Appendix

Table A.1: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) of **CI[1]**

	x	*y*	*z*	U_{iso}*/U_{eq}
Cr1	0.40542 (6)	0.60336 (5)	0.62841 (5)	0.0131 (2)
Cr2	0.17034 (6)	0.56625 (5)	0.73703 (5)	0.0135 (2)
Cr3	0.18005 (6)	0.73269 (6)	0.58877 (5)	0.0140 (2)
O1	0.4536 (3)	0.6151 (3)	0.7549 (2)	0.0198 (8)
O2	0.2966 (3)	0.5724 (3)	0.8261 (3)	0.0205 (8)
O3	0.3914 (3)	0.4689 (3)	0.6374 (3)	0.0184 (7)
O4	0.2208 (3)	0.4442 (3)	0.6949 (3)	0.0198 (8)
O5	0.1056 (3)	0.6751 (3)	0.7966 (3)	0.0195 (7)
O6	0.0969 (3)	0.7819 (3)	0.6894 (3)	0.0195 (8)
O7	0.0316 (3)	0.5543 (3)	0.6608 (3)	0.0189 (7)
O8	0.0452 (3)	0.6588 (3)	0.5512 (3)	0.0192 (7)
O9	0.3030 (3)	0.8221 (3)	0.6195 (2)	0.0174 (7)
O10	0.4560 (3)	0.7309 (3)	0.6132 (3)	0.0193 (8)
O11	0.2517 (3)	0.7039 (3)	0.4743 (2)	0.0176 (7)
O12	0.3748 (3)	0.5871 (3)	0.4972 (2)	0.0172 (7)
O13	0.2517 (3)	0.6341 (2)	0.6511 (2)	0.0147 (7)
O1W	0.5731 (3)	0.5752 (3)	0.6032 (2)	0.0172 (7)
O2W	0.0843 (3)	0.4914 (3)	0.8268 (3)	0.0200 (8)
O3W	0.1111 (3)	0.8387 (3)	0.5119 (3)	0.0222 (8)
C1	0.3976 (4)	0.6011 (3)	0.8241 (3)	0.0161 (9)
C2	0.4557 (5)	0.6207 (4)	0.9128 (4)	0.0213 (10)
C3	0.3122 (4)	0.4166 (4)	0.6615 (3)	0.0163 (9)
C4	0.3268 (5)	0.3144 (4)	0.6485 (4)	0.0233 (11)
C5	0.0764 (4)	0.7537 (4)	0.7646 (4)	0.0175 (10)
C6	0.0117 (5)	0.8165 (4)	0.8254 (4)	0.0213 (11)
C7	−0.0024 (4)	0.5925 (4)	0.5887 (3)	0.0173 (10)
C8	−0.1111 (4)	0.5551 (4)	0.5464 (4)	0.0217 (11)
C9	0.4087 (4)	0.8085 (4)	0.6238 (3)	0.0163 (9)
C10	0.4856 (5)	0.8895 (4)	0.6411 (4)	0.0214 (11)
C11	0.3182 (4)	0.6420 (3)	0.4472 (3)	0.0154 (9)
C12	0.3291 (5)	0.6330 (4)	0.3480 (3)	0.0213 (10)

Table A.2: Atomic displacement parameters (Å^2) of **CI[1]**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0129 (4)	0.0149 (4)	0.0115 (4)	0.0003 (3)	0.0011 (3)	0.0001 (3)
Cr2	0.0135 (4)	0.0149 (4)	0.0123 (4)	0.0005 (3)	0.0018 (3)	−0.0001 (3)
Cr3	0.0134 (4)	0.0149 (4)	0.0136 (4)	0.0010 (3)	0.0001 (3)	−0.0013 (3)
O1	0.0163 (16)	0.029 (2)	0.0142 (17)	−0.0013 (14)	0.0007 (13)	0.0001 (15)
O2	0.0194 (18)	0.027 (2)	0.0154 (17)	−0.0023 (15)	0.0007 (14)	0.0032 (15)
O3	0.0155 (16)	0.0158 (17)	0.0241 (19)	0.0014 (13)	0.0044 (14)	0.0029 (14)
O4	0.0209 (18)	0.0149 (17)	0.0239 (19)	−0.0013 (14)	0.0088 (15)	−0.0018 (14)
O5	0.0207 (17)	0.0184 (18)	0.0194 (18)	0.0023 (14)	0.0033 (14)	−0.0001 (15)
O6	0.0187 (17)	0.0204 (18)	0.0196 (19)	0.0021 (14)	0.0020 (14)	−0.0027 (15)
O7	0.0152 (16)	0.0233 (19)	0.0182 (18)	−0.0021 (14)	0.0017 (13)	0.0031 (15)
O8	0.0177 (17)	0.0194 (18)	0.0205 (18)	0.0000 (14)	−0.0014 (14)	−0.0024 (15)
O9	0.0172 (17)	0.0167 (17)	0.0182 (17)	−0.0009 (13)	−0.0010 (13)	0.0004 (14)
O10	0.0164 (17)	0.0166 (17)	0.025 (2)	0.0004 (13)	0.0038 (14)	0.0010 (15)
O11	0.0204 (17)	0.0190 (18)	0.0136 (17)	0.0005 (14)	0.0010 (13)	0.0003 (14)
O12	0.0171 (17)	0.0208 (18)	0.0136 (16)	0.0012 (14)	0.0011 (13)	−0.0022 (14)
O13	0.0131 (15)	0.0175 (17)	0.0135 (16)	0.0007 (13)	0.0020 (12)	−0.0006 (13)
O14	0.0195 (18)	0.029 (2)	0.029 (2)	−0.0017 (16)	0.0010 (16)	−0.0053 (17)
O15	0.022 (2)	0.042 (3)	0.025 (2)	0.0091 (18)	−0.0012 (16)	−0.0096 (19)
O16	0.0219 (19)	0.026 (2)	0.032 (2)	−0.0049 (16)	−0.0010 (17)	0.0024 (18)
O17	0.043 (2)	0.028 (2)	0.0164 (19)	0.0016 (18)	0.0006 (17)	0.0017 (16)
O18	0.051 (3)	0.026 (2)	0.030 (2)	−0.017 (2)	−0.010 (2)	0.0036 (19)
O1W	0.0153 (16)	0.0180 (17)	0.0184 (18)	−0.0002 (13)	0.0038 (13)	−0.0010 (14)
O2W	0.0204 (17)	0.0196 (18)	0.0205 (18)	0.0039 (14)	0.0079 (14)	0.0009 (15)
O3W	0.0213 (18)	0.0214 (19)	0.024 (2)	0.0047 (15)	−0.0029 (15)	−0.0008 (16)
N1	0.028 (2)	0.021 (2)	0.016 (2)	−0.0016 (18)	0.0057 (18)	−0.0024 (18)
C1	0.018 (2)	0.017 (2)	0.013 (2)	0.0040 (18)	−0.0013 (18)	−0.0018 (18)
C2	0.020 (2)	0.025 (3)	0.018 (3)	0.001 (2)	−0.0008 (19)	−0.005 (2)
C3	0.017 (2)	0.018 (2)	0.013 (2)	0.0020 (18)	−0.0011 (18)	−0.0007 (18)
C4	0.023 (3)	0.016 (2)	0.032 (3)	−0.001 (2)	0.008 (2)	−0.004 (2)
C5	0.013 (2)	0.019 (2)	0.020 (2)	−0.0014 (18)	−0.0020 (18)	−0.005 (2)
C6	0.025 (3)	0.023 (3)	0.016 (2)	0.007 (2)	0.002 (2)	−0.006 (2)
C7	0.013 (2)	0.022 (2)	0.017 (2)	0.0019 (18)	0.0024 (18)	−0.0037 (19)
C8	0.018 (2)	0.023 (3)	0.024 (3)	0.0000 (19)	−0.001 (2)	−0.003 (2)
C9	0.018 (2)	0.021 (2)	0.010 (2)	−0.0031 (18)	0.0006 (17)	0.0007 (18)
C10	0.020 (2)	0.021 (3)	0.023 (3)	−0.004 (2)	0.001 (2)	−0.002 (2)
C11	0.014 (2)	0.016 (2)	0.016 (2)	−0.0016 (17)	0.0007 (17)	−0.0026 (18)
C12	0.026 (3)	0.027 (3)	0.011 (2)	0.004 (2)	0.0006 (19)	−0.001 (2)
C13	0.019 (2)	0.018 (2)	0.022 (3)	−0.0010 (18)	−0.002 (2)	0.001 (2)
C14	0.024 (3)	0.027 (3)	0.015 (2)	−0.002 (2)	−0.001 (2)	−0.002 (2)

