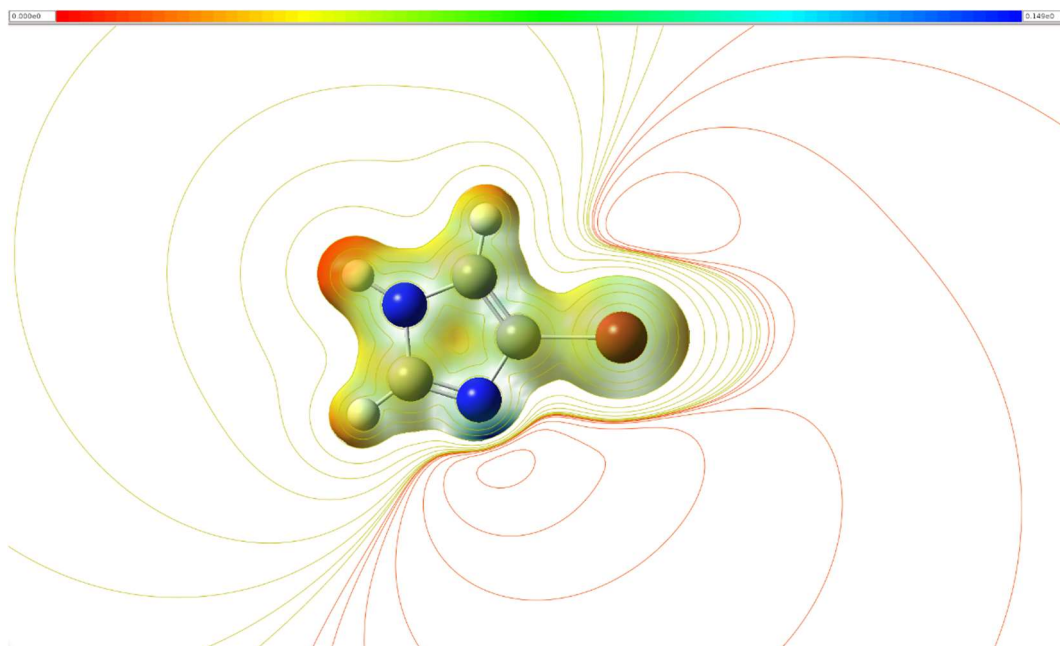


Figure B.139 - Molecular electrostatic potential map of 4-bromoimidazole.

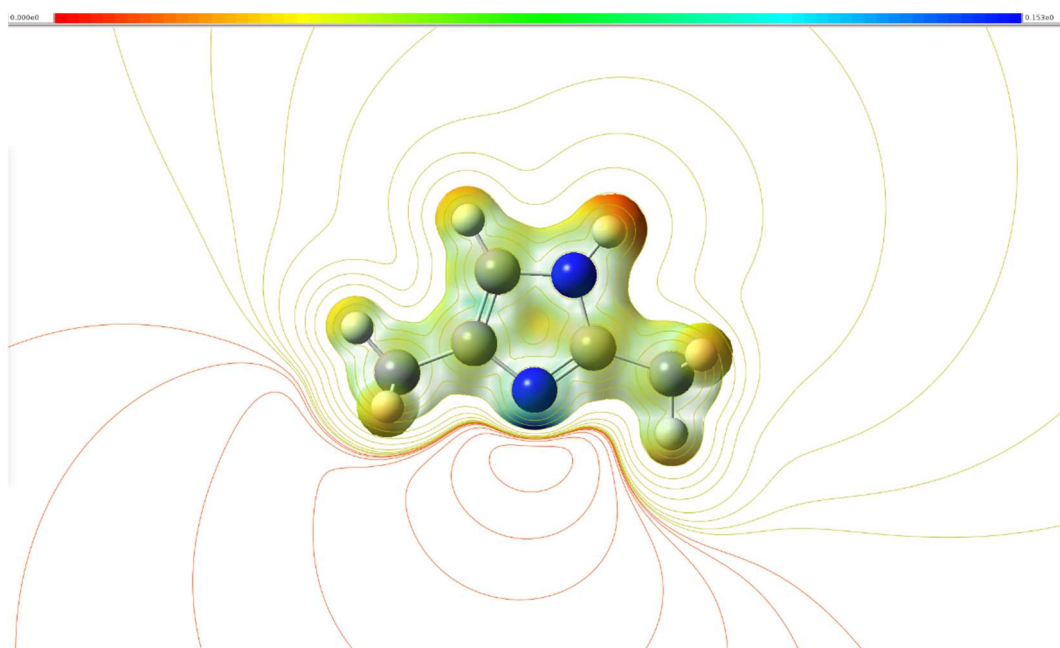


Figure B.140 - Molecular electrostatic potential map of 2,4-dimethylimidazole.

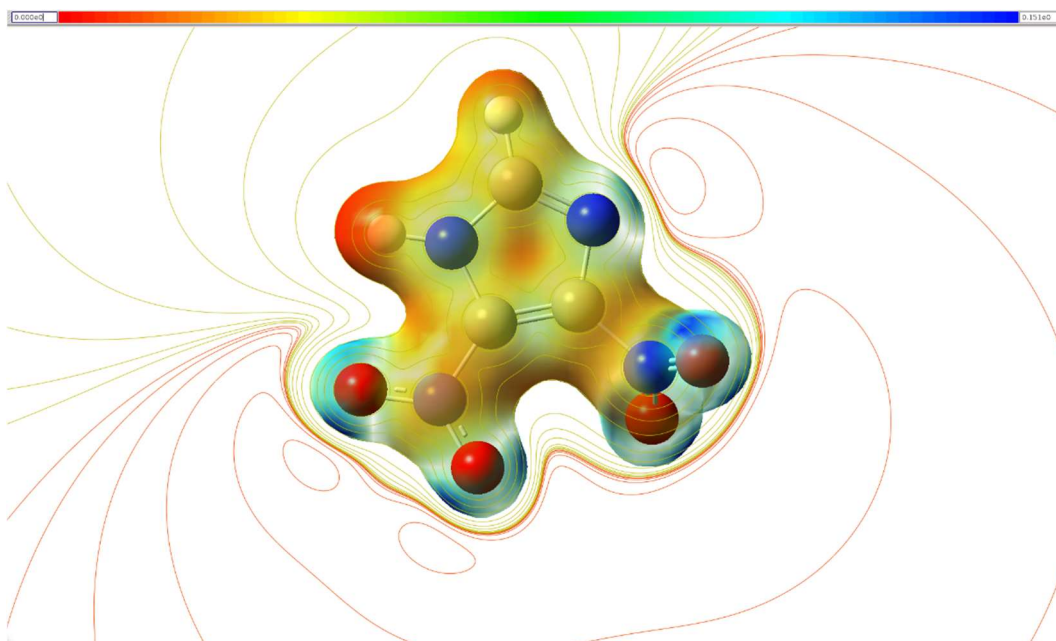


Figure B.141 - Molecular electrostatic potential map of 4,5-dinitroimidazole.

