

# A simple model for reliable prediction of the specific heat release capacity of polymers as an important characteristic of their flammability

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Abstract The heat release capacity (HRC) is the ratio of specific heat release rate by the rate of the temperature rise of a sample polymer during a test. It is an important factor for the determination of fire safety and flame retardancy of polymeric materials because it can help to develop new polymers with desired flame-retardant properties. A simple and reliable model is introduced to predict the HRC of different polymers on the basis of their repeat units that may contain chemical groups/moieties such as methyl, phenyl, carbonyl, ether, amide and ester. It simply requires only molecular structure of repeat unit of a desired polymer without using complex molecular descriptors and computer codes where they need expert users. Model building has been constructed on the basis of the measured HRC of 111 polymers and compared with the predicted results of two group additivity methods. The root-mean-square (RMS) deviation of the new model is 80 J  $g^{-1}$  K<sup>-1</sup>, which is lower than those predicted by two group additivity methods, i.e., 147 and 208 J g<sup>-1</sup> K<sup>-1</sup> corresponding to application of group additivity methods for 110 and 101 polymers, respectively. The new method has also been examined for 11 new synthesized polymers that its RMS value is lower than those obtained by group additivity methods.

**Keywords** Heat release capacity · Repeat unit of polymer · Correlation · Molecular structure · Fire safety

# Introduction

Determination of fire safety and flame retardancy of polymeric materials is important for the development of new polymers with desired flame-retardant properties. Specific heat release rate (HRR), heat release capacity (HRC) and total heat release (THR) are important parameters to reflect the combustion properties of materials. Microscale combustion calorimeter (MCC) is a small-scale flammability testing technique to screen polymer flammability prior to scale-up, which measures the values of HRR, HRC and THR on the basis of principle of oxygen consumption as well as cone calorimeter to determine the rate and amount of heat during combustion [1]. The thermogravimetric analysis (TG) and derivative TG (DTG) data of polymers are also adopted to assist the assessment of data from the MCC [2]. The HRR is the molecular-level fire response of a burning polymer, which can be obtained through analyzing the oxygen consumed by the complete combustion of the pyrolysis gases during a linear heating program. It can be divided by the rate of the temperature rise of a sample during a test to determine the HRC. However, the HRC appears to be a good predictor of the fire response and flammability of polymers. The HRC is a combination of the thermal stability and combustion properties, which can be obtained by the following equation [3–5]:

$$HRC = \frac{Q_{\rm c}^{\circ}(1-\mu)E_{\rm a}}{eRT_{\rm p}^2}$$
(1)

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where  $Q_c^{\circ}$  is the heat of complete combustion of the pyrolysis gases;  $\mu$  is the weight fraction of the solid residue after pyrolysis or burning;  $E_a$  is the global activation energy for the single-step mass-loss process or pyrolysis;  $T_p$  is the temperature at the peak mass-loss rate in a linear heating program at a constant rate; e is the natural number; and R is the gas constant.

Additive molar group contributions and quantitative structure-property relationships (QSPR) methodology are two different approaches, which have been recently developed for prediction of the HRC [6-9]. The molar group contribution method is an easy approach, which uses additive contribution from a variety of functional groups. This method cannot be applied for prediction of the HRC of those polymers containing a particular functional group where it is missed from the used database of functional groups to build the model. Parandekar et al. [9] used QSPR approaches to predict the HRC as well as total heat release and % char using genetic function algorithms. In contrast to available additive molar group contribution methods, two QSPR models of Parandekar et al. [9] for estimation of the HRC are based on complex/unfamiliar descriptors such as AlogP98 and LUMO-HOMO energy, which require specific computer codes and expert users.

Since searching for new heat- and flame-resistant polymers has attracted considerable research activity during recent years, it is important to develop new approach for prediction of the HRC. The purpose of this work is to introduce a simple and reliable model for the prediction of the HRC of different polymers with their repeat units that are comprised of chemical groups/moieties such as methyl, phenyl, carbonyl, ether, amide and ester. The model is based on a molecular basis for polymer flammability that correlates the HRC test results.

#### Materials and methods

Experimental data of the HRC for 111 polymers with their repeat units containing chemical groups/moieties such as methyl, phenyl, carbonyl, ether, amide and ester are given in Table 1, which were taken from previous works where these data have been used to provide over 40 different empirical molar group contributions as well as (QSPR) methodology for prediction of the heat release capacity [6–9]. These data were taken as training set for building the new model. Since each new model is frequently tested on some chemicals that were not used in the model building, further an external dataset of 11 polymers compiled from several new experimental studies was considered to compare the new model predictions with molar group contribution methods.