Table A.3: Bond length of **CI[1]**

Atom	Distance (Å)	Atom	Distance (Å)
Cr1—O13	1.893 (3)	O1—C1	1.260 (6)
Cr1—O10	1.959 (4)	O2—C1	1.255 (7)
Cr1—O3	1.962 (4)	O3—C3	1.259 (6)
Cr1—O1	1.978 (4)	O4—C3	1.259 (6)
Cr1—O12	2.010 (4)	O5—C5	1.281 (7)
Cr1—O1W	2.049 (4)	O6—C5	1.233 (7)
Cr2—O13	1.901 (4)	O7—C7	1.272 (6)
Cr2—O2	1.969 (4)	O8—C7	1.254 (7)
Cr2—O7	1.970 (4)	O9—C9	1.254 (6)
Cr2—O5	1.976 (4)	O10—C9	1.267 (7)
Cr2—O4	1.977 (4)	O11—C11	1.263 (6)
Cr2—O2W	2.022 (4)	O12—C11	1.269 (6)
Cr3—O13	1.894 (4)	C1—C2	1.509 (7)
Cr3—O6	1.956 (4)	C3—C4	1.506 (7)
Cr3—O8	1.978 (4)	C7—C8	1.508 (7)
Cr3—O11	1.980 (4)	C9—C10	1.498 (7)
Cr3—O9	1.982 (4)	C11—C12	1.507 (7)
Cr3—O3W	2.075 (4)		

Table A.4: Bond angles of **CI[1]**

Atom 1	Atom 2	Atom 3	Angle (^{O})	Atom 1	Atom 2	Atom 3	Angle(^{O})
O13	Cr1	O10	95.17 (16)	O11	Cr3	O9	91.12 (16)
O13	Cr1	O3	98.06 (15)	O13	Cr3	O3W	175.13 (16)
O10	Cr1	O3	166.77 (16)	O6	Cr3	O3W	88.07 (16)
O13	Cr1	O1	93.10 (15)	O8	Cr3	O3W	86.97 (16)
O10	Cr1	O1	87.24 (17)	O11	Cr3	O3W	80.73 (16)
O3	Cr1	O1	92.37 (17)	O9	Cr3	O3W	85.05 (16)
O13	Cr1	O12	93.38 (15)	C1	O1	Cr1	129.8 (3)
O10	Cr1	O12	92.45 (16)	C1	O2	Cr2	133.6 (3)
O3	Cr1	O12	86.44 (16)	C3	O3	Cr1	133.1 (3)
O1	Cr1	O12	173.51 (15)	C3	O4	Cr2	132.6 (3)
O13	Cr1	O1W	177.86 (16)	C5	O5	Cr2	130.0 (4)
O10	Cr1	O1W	82.69 (15)	C5	O6	Cr3	134.5 (4)
O3	Cr1	O1W	84.09 (15)	C7	O7	Cr2	133.8 (3)
O1	Cr1	O1W	86.87 (15)	C7	O8	Cr3	130.4 (3)
O12	Cr1	O1W	86.66 (15)	C9	O9	Cr3	128.2 (3)
O13	Cr2	O2	93.38 (15)	C9	O10	Cr1	133.7 (3)
O13	Cr2	O7	93.98 (15)	C11	O11	Cr3	135.2 (3)
O2	Cr2	O7	172.47 (16)	C11	O12	Cr1	125.8 (3)
O13	Cr2	O5	95.72 (16)	Cr1	O13	Cr3	119.96 (19)
O2	Cr2	O5	86.87 (17)	Cr1	O13	Cr2	119.74 (18)
O7	Cr2	O5	90.83 (16)	Cr3	O13	Cr2	120.30 (18)
O13	Cr2	O4	94.97 (16)	O2	C1	O1	125.7 (5)
O2	Cr2	O4	91.88 (17)	O2	C1	C2	116.4 (5)
O7	Cr2	O4	89.05 (17)	O1	C1	C2	117.9 (5)
O5	Cr2	O4	169.29 (17)	O4	C3	O3	124.2 (5)
O13	Cr2	O2W	178.67 (16)	O4	C3	C4	117.7 (5)
O2	Cr2	O2W	87.02 (16)	O3	C3	C4	118.0 (5)
O7	Cr2	O2W	85.66 (16)	O6	C5	O5	125.8 (5)
O5	Cr2	O2W	85.56 (16)	O6	C5	C6	117.9 (5)
O4	Cr2	O2W	83.75 (16)	O5	C5	C6	116.3 (5)
O13	Cr3	O6	96.66 (16)	O8	C7	O7	125.8 (5)
O13	Cr3	O8	94.10 (15)	O8	C7	C8	117.8 (5)
O6	Cr3	O8	90.55 (16)	O7	C7	C8	116.4 (5)
O13	Cr3	O11	94.52 (15)	O9	C9	O10	124.6 (5)
O6	Cr3	O11	168.79 (16)	O9	C9	C10	118.2 (5)
O8	Cr3	O11	89.43 (16)	O10	C9	C10	117.2 (4)
O13	Cr3	O9	94.02 (15)	O11	C11	O12	124.9 (5)
O6	Cr3	O9	87.33 (16)	O11	C11	C12	116.7 (5)
O8	Cr3	O9	171.80 (16)	O12	C11	C12	118.4 (4)