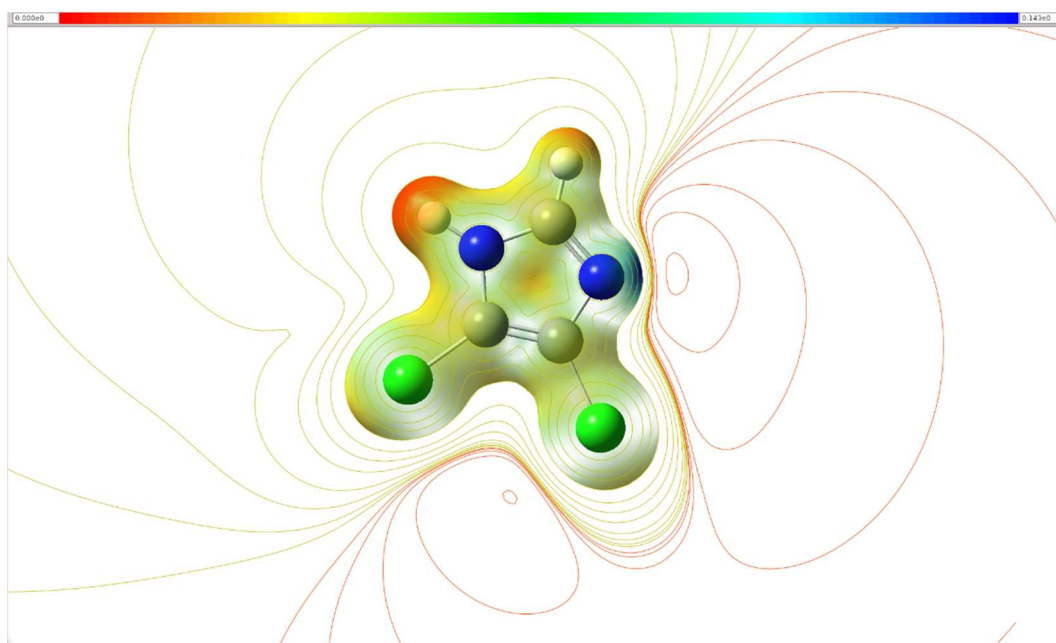


Figure B.142 - Molecular electrostatic potential map of 4,5-dichloroimidazole.

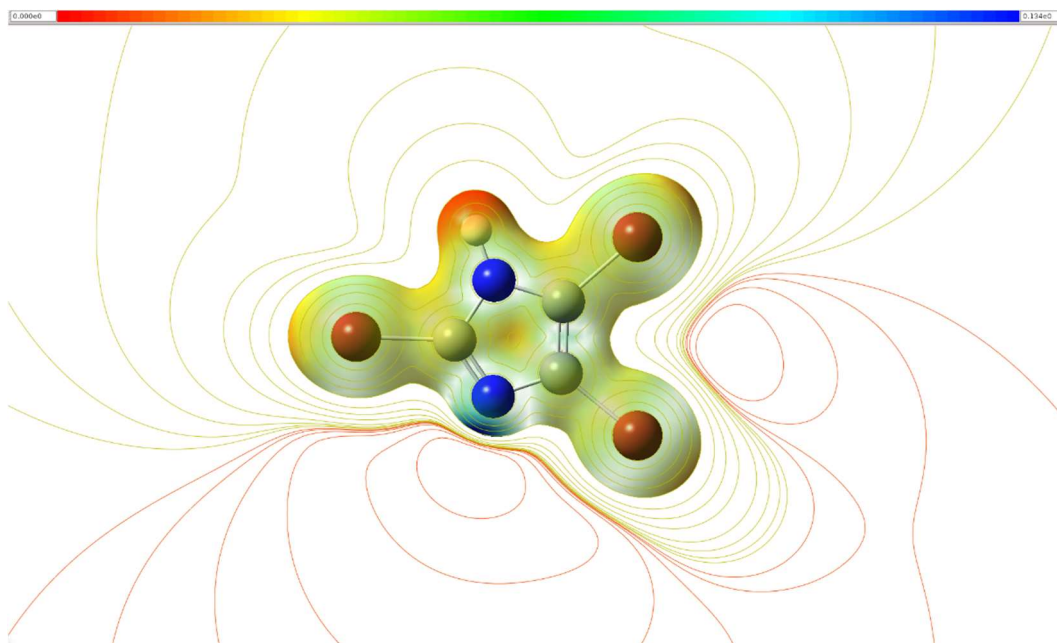


Figure B.143 - Molecular electrostatic potential map of 2,4,5-tribromoimidazole.

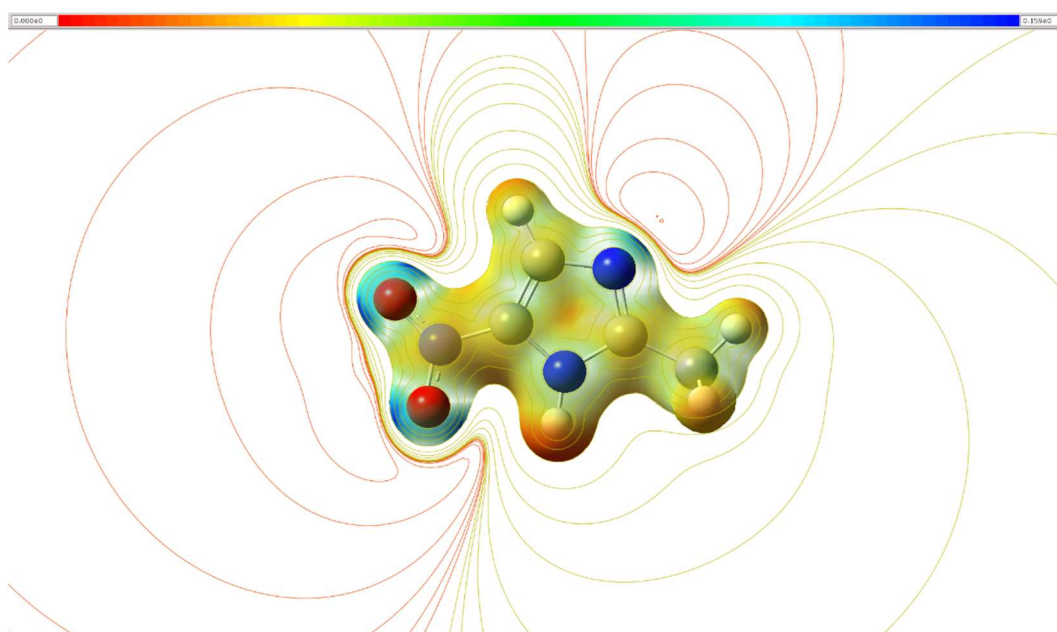


Figure B.144 - Molecular electrostatic potential map of 2-methyl-5-nitroimidazole.