## **Results and discussion**

#### Development of the new model

Parandekar et al. [9] introduced the following correlations on the basis of complex descriptors for prediction of the HRC:

$$HRC = [-2.03W(19.93 - \%H) + 2.76W(\%C - 87.02) - 1.05W(AlogP98 - 1.615) - 8.55W(0.668 - AlogP98) - 1.12W(12 - Rbonds) - 2.48W(Hbond donor) + 5.46]2 (2)$$

$$HRC = [67.55W(E_{LUMO-HOMO} - 0.104) + 0.743 R_{bonds} - 0.647W(R_{bonds} - 26) + 0.00128VDE - 0.00056VDM - 0.6853Kap + 0.347\%C + 4.38W(\%C - 90.5) - 0.084MR + 0.248AC + 5.473W(0.95 - DM) + 1.07W(5.372 - S_sNH_2) - 15.73]^2$$
(3)

where W is the ramp function; %H is mass percent of hydrogen atoms; %C is mass percent of carbon atoms; AlogP98 is the log of the octanol-water partition coefficient that is calculated from empirical atomic contributions;  $R_{\text{bonds}}$  is rotatable bonds;  $H_{\text{bond donor}}$  is hydrogen bond donor;  $E_{LUMO-HOMO}$  is LUMO-HOMO energy (au); VDE is vertex distance/equality; VDM is vertex distance/magnitude; Kap is kappa-1; MR is molecular refractivity; AC is atomic composition (total); and DM is dipole moment (au). Equation (2) was generated by genetic function algorithm containing six variables. Meanwhile, Eq. (3) was obtained by using trimer structures including 12 variables where the geometry was optimized with density functional method GGA/PW91 (L56). Although complexity of Eq. (3) is higher than Eq. (2), it provides more reliable predictions. Beside complexity of descriptors, these QSPR models require special computer codes and expert users.

It was indicated that the flash point and the auto-ignition temperature as two flammability characteristics of organic compounds depend on elemental composition and the contribution of some structural parameters, which are related to intra- and intermolecular interactions [10–13]. A careful examination of the HRC of many polymers revealed that the elemental composition as well as the specific structural parameters can be used to construct the new model. Among different elements, the number of carbon, hydrogen, nitrogen, oxygen, chlorine and silicon

Table 1 Comparison of the predicted results of HRC in J  $g^{-1} K^{-1}$  for the new model as well as two molar group contributions of Walters and Lyon [6] and Lyon et al. [8] with experimental data