Table A.5: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) of **CI[4]**

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.40419 (2)	0.60220 (2)	0.129438 (17)	0.00843 (7)
Fe2	0.17888 (2)	0.73247 (2)	0.090068 (16)	0.00844 (7)
Fe3	0.16926 (2)	0.56560 (2)	0.236988 (17)	0.00858 (7)
O1	0.25064 (10)	0.63291 (10)	0.15059 (8)	0.0092 (3)
O2	0.45619 (11)	0.73084 (10)	0.11201 (9)	0.0146 (3)
O3	0.30503 (11)	0.82349 (10)	0.11945 (8)	0.0122 (3)
O4	0.37105 (11)	0.58560 (10)	−0.00509 (8)	0.0117 (3)
O5	0.25122 (11)	0.70406 (10)	−0.02709 (8)	0.0121 (3)
O6	0.09731 (11)	0.78451 (10)	0.19119 (8)	0.0123 (3)
O7	0.10095 (12)	0.67591 (10)	0.29677 (9)	0.0153 (3)
O8	0.03982 (11)	0.66008 (10)	0.05222 (8)	0.0127 (3)
O9	0.02914 (11)	0.55304 (10)	0.15840 (8)	0.0137 (3)
O10	0.39230 (11)	0.46557 (10)	0.13640 (9)	0.0142 (3)
O11	0.22475 (11)	0.44121 (10)	0.19769 (9)	0.0147 (3)
O12	0.29657 (12)	0.57476 (11)	0.32827 (9)	0.0182 (3)
O13	0.45411 (11)	0.61259 (11)	0.25732 (8)	0.0162 (3)
C1	0.41120 (16)	0.80855 (15)	0.12314 (11)	0.0106 (4)
C2	0.48869 (17)	0.88825 (15)	0.14216 (13)	0.0164 (4)
C3	0.31601 (15)	0.64213 (14)	−0.05454 (12)	0.0096 (4)
C4	0.32829 (18)	0.63401 (16)	−0.15304 (12)	0.0175 (5)
C5	0.07364 (15)	0.75476 (15)	0.26715 (12)	0.0114 (4)
C6	0.00862 (17)	0.81694 (16)	0.32566 (12)	0.0145 (4)
C7	−0.00686 (15)	0.59229 (14)	0.08820 (12)	0.0107 (4)
C8	−0.11353 (16)	0.55361 (16)	0.04538 (13)	0.0153 (4)
C9	0.31398 (16)	0.41317 (15)	0.16228 (12)	0.0115 (4)
C10	0.32888 (18)	0.31191 (15)	0.14963 (14)	0.0178 (4)
C11	0.39815 (16)	0.60130 (14)	0.32672 (12)	0.0116 (4)
C12	0.45624 (17)	0.62180 (16)	0.41426 (12)	0.0164 (5)