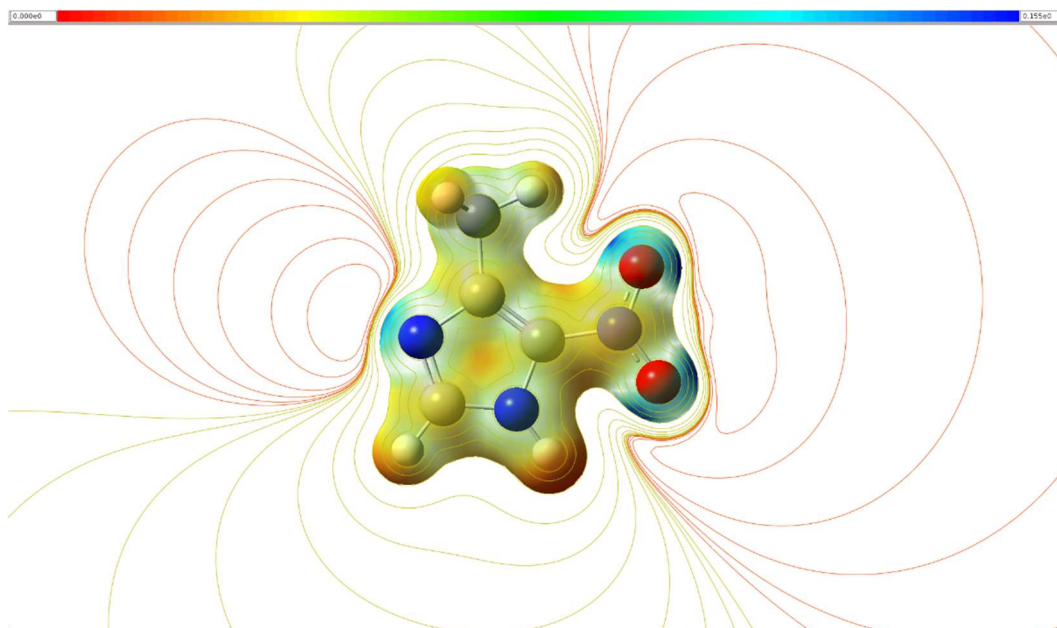


Figure B.145 - Molecular electrostatic potential map of 4-methyl-5-nitroimidazole.

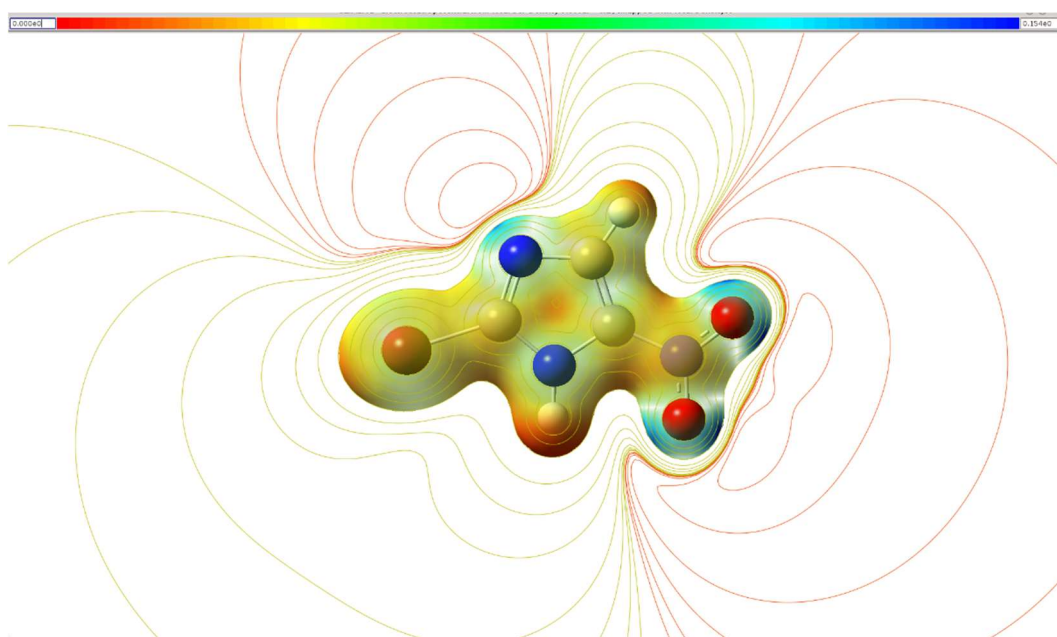


Figure B.146 - Molecular electrostatic potential map of 2-bromo-5-nitroimidazole.

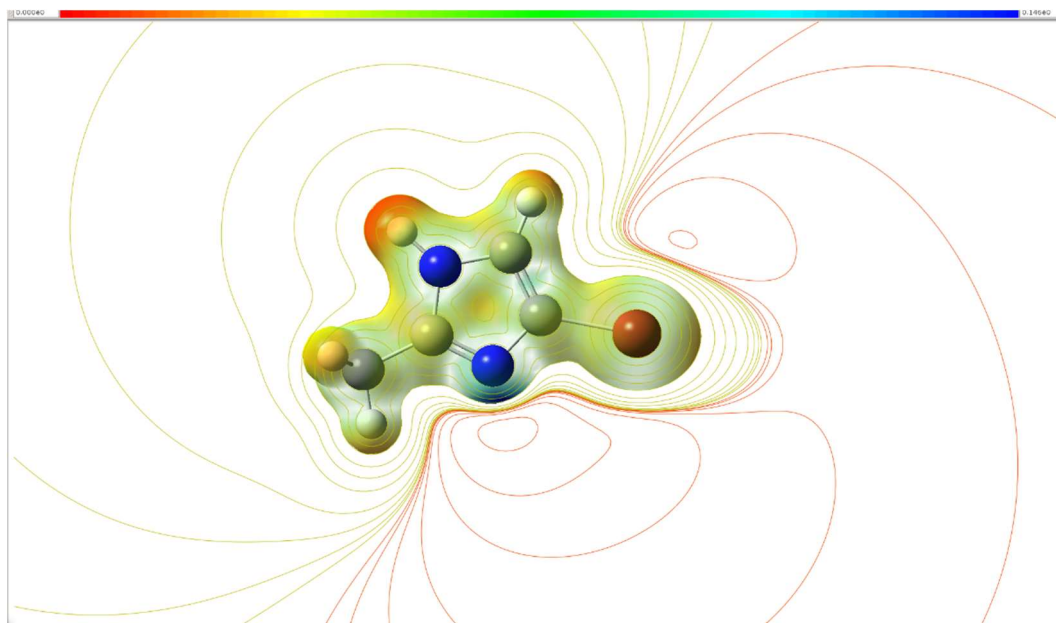


Figure B.147 - Molecular electrostatic potential map of 4-bromo-2-methylimidazole.