Notesthylene (PE) $C_5H_4$ 1676 [7]         1711         35         1285 $-391$ 1029 $-647$ Polyprognice (POM) $C_4H_6$ 1571 [7]         1617         461         170         1         80         081           Poly(end)lacohd) (9%; PVOH) $C_4H_0$ 533 [7]         533         20         532 $-157$ 97         225           Poly(end)lene oxide) $C_4H_0$ 532 [7]         671         19         495 $-157$ 97         225           Poly(end)lene oxide) $C_4H_0$ 1000 [7]         1025         23         1607         605         823 $-179$ Poly(end)lene oxide) $C_4H_0$ 131 [7]         31         18         74         61         41         118           Poly(end)lene oxide) $C_4H_0$ 416 [7]         413         18         74         61         41         118           Poly(end)lene oxide) $C_4H_0$ 416 [7]         415         24         -64         75         90         -25         53         92         36         -15           Poly(end)mehene oxide) $C_4H_0$ <t< th=""><th>Name</th><th>Elemental composition in repeat unit composition</th><th>Exp.</th><th>New model</th><th>Dev</th><th>Walters– Lyon</th><th>Dev</th><th>Lyon et al.</th><th>Dev</th></t<>	Name	Elemental composition in repeat unit composition	Exp.	New model	Dev	Walters– Lyon	Dev	Lyon et al.	Dev
Polycognethylene (POM)         CI <sub>4</sub> D         150 [7]         217         68         170         1         8.00         68.1           Polytropylene (PP)         C <sub>3</sub> H <sub>4</sub> D         533 [7]         1617         533         20         52         -1         56         33           Polytopylachacholl (99%; PVOH)         C <sub>3</sub> H <sub>4</sub> D         052 [7]         671         19         495         -117         61         40         83         71           Polytopylachacholl (99%; PVOH)         C <sub>3</sub> H <sub>4</sub> D         102 [7]         671         19         49         -157         907         255           Polytopylachacholl (110)         C <sub>4</sub> H <sub>4</sub> D         102 [7]         671         138         70         405         72         28         64         -71         138         70         61         131         188         71         148         71         66         138         71         161         16         70         72         72         72         71         71         716         71         716         71         716         71         716         71         716         71         716         71         716         71         717         717         717         717         <	Polyethylene (PE)	$C_2H_4$	1676 [ <mark>7</mark> ]	1711	35	1285	-391	1029	-647
Polygonglene (PP)         C <sub>1</sub> H <sub>4</sub> IST1 [7]         IG1         G         ISS3         Q         ISS3         Q         ISS3         Q         ISS3         Q         S         Q         S           Polytinyla lachnl) (9%; PVOH)         C <sub>3</sub> H <sub>4</sub> O         GS2 [7]         G71         19         495         -157         907         255           Polytinylchinen oxide)         C <sub>3</sub> H <sub>4</sub> C1         138 [7]         S33         168         0         133         -5           Polytinylchiner         C <sub>4</sub> H <sub>4</sub> C1         138 [7]         G4         -74         188         0         133         -5           Polytinylchiner         C <sub>4</sub> H <sub>4</sub> O         165 [7]         133         -32         1         -14         61         41         1         16           Polytinyl acatab (PVAc)         C <sub>4</sub> H <sub>4</sub> O         165 [7]         133         -32         1         -15         30         -23         -23           Polytingthiacatab (PVAc)         C <sub>4</sub> H <sub>4</sub> O         35 [7]         16         -19         36         1         50         -23         -23         -23         -24         -24         -24         -25         53         90         -25         53         90         -25	Polyoxymethylene (POM)	CH <sub>2</sub> O	169 [7]	237	68	170	1	850	681