Table A.6: Atomic displacement parameters (Å^2) of **CI[4]**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.00752(13)	0.00877(17)	0.00907(13)	0.00070(10)	0.00138(9)	0.00040(10)
Fe2	0.00876(13)	0.00801(17)	0.00860(12)	0.00090(11)	0.00096(9)	0.00010(10)
Fe3	0.00827(13)	0.00836(17)	0.00923(13)	0.00028 11)	0.00205(9)	0.00028(10)
O1	0.0077 (6)	0.0108 (8)	0.0090 (6)	0.0001 (5)	0.0011 (5)	0.0008 (5)
O2	0.0105 (7)	0.0104 (9)	0.0233 (7)	0.0010 (6)	0.0047 (5)	0.0012 (6)
O3	0.0114 (7)	0.0106 (9)	0.0147 (7)	0.0003 (5)	0.0011 (5)	0.0001 (5)
O4	0.0132 (7)	0.0104 (9)	0.0114 (6)	0.0028 (5)	0.0008 (5)	0.0002 (5)
O5	0.0134 (7)	0.0128 (9)	0.0101 (6)	0.0023 (6)	0.0020 (5)	0.0001 (5)
O6	0.0129 (7)	0.0121 (9)	0.0120 (6)	0.0027 (6)	0.0025 (5)	−0.0008 (5)
O7	0.0195 (7)	0.0102 (9)	0.0167 (7)	0.0031 (6)	0.0073 (6)	0.0002 (5)
O8	0.0116 (7)	0.0133 (9)	0.0130 (7)	−0.0007 (6)	−0.0011(5)	0.0009 (5)
O9	0.0107 (7)	0.0149 (9)	0.0154 (7)	−0.0014 (6)	−0.0005(5)	0.0041 (6)
O10	0.0111 (7)	0.0104 (9)	0.0216 (7)	0.0010 (6)	0.0062 (5)	0.0016 (6)
O11	0.0141 (7)	0.0088 (9)	0.0217 (7)	0.0006 (6)	0.0082 (6)	−0.0008 (6)
O12	0.0154 (7)	0.0268 (10)	0.0123 (7)	−0.0057 (6)	−0.0026(5)	0.0053 (6)
O13	0.0120 (7)	0.0262 (10)	0.0106 (6)	0.0016 (6)	0.0006 (5)	−0.0012 (6)
O14	0.0394 (10)	0.0156 (10)	0.0212 (8)	−0.0138 (8)	−0.0051(7)	0.0023 (6)
O15	0.0340 (9)	0.0202 (11)	0.0149 (7)	0.0005 (7)	0.0013 (6)	0.0032 (6)
O16	0.0165 (7)	0.0191 (10)	0.0275 (8)	−0.0056 (6)	−0.0013(6)	0.0007 (6)
O17	0.0119 (7)	0.0193 (10)	0.0176 (7)	−0.0011 (6)	0.0023 (5)	−0.0044 (6)
O18	0.0154 (7)	0.0295 (11)	0.0207 (8)	0.0064 (7)	−0.0003(6)	−0.0086 (7)
N1	0.0205 (9)	0.0132 (11)	0.0147 (8)	−0.0021 (7)	0.0061 (7)	−0.0019 (7)
C1	0.0134 (9)	0.0122 (12)	0.0063 (8)	−0.0019 (8)	0.0014 (7)	0.0013 (7)
C2	0.0163 (10)	0.0144 (13)	0.0186 (10)	−0.0054 (8)	0.0003 (8)	−0.0023 (8)
C3	0.0090 (8)	0.0092 (12)	0.0107 (9)	−0.0042 (7)	0.0011 (7)	0.0003 (7)
C4	0.0201 (10)	0.0226 (14)	0.0099 (9)	0.0045 (9)	0.0015 (8)	−0.0005 (8)
C5	0.0075 (8)	0.0133 (12)	0.0136 (9)	−0.0018 (7)	−0.0003(7)	−0.0023 (7)
C6	0.0185 (10)	0.0135 (13)	0.0115 (9)	0.0068 (8)	0.0018 (7)	−0.0029 (7)
C7	0.0092 (8)	0.0122 (12)	0.0109 (9)	0.0018 (7)	0.0019 (7)	−0.0031 (7)
C8	0.0113 (9)	0.0155 (13)	0.0189 (10)	−0.0016 (8)	−0.0014(7)	−0.0029 (8)
C9	0.0124 (9)	0.0121 (12)	0.0098 (8)	0.0010 (8)	−0.0007(7)	−0.0010 (7)
C10	0.0177 (10)	0.0100 (13)	0.0262 (11)	−0.0003 (8)	0.0076 (8)	−0.0030 (8)
C11	0.0141 (9)	0.0080 (12)	0.0126 (9)	0.0037 (8)	−0.0011(7)	−0.0005 (7)
C12	0.0161 (10)	0.0216 (14)	0.0115 (9)	0.0026 (9)	−0.0010(7)	−0.0027 (8)
C13	0.0201 (10)	0.0161 (13)	0.0159 (10)	−0.0024 (9)	−0.0001(8)	−0.0020 (8)
C14	0.0147 (9)	0.0095 (12)	0.0167 (10)	−0.0015 (8)	0.0026 (7)	0.0021 (8)
O1W	0.0099 (6)	0.0111 (9)	0.0173 (7)	−0.0006 (6)	0.0027 (5)	−0.0014 (6)
O2W	0.0158 (7)	0.0157 (9)	0.0156 (7)	0.0058 (6)	0.0012 (6)	0.0036 (6)
O3W	0.0149 (7)	0.0116 (9)	0.0158 (7)	0.0041 (6)	0.0063 (6)	0.0036 (6)

Table A.7: Bond length of **CI[4]**

Atom	Distance (Å)	Atom	Distance (Å)
Fe1—O1	1.8982 (13)	O18—H18	0.8400
Fe1—O2	1.9867 (15)	C1—C2	1.496 (3)
Fe1—O10	1.9928 (15)	C2—H2A	0.9800
Fe1—O13	2.0069 (13)	C2—H2B	0.9800
Fe1—O4	2.0714 (13)	C2—H2C	0.9800
Fe1—O1W	2.0820 (13)	C3—C4	1.504 (3)
Fe2—O1	1.8951 (13)	C4—H4A	0.9800
Fe2—O6	1.9800 (13)	C4—H4B	0.9800
Fe2—O8	2.0126 (13)	C4—H4C	0.9800
Fe2—O3	2.0266 (14)	C5—C6	1.492 (3)
Fe2—O5	2.0308 (13)	C6—H6A	0.9800
Fe2—O2W	2.1158 (14)	C6—H6B	0.9800
Fe3—O1	1.9124 (13)	C6—H6C	0.9800
Fe3—O12	2.0078 (13)	C7—C8	1.503 (3)
Fe3—O9	2.0090 (13)	C8—H8A	0.9800
Fe3—O11	2.0174 (15)	C8—H8B	0.9800
Fe3—O7	2.0190 (14)	C8—H8C	0.9800
Fe3—O3W	2.0392 (14)	C9—C10	1.494 (3)
O2—C1	1.260 (2)	C10—H10A	0.9800
O3—C1	1.267 (2)	C10—H10B	0.9800
O4—C3	1.273 (2)	C10—H10C	0.9800
O5—C3	1.258 (2)	C11—C12	1.499 (3)
O6—C5	1.266 (2)	C12—H12A	0.9800
O7—C5	1.268 (2)	C12—H12B	0.9800
O8—C7	1.259 (2)	C12—H12C	0.9800
O9—C7	1.265 (2)	C13—C14	1.495 (3)
O10—C9	1.267 (2)	C13—H13A	0.9800
O11—C9	1.261 (2)	C13—H13B	0.9800
O12—C11	1.257 (2)	C13—H13C	0.9800
O13—C11	1.267 (2)	O1W—H1WA	0.8353
O14—N1	1.275 (2)	O1W—H1WB	0.7748
O15—N1	1.227 (2)	O2W—H2WA	0.8628
O16—N1	1.253 (2)	O2W—H2WB	0.7826
O17—C14	1.226 (2)	O3W—H3WA	0.7807
O18—C14	1.307 (2)	O3W—H3WB	0.7437