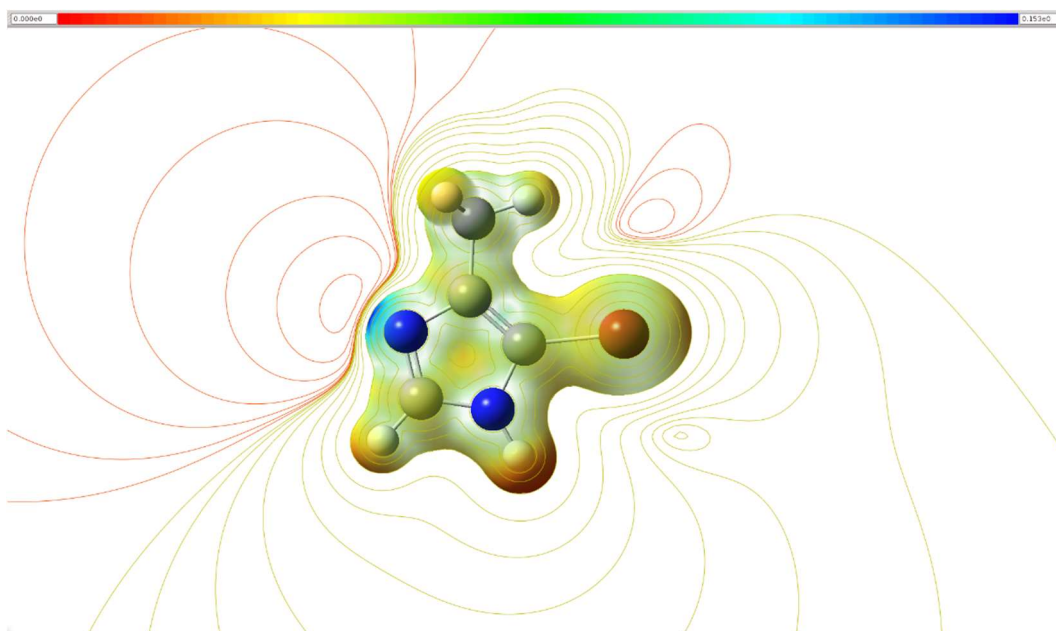


Figure B.148 - Molecular electrostatic potential map of 5-bromo-4-methylimidazole.

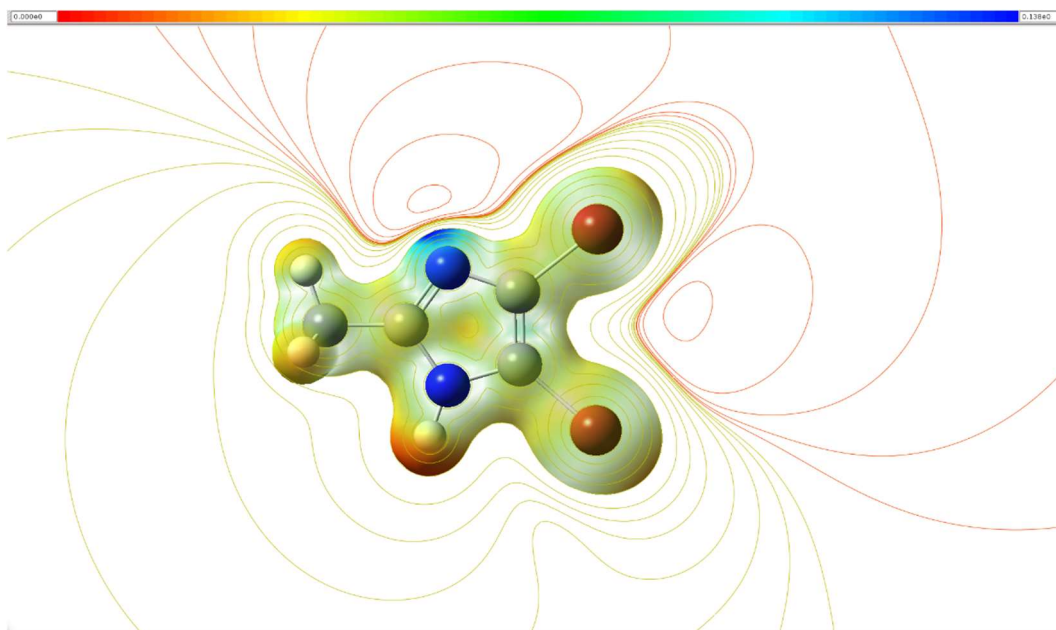


Figure B.149 - Molecular electrostatic potential map of 4,5-dibromo-2-methylimidazole.

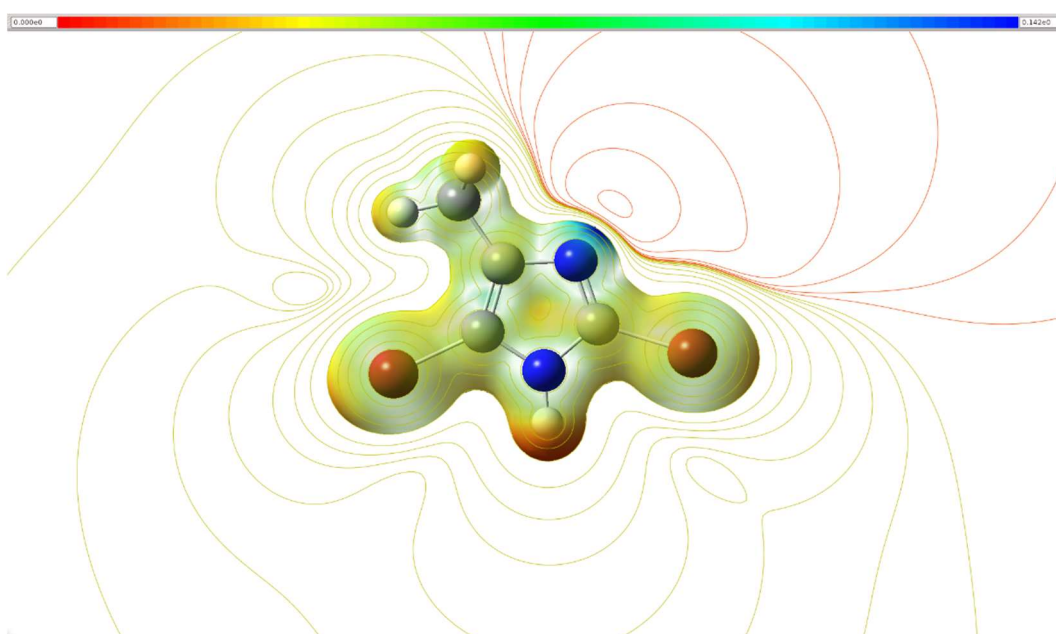


Figure B.150 - Molecular electrostatic potential map of 2,5-dibromo-4-methylimidazole.