Poly(cin)         C <sub>2</sub> H <sub>4</sub> O         533         Γ1         553         20         532         -1         566         33           Poly(cin)(sen oxide)         C <sub>2</sub> H <sub>4</sub> O         652         [7]         671         109         495         -157         907         255           Poly(ciny)(i chiofide)         C <sub>2</sub> H <sub>4</sub> C <sub>1</sub> 138         [7]         64         -74         138         0         33         -5           Poly(ciny) chiofide)         C <sub>2</sub> H <sub>4</sub> C <sub>2</sub> 311         [7]         280         -22         244         -47           Poly(ciny) chiofide)         C <sub>2</sub> H <sub>4</sub> C <sub>2</sub> 313         [7]         331         83         74         61         131         118           Poly(cins) catcink) (PVAC)         C <sub>4</sub> H <sub>4</sub> C <sub>2</sub> 451         118         877         166         -12         364         161 <td>Polypropylene (PP)</td> <td><math>C_3H_6</math></td> <td>1571 [7]</td> <td>1617</td> <td>46</td> <td>1567</td> <td>-4</td> <td>919</td> <td>-652</td>	Polypropylene (PP)	$C_3H_6$	1571 [7]	1617	46	1567	-4	919	-652
Paly(ch)me axide)         C <sub>3</sub> H <sub>2</sub> O         652         Γ1         61         967         615         970         925           Polyisolutylene         C <sub>4</sub> H <sub>8</sub> 1002         [7]         1023         23         1607         605         823         -179           Polyixolylene fluoride)         C <sub>3</sub> H <sub>5</sub> C         311         [7]         64         -74         138         0         0         86         -18           Polyixorylanide         C <sub>3</sub> H <sub>5</sub> C         131         [1]         25         21         -144         17         6           Polyixorylanide         C <sub>3</sub> H <sub>5</sub> C         131         [1]         31         18         74         61         41         18           Polyixorylanide         C <sub>4</sub> H <sub>5</sub> C         461         [1]         472         8         533         30         26         -188           Polyixorylanide         C <sub>4</sub> H <sub>5</sub> C         513         [1]         516         52         533         92         26         -135           Polyixorharylane/PMMA         C <sub>4</sub> H <sub>2</sub> C         531         [1]         516         -13         56         -157         917         911         530         12         530         26         183	Poly(vinyl alcohol) (99%; PVOH)	$C_2H_4O$	533 [7]	553	20	532	-1	566	33
Polyizobuychen         C,H <sub>6</sub> 1002         Γ17         1025         2.3         16.07         605         82.3         -179           Poly(vinylichoride)         C,H <sub>7</sub> C         311         7         6.4         -7.4         138         77         6.4         -7.4         138         7.4         128         7.4         128         7.4         128         7.4         6.4         -7.5           Polycopulanide         C,H <sub>5</sub> O         165         71         133         -32         21         -1.44         0.7         6.7           Polychacylic acid)         C,H <sub>5</sub> O         313         717         13         18         8.7         -1.65         230         -2.3         9.7         9.7           Polychacylic acid)         C,H <sub>5</sub> O         4.64         7.1         1.8         1.7         1.6         -7.2         1.97         9.7         9.8         1.60         1.8         1.86         -7.2         1.97         9.0         2.2         5.53         9.20         2.2         1.80         7.1         1.80         7.7         1.80         7.8         1.80         7.8         1.80         7.8         1.80         7.80         1.20         9.02         2.2 <td>Poly(ethylene oxide)</td> <td><math>C_2H_4O</math></td> <td>652 [<b>7</b>]</td> <td>671</td> <td>19</td> <td>495</td> <td>-157</td> <td>907</td> <td>255</td>	Poly(ethylene oxide)	$C_2H_4O$	652 [ <b>7</b> ]	671	19	495	-157	907	255
Poly(inity) chloride)         C <sub>2</sub> H <sub>2</sub> C1         138         C1         C34         C3         C3           Poly(inity) idene fluoride)         C <sub>2</sub> H <sub>2</sub> C         311         [7]         280         -31         289         -22         264         -67           Poly(acry)anical         C <sub>2</sub> H <sub>2</sub> O         165         [7]         133         -52         114         0         86         -18           Poly(acry)in actia)         C <sub>2</sub> H <sub>2</sub> O         313         [7]         331         18         37         61         -143         11         18           Poly(inclus)(rice acid)         C <sub>2</sub> H <sub>2</sub> O         