Table A.8: Bond angles of **CI[4]**

Atom	Angle (^{O})	Atom	Angle (^{O})
O1—Fe1—O2	95.74 (6)	O12—Fe3—O7	86.51 (6)
O1—Fe1—O10	99.00 (6)	O9—Fe3—O7	90.32 (6)
O2—Fe1—O10	165.11 (6)	O11—Fe3—O7	168.51 (6)
O1—Fe1—O13	94.08 (5)	O1—Fe3—O3W	177.84 (6)
O2—Fe1—O13	88.57 (6)	O12—Fe3—O3W	87.29 (6)
O10—Fe1—O13	92.46 (6)	O9—Fe3—O3W	86.00 (5)
O1—Fe1—O4	92.42 (5)	O11—Fe3—O3W	83.11 (6)
O2—Fe1—O4	91.64 (6)	O7—Fe3—O3W	85.53 (6)
O10—Fe1—O4	85.67 (6)	Fe2—O1—Fe1	120.67 (7)
O13—Fe1—O4	173.45 (6)	Fe2—O1—Fe3	119.63 (7)
O1—Fe1—O1W	176.64 (6)	Fe1—O1—Fe3	119.66 (7)
O2—Fe1—O1W	81.36 (6)	C1—O2—Fe1	133.83 (13)
O10—Fe1—O1W	83.85 (6)	C1—O3—Fe2	127.73 (13)
O13—Fe1—O1W	87.56 (5)	C3—O4—Fe1	125.23 (13)
O4—Fe1—O1W	86.00 (5)	C3—O5—Fe2	135.07 (12)
O1—Fe2—O6	97.97 (6)	C5—O6—Fe2	134.06 (14)
O1—Fe2—O8	94.81 (6)	C5—O7—Fe3	131.26 (12)
O6—Fe2—O8	90.51 (6)	C7—O8—Fe2	130.38 (12)
O1—Fe2—O3	94.61 (6)	C7—O9—Fe3	134.50 (13)
O6—Fe2—O3	87.23 (6)	C9—O10—Fe1	131.90 (13)
O8—Fe2—O3	170.53 (6)	C9—O11—Fe3	134.10 (14)
O1—Fe2—O5	94.17 (5)	C11—O12—Fe3	134.15 (12)
O6—Fe2—O5	167.72 (6)	C11—O13—Fe1	130.04 (13)
O8—Fe2—O5	90.33 (5)	O15—N1—O16	122.30 (19)
O3—Fe2—O5	89.94 (5)	O15—N1—O14	120.46 (17)
O1—Fe2—O2W	173.01 (6)	O16—N1—O14	117.24 (17)
O6—Fe2—O2W	88.95 (6)	O2—C1—O3	124.41 (18)
O8—Fe2—O2W	86.02 (6)	O2—C1—C2	117.57 (17)
O3—Fe2—O2W	84.74 (6)	O3—C1—C2	118.02 (19)
O5—Fe2—O2W	78.88 (5)	C1—O2—Fe1	133.83 (13)
O1—Fe3—O12	93.22 (6)	O5—C3—O4	124.76 (17)
O1—Fe3—O9	93.58 (5)	O5—C3—C4	117.42 (17)
O12—Fe3—O9	172.79 (6)	O4—C3—C4	117.82 (18)
O1—Fe3—O11	94.78 (6)	O6—C5—O7	124.61 (18)
O12—Fe3—O11	91.15 (6)	O6—C5—C6	117.55 (18)
O9—Fe3—O11	90.68 (6)	O7—C5—C6	117.84 (17)
O1—Fe3—O7	96.59 (6)		

Calculation for Maximum Initial Activity

i. Actual pressure drop (atm)

Actual pressure drop = {(Initial reading – final reading) x 2} – controlled pressure drop
= [{(77.50 – 76.90) x 2} – 4.00] cmHg
= 2.60 cmHg

Actual pressure drop (in atm) = 2.60 cmHg (1/76 atm/cmHg)
= 0.0342 atm

ii. Weight of PE (gPE)

By using the ideal gas law, $\Delta n = \Delta P(V/RT)$, and Δn = weight/molar mass. So;

Weight = $\Delta P(V/RT)$ x (molar mass)
= (0.0342 atm) x (2.906 L / (0.0821 L atm K^{-1} mol^{-1} x 303 K)) x (48 g mol^{-1})
= 0.1122 g

iii. Weight of Cr in catalysts (gCr)

Based on elemental analysis, there are 22.19 % of Cr in **CI[1]**

Weight = 22.19 % (0.0207 g)
= 0.0046 g

iv. Catalytic activity (gPE/gCr/hr/atm)

Example for 0.5 minutes of polymerization process.

0.5 minutes = 0.0083 hours

Activity = gPE/gCr/hr/atm
= 0.1122 g / 0.0046 g / 0.0083 hours / 1 atm
= 2931 gPE/gCr/hr/atm

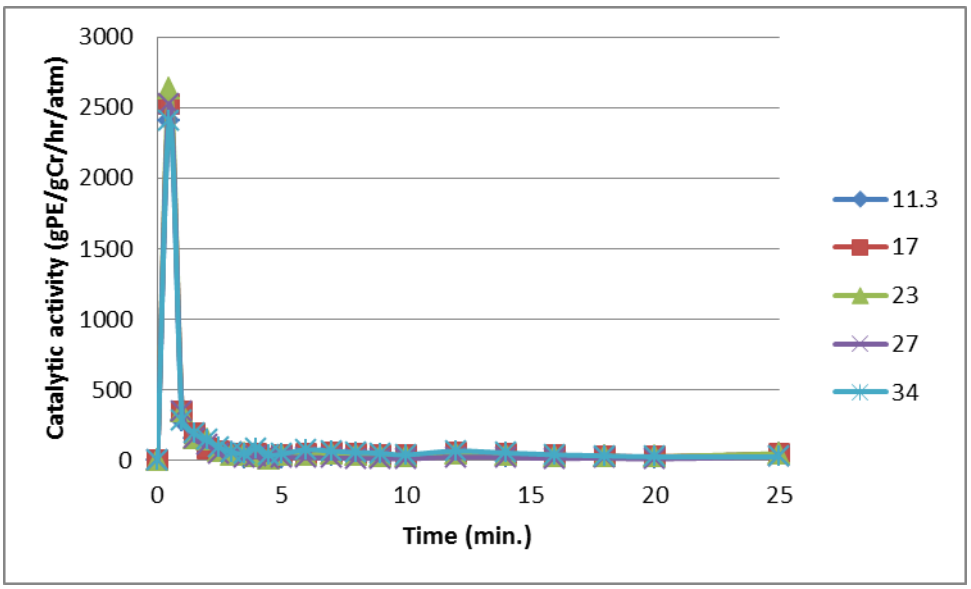

Figure A.1: Kinetic curve for the polymerization of ethylene using **CI[2]** at 30°C with different Al/Cr molar ratios