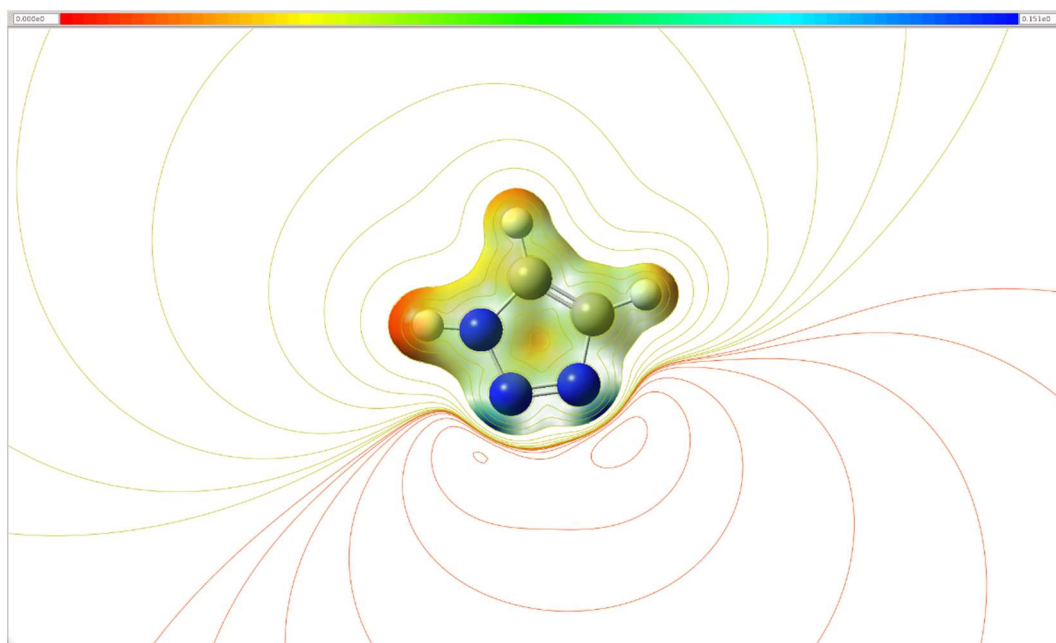


Figure B.151 - Molecular electrostatic potential map of 1,2,3-triazole.

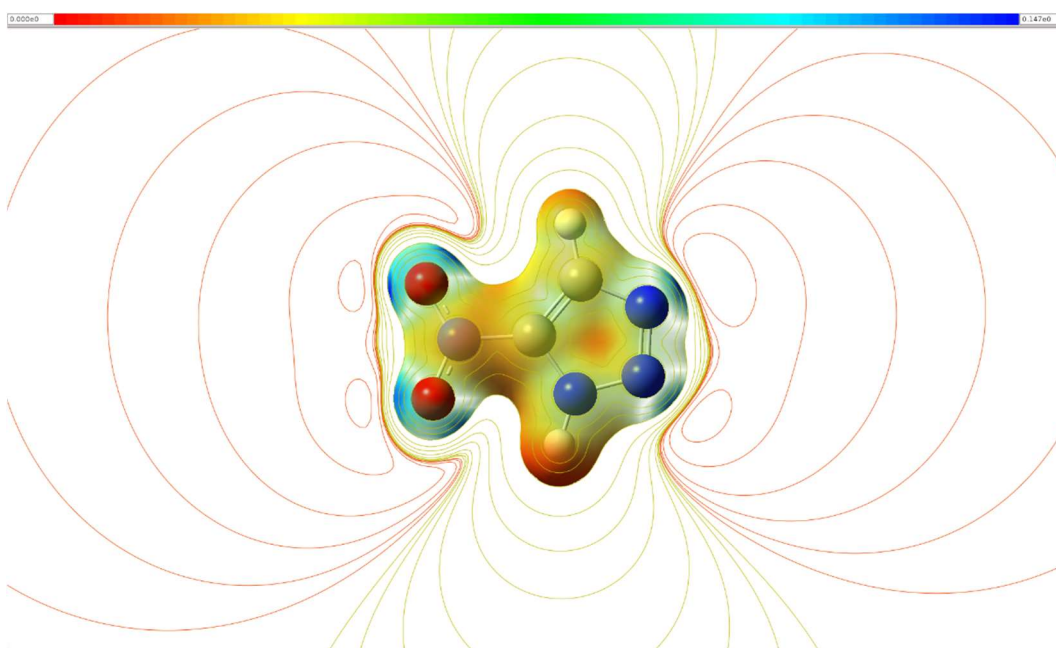


Figure B.152 - Molecular electrostatic potential map of 5-nitro-1,2,3-triazole.

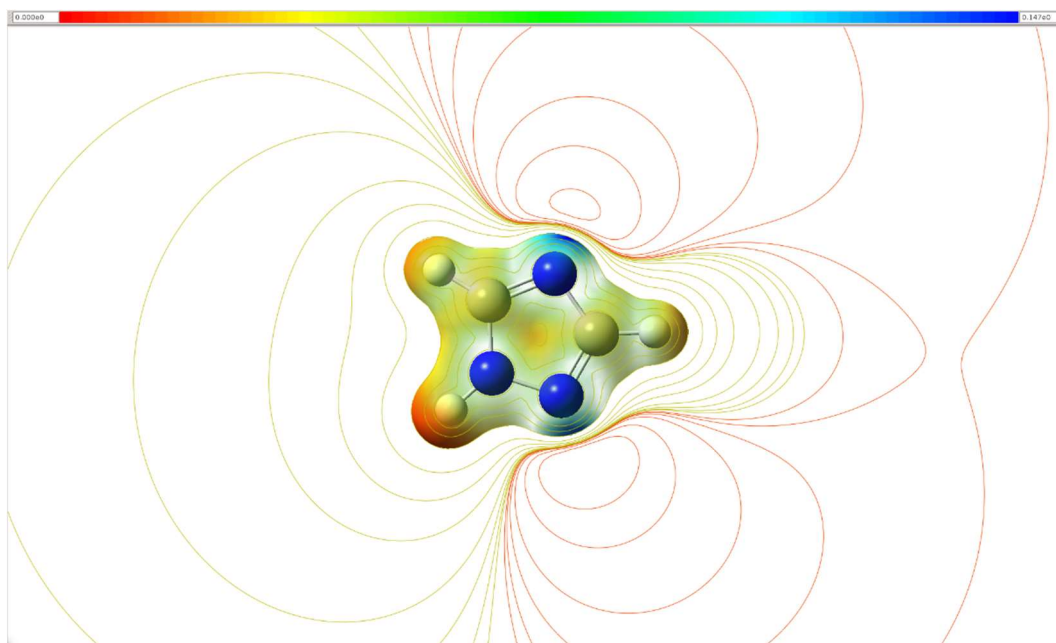


Figure B.153 - Molecular electrostatic potential map of 1,2,4-triazole.