313         [7]         314         86         -22         99         -165         230         -234           Poly(inclus)(rice acid)         C <sub>2</sub> H <sub>4</sub> O         416         17         486         -28         53         90         326         -135           Poly(inclus)(rice planchary)tare) (PMMA)         C <sub>2</sub> H <sub>4</sub> O         321         171         415         92         548         -137         313         -614           Poly(acry)[1] pridine         C <sub>3</sub> H <sub>8</sub> O         217         901         -25         559         -22         568         -44           Poly(acry)[1] pridine	Polyisobutylene	$C_4H_8$	1002 [7]	1025	23	1607	605	823	-179
Poly(vinylidene fluoride)         C,H,F <sub>2</sub> 311 [7]         280         -31         289         -22         264         -47           Polyacrylianide         C,H,Q0         106 [7]         133         -32         21         -144         171         6           Poly(vinyl acetale) (PVAc)         C,H,Q0         313 [7]         331         18         374         61         431         118           Poly(methacrylic acid)         C,H,Q0         464 [7]         472         8         29         -165         230         -234           Poly(detrafluorocethylene) (PTFE)         C,H,Q0         464 [7]         486         -28         553         90         32         71           Poly(detrafluorocethylene) (PTMA)         C,H,Q0         313 [7]         180         71         88         91         30         68           Poly(detrafluorocethylene) (PMMA)         C,H,Q0         313 [7]         180         71         89         51         68         715         80         -22         58         -333         33         -61           Poly(detrafluorocethyl methacrylate)         C,H,N0         133 [7]         313         148         161         191         9         340         -55	Poly(vinyl chloride)	C <sub>2</sub> H <sub>3</sub> Cl	138 [7]	64	-74	138	0	133	-5
Polyacrylamide         C,H,NO         104 [7]         156         52         104         0         86         -18           Poly(carplic acid)         C,H,Qo         165 [7]         133         -32         2         -144         17         6           Poly(methacrylic acid)         C,H,Qo         313 [7]         31         18         374         61         431         18           Poly(methacrylic acid)         C,H,Qo         446 [7]         472         8         299         -165         230         -234           Poly(methorylene) (PTFF)         C,F,4         351 [7]         16         -19         36         1         50         -188           Poly(methyl methacrylate) (PMMA)         C,H,Qo         231 [7]         180         77         198         95         126         23           Poly(carving) expland         C,H,NO         331 [7]         180         77         198         95         126         24           Poly(carving) expland         C,H,NO         331 [7]         180         73         313         -614           Poly(carving) pyridine)         C,H,NO         481 [7]         90         -25         54         -373         313         -614	Poly(vinylidene fluoride)	$C_2H_2F_2$	311 [7]	280	-31	289	-22	264	-47
Poly(acrylic acid)       C3H4O2       165 [7]       133       -32       21       -144       171       6         Poly(intacylip acetid) (PVAc)       C4H4O2       313 [7]       331       18       74       61       431       118         Poly(intacylip acetid)       C4H5C1       188 [7]       206       18       186       -23       93       30       32       -155       30       326       -135         Poly(interind indexcylist) (PMMA)       C3H4O2       511 [7]       486       -28       553       92       326       -135         Poly(methin dinkacylist) (PMMA)       C3H4O2       323 [7]       415       92       484       161       391       62       23         Poly(methin dinkacylist) (PMMA)       C3H4O2       323 [7]       416       74       84       161       391       62       23         Poly(acrylip arylate)       C4HaO2       C4Ha       800 [7]       901       -26       54       -333       33       -614         Isotacic polystyrene (PS)       C4Ha       800 [7]       901       -21       55       63       -44         Poly(1-nyin) pyridino)       C7HN       56 [7]       580       12       125       56	Polyacrylamide	C <sub>3</sub> H <sub>5</sub> NO	104 [7]	156	52	104	0	86	-18