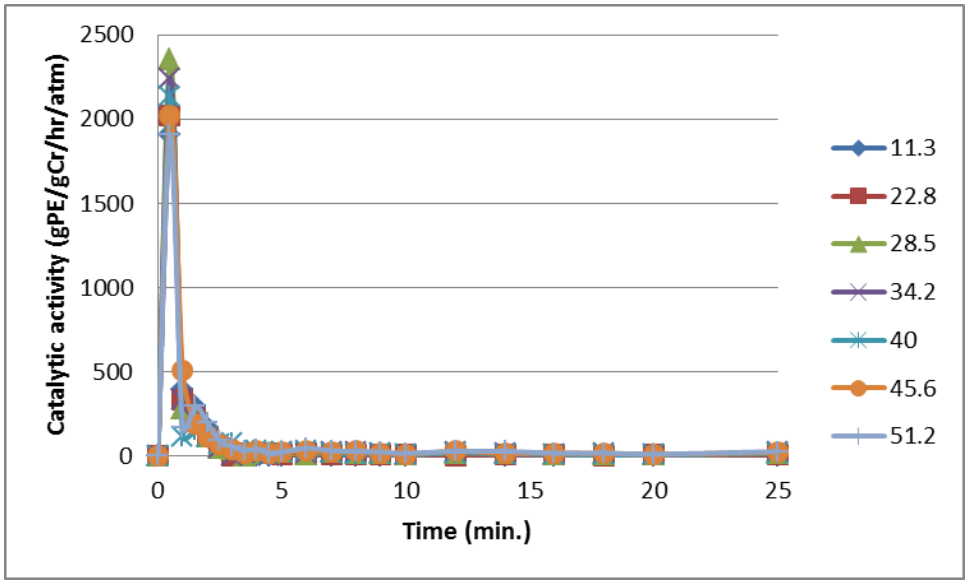

Figure A.2: Kinetic curve for the polymerization of ethylene using **CI[3]** at 30°C with different Al/Cr molar ratios

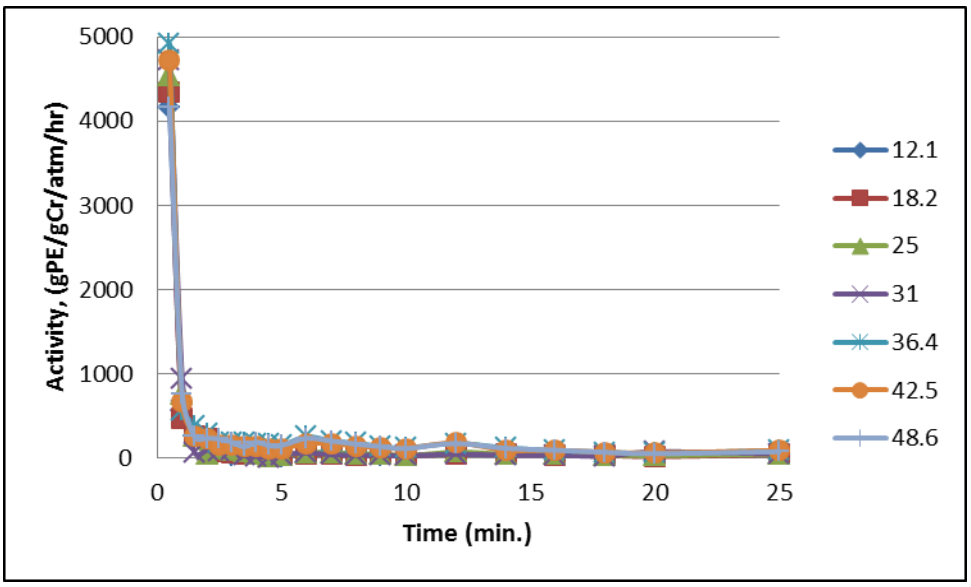

Figure A.3: Kinetic curve for polymerization of ethylene using **CI[5]** at 30ºC with different Al/Cr molar ratios

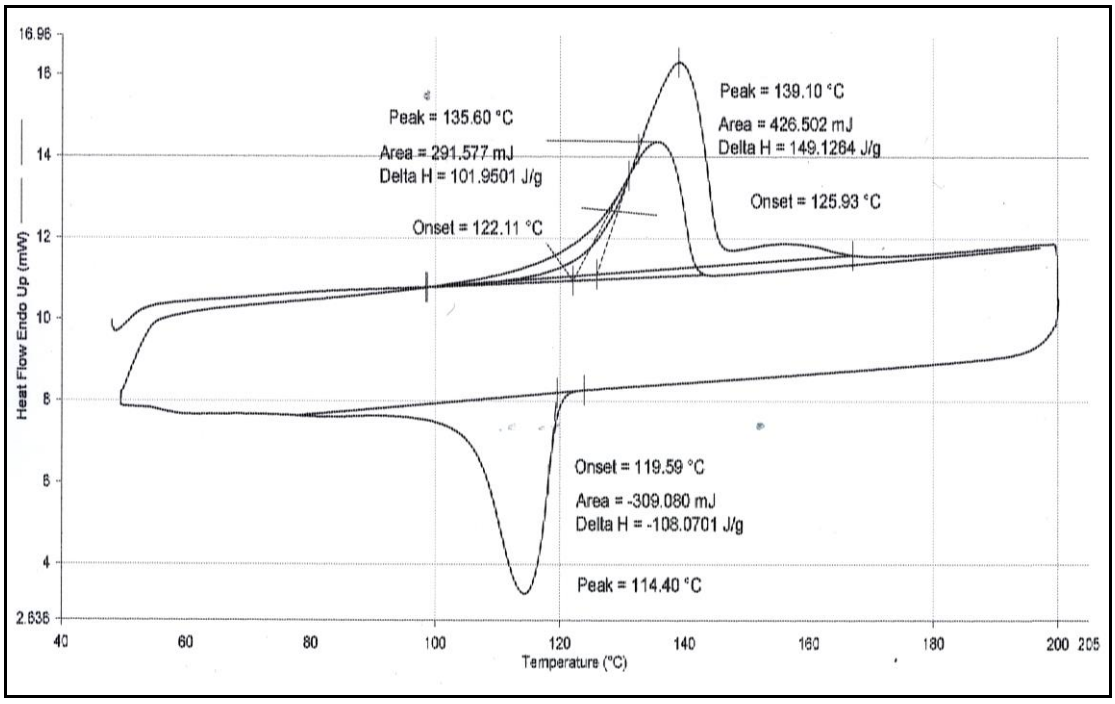

Figure A.4: DSC thermogram of PE-**CI[1]** (Al/Cr=11.2)