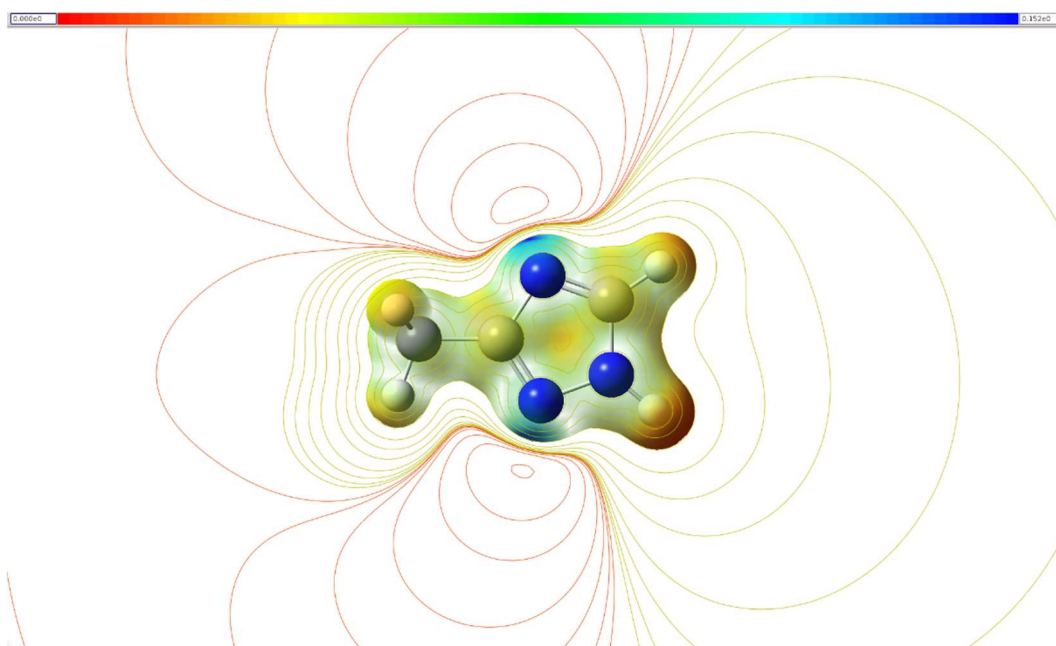


Figure B.154 - Molecular electrostatic potential map of 3-methyl-1,2,4-triazole.

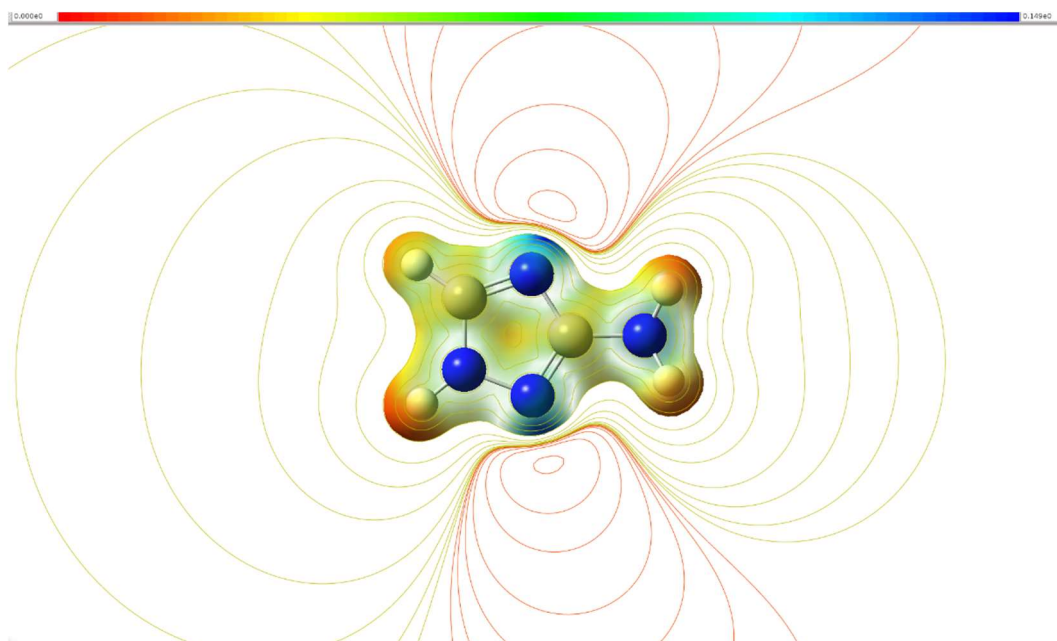


Figure B.155 - Molecular electrostatic potential map of 1,2,4-triazol-3-amine.

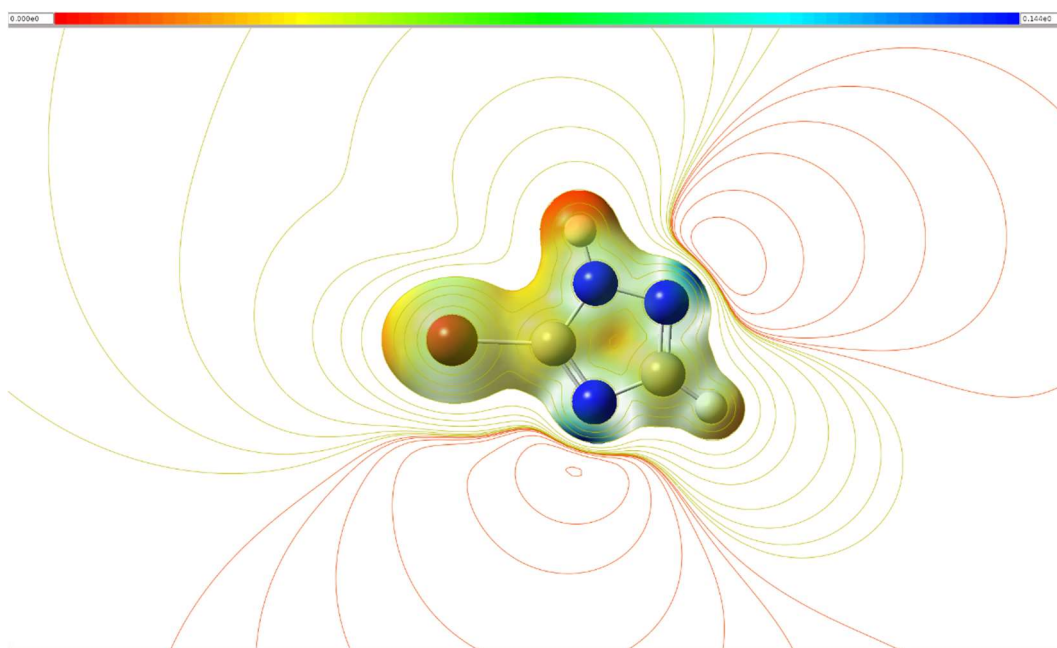


Figure B.156 - Molecular electrostatic potential map of 5-bromo-1,2,4-triazole.