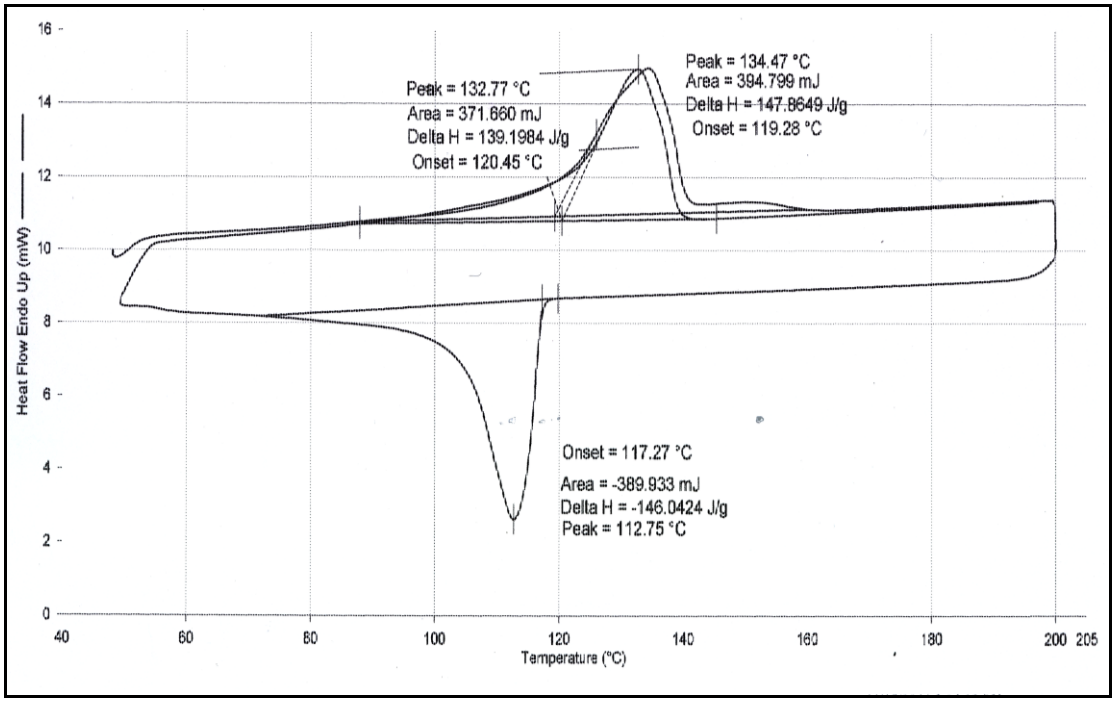

Figure A.5: DSC thermogram of PE-**CI[1]** (Al/Cr=30.0)

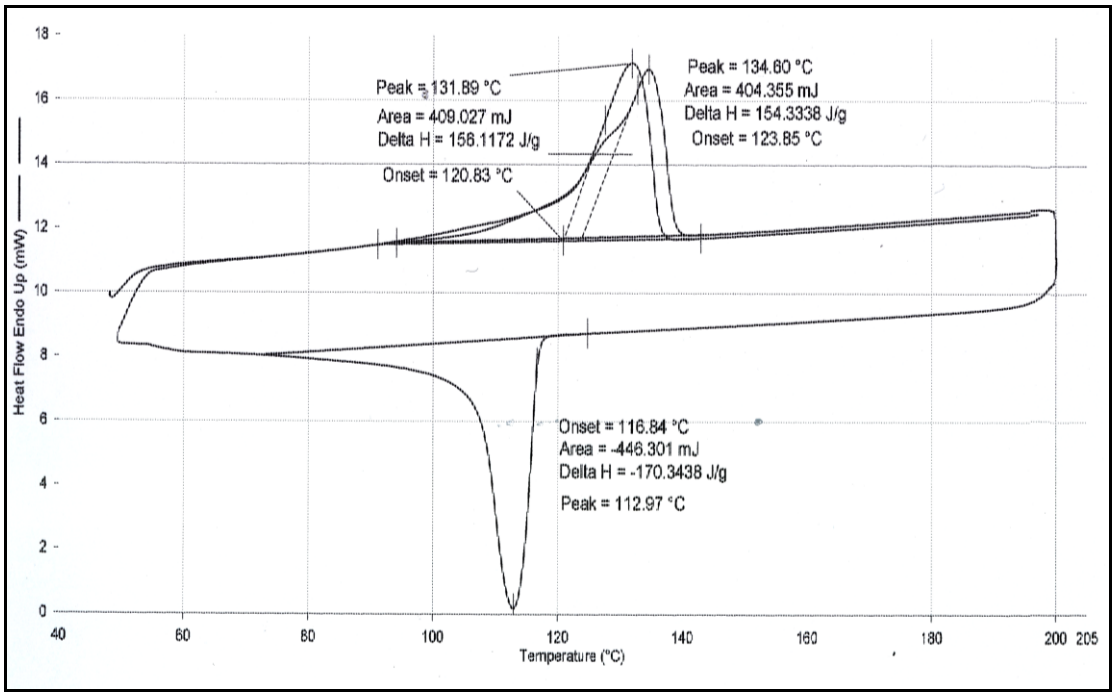

Figure A.6: DSC thermogram of PE-**CI[1]** (Al/Cr=33.7)

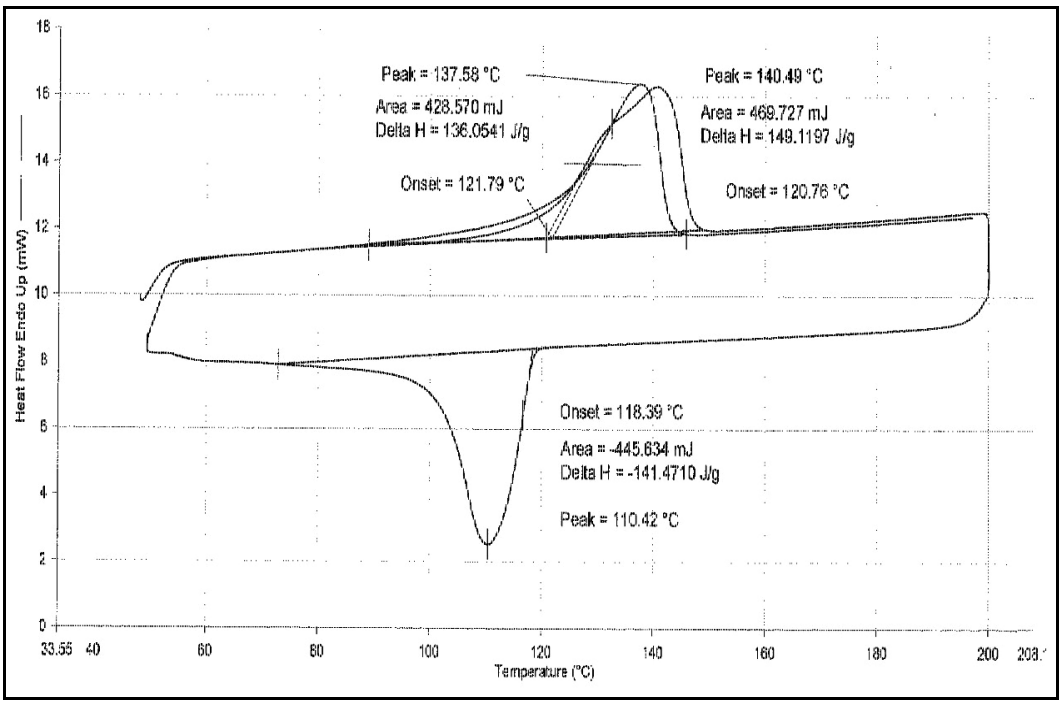

Figure A.7: DSC thermogram of PE-**CI[2]**

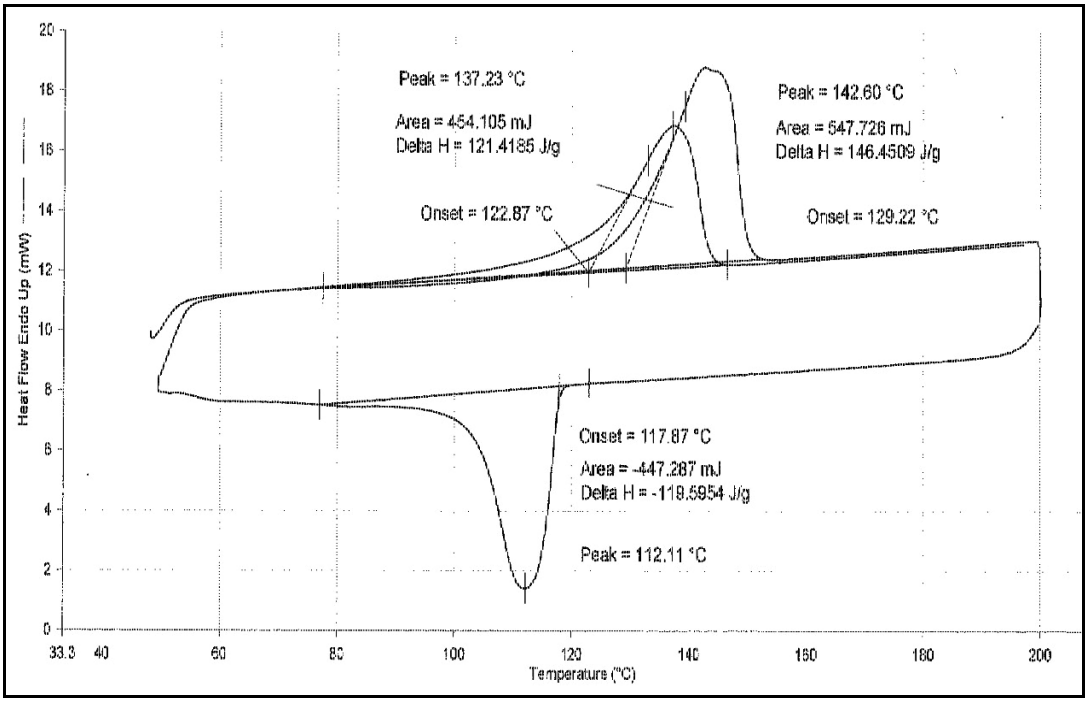

Figure A.8: DSC thermogram of PE-**CI[3]**

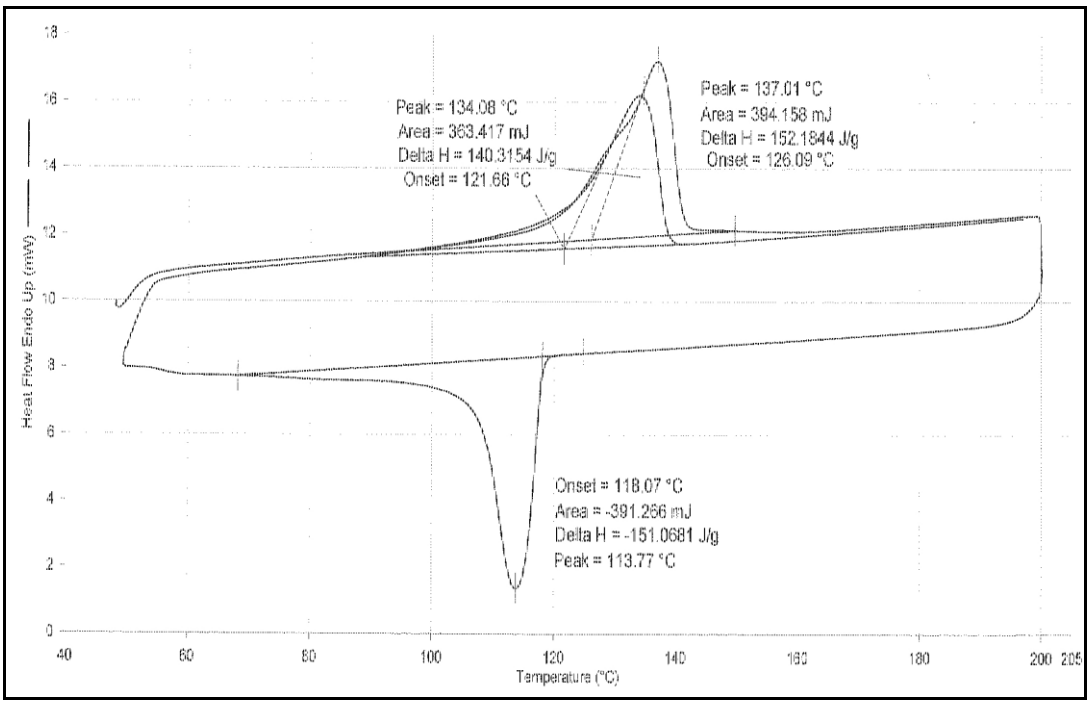

Figure A.9: DSC thermogram of PE-**CI[5]**