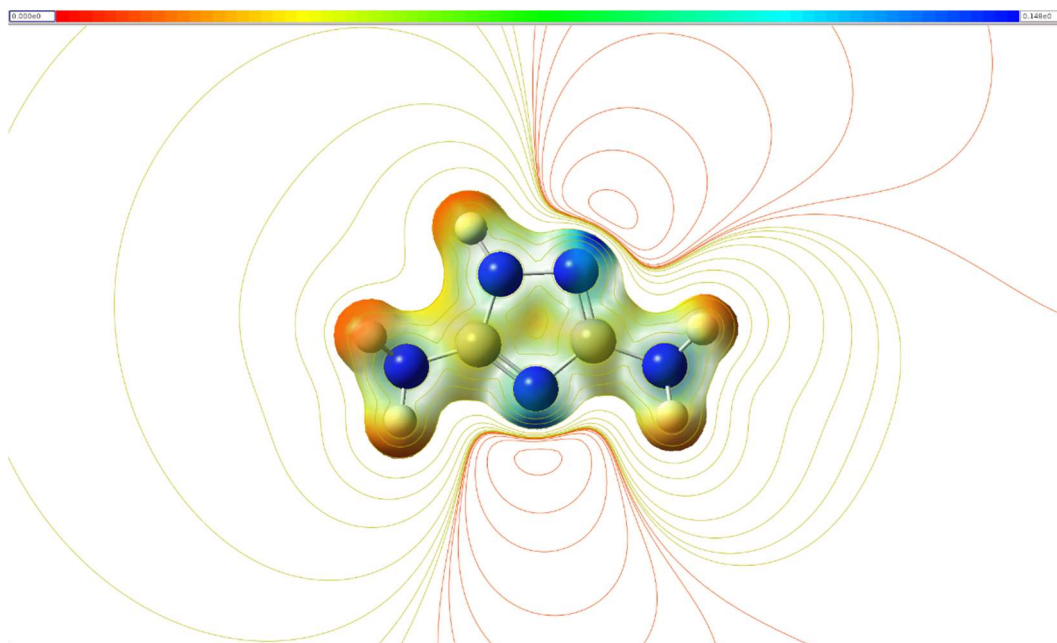


Figure B.157 - Molecular electrostatic potential map of 1,2,4-triazol-3,5-diamine.

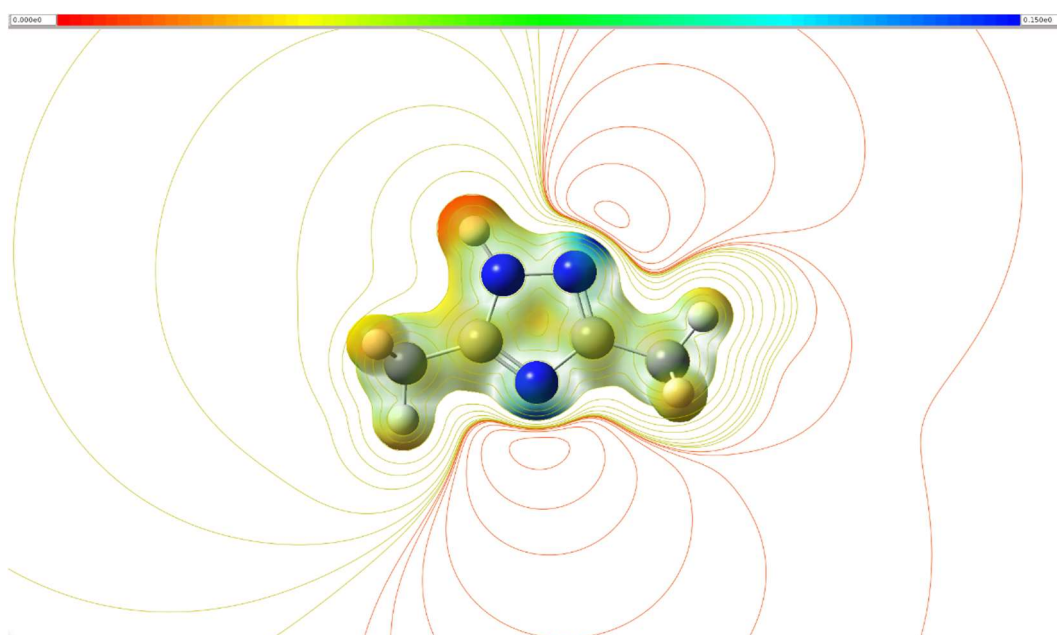


Figure B.158 - Molecular electrostatic potential map of 3,5-dimethyl-1,2,4-triazole.

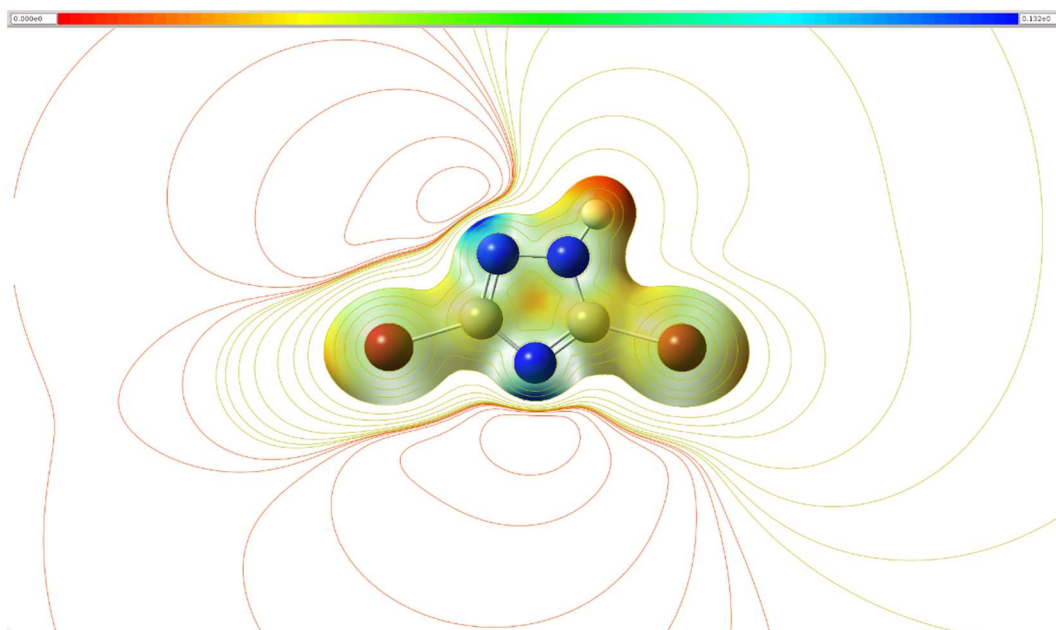


Figure B.159 - Molecular electrostatic potential map of 3,5-dibromo-1,2,4-triazole.

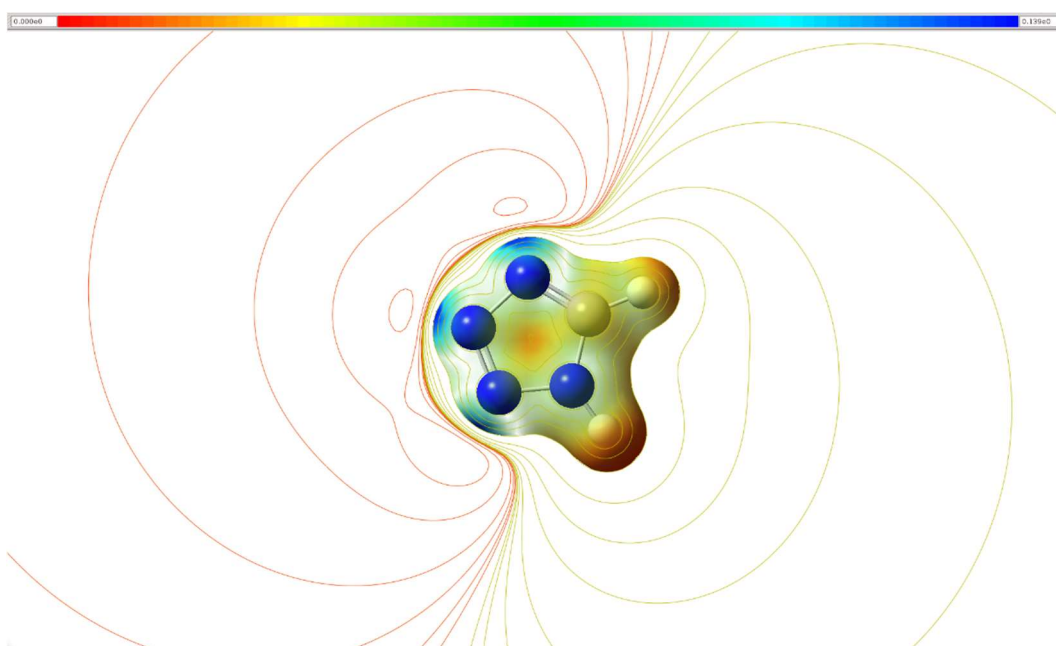


Figure B.160 - Molecular electrostatic potential map of 1,2,3,4-tetrazole.

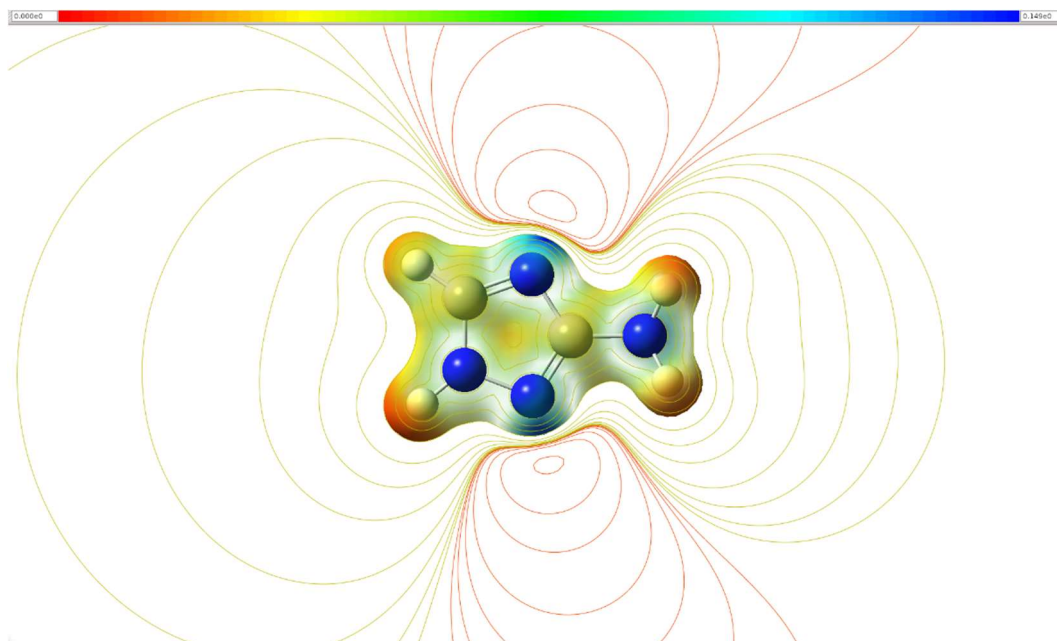


Figure B.161 - Molecular electrostatic potential map of 1,2,3,4-tetrazol-5-amine.

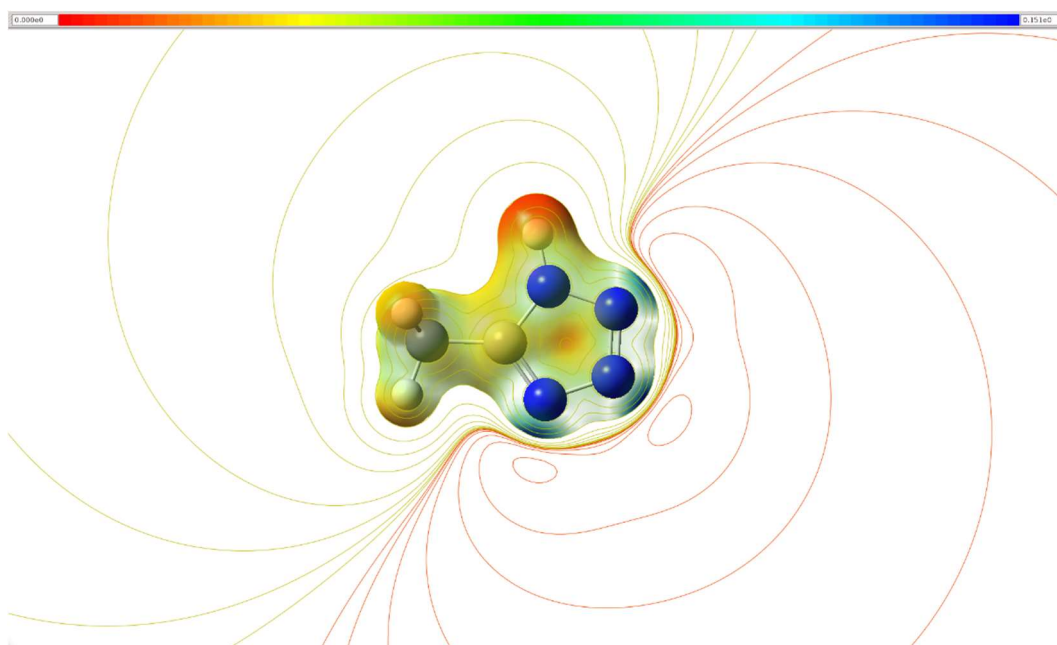


Figure B.162 - Molecular electrostatic potential map of 5-methyl-1,2,3,4-tetrazole.