Poly(vinyl acetate) (PVAc) $C_4H_6O_2$ 313 [7]313 [7]313 [1837461431118Poly(methacrylic acid) $C_4H_4O_2$ 464 [7]472899-165230-224Poly(netrafluoroethylene) (PTEE) $C_2F_4$ 35 [7]16-193615015Poly(tetrafluoroethylene) (PTEE) $C_2F_4$ 35 [7]146-193615015Poly(tetrafluoroethyl methacrylate) (PMMA) $C_3H_8O_2$ 321 [7]4159248416139168Poly(methacrylate) (PMMA) $C_3H_8O_2$ 103 [7]180771989512623Poly(methacrylate) (PMMA) $C_3H_8O_2$ 103 [7]180771989512623Poly(arbitalte) $C_3H_8O_2$ 103 [7]800 [7]90121554-323313-567Poly(2-vinyl pyridine) $C_7H_7N$ 612 [7]580-32590-22568-44Poly(1-vinyl pyridine) $C_4H_8N$ 568 [7]313148166114449Poly(1-vinyl pyridine) $C_4H_8N$ 568 [7]313148166114449Poly(a-vinyl pyridine) $C_4H_8N$ 322 [7]34513256-76441109Poly(a-vinyl pyridine) $C_4H_8N$ 487 [7]4925<	Poly(acrylic acid)	$C_3H_4O_2$	165 [7]	133	-32	21	-144	171	6
Poly(methacrylic acid) $C_4H_0O_2$ 464 [7]4728299-165230-234Poly(chrolpropene $C_4H_1C_1$ 188 [7]16-1936-21979Poly(methy) methacrylate) (PMMA) $C_3H_4O_2$ 514 [7]486-2855392326-138Poly(methy) methacrylate) (PMMA) $C_3H_4O_2$ 323 [7]4159254416139168Poly(methy) methacrylate) $C_3H_4O_2$ 323 [7]4159254-733313-616Polymethacrylamide $C_4H_NO_2$ 103 [7]180771989512623Polytarvene (PS) $C_3H_8$ 880 [7]901-2654-733313-567Poly(2-vinyl pyridine) $C_7H_N$ 568 [7]5801259022568-44Poly(4-vinyl pyridine) $C_6H_1NO$ 487 [7]492561212558093Poly(a-vinyl pyrolione) $C_6H_1NO$ 487 [7]492561212558093Poly(a-vinyl pyrolione) $C_6H_1O_2$ 380 [7]4788646164109Poly(a-vinyl pyrolione) $C_6H_1O_2$ 380 [7]4788646176412-58Poly(a-winyl pyrolione) $C_6H_1O_2$ 380 [7]4788646176412-58Poly(a-winyl pyrolione) $C_6H_1O_2$ 380 [7]4788646176412-58 </td <td>Poly(vinyl acetate) (PVAc)</td> <td><math>C_4H_6O_2</math></td> <td>313 [7]</td> <td>331</td> <td>18</td> <td>374</td> <td>61</td> <td>431</td> <td>118</td>	Poly(vinyl acetate) (PVAc)	$C_4H_6O_2$	313 [7]	331	18	374	61	431	118
PolychloropreneC4H3Cl188[7]20618186 $-2$ 1979Polytertarluoroethylene) (PTFE)C2F43535116 $-19$ 3615015Polytenthyl methacrylate) (PMMA)C4H4O251471486 $-28$ 55392326 $-188$ Polytenthyl methacrylate) (PMMA)C3H4O2323714159248416139168Polytenthyl aerylate)C4H2O21037118097198 $-326$ 313 $-614$ PolytenthacrylamideC4H3NO21037118097198 $-326$ 313 $-667$ Polyteyrene (PS)C4H48807190121554 $-373$ 313 $-667$ Poly(1-4)penylene sulfide) (PPS)C7H3N61275801259022568 $-44$ Poly(1-4)penylene sulfide) (PPS)C4H4S165131481661109 $91$ Poly(a-ninyl pyrolidone)C4H4NO3327134513256 $-76$ 441109PolycaprolactamC4H10O2380714925561213131481661109Polycachinethyl styrene)C4H10O23807147886466166142258Polycachinethyl styreneC4H10O2380714784864616613223Polycachinethyl styrene<	Poly(methacrylic acid)	$C_4H_6O_2$	464 [7]	472	8	299	-165	230	-234
Poly(tetrafluoroethylene) (PTFE) $C_2F_4$ $35$ [7] $16$ $-19$ $36$ $1$ $50$ $15$ Poly(methyl methacrylate) (PMMA) $C_3H_0O_2$ $514$ [7] $486$ $-28$ $553$ $92$ $326$ $-138$ Poly(methyl methacrylate) (PMMA) $C_3H_0O_2$ $321$ [7] $180$ $77$ $198$ $95$ $126$ $23$ Poly(actyl acrylarc) $C_3H_8$ $927$ [7] $901$ $-26$ $554$ $-373$ $313$ $-614$ Isotactic polystyrene $C_3H_8$ $800$ [7] $901$ $211$ $554$ $-326$ $313$ $-614$ Isotactic polystyrene $C_7H_8N$ $568$ [7] $580$ $-32$ $590$ $-22$ $568$ $-44$ Poly(4-vinyl pyridine) $C_7H_8N$ $568$ [7] $580$ $12$ $590$ $-22$ $568$ $-04$ Poly(4-vinyl pyridine) $C_6H_8O$ $322$ [7] $345$ $132$ $560$ $-76$ $444$ $109$ Poly(a-vinyl pyrolidone) $C_6H_9O_2$ $526$ [7] $525$ $-14$ $438$ $-88$ $513$ $-13$ Poly(abult methacrylate) $C_6H_1O_2$ $307$ [7] $748$ $86$ $646$ $266$ $126$ $256$ Poly(a-vinyl pyrolidone) $C_8H_8O$ $261$ [7] $525$ $-14$ $438$ $-88$ $513$ $-13$ Poly(a-ving methacrylate) $C_6H_1O_2$ $307$ [7] $748$ $86$ $646$ $266$ $126$ $256$ Poly(a-ving methyl $1-4phenyleneC_8H_0O_23807[7]$	Polychloroprene	C <sub>4</sub> H <sub>5</sub> Cl	188 [ <b>7</b> ]	206	18	186	-2	197	9
Poly(methyl methacrylate) (PMMA) $C_3H_8O_2$ 514 [7]486-2855339326-188Poly(methyl methacrylate) (PMMA) $C_3H_8O_2$ 323 [7]4155255392326-135Poly(ethyl acrylate) $C_3H_8O_2$ 323 [7]4159248416139168Polymethacrylamide $C_4H_7NO_2$ 103 [7]180771989512623Polystyrene (PS) $C_8H_8$ 880 [7]901-26554-373313-614Isotactic polystyrene $C_3H_8$ 880 [7]901-26554-372313-614Poly(2-vinyl pyridine) $C_7H_7N$ 568 [7]58012590-22568-44Poly(1-xinyl pyridine) $C_7H_7N$ 568 [7]313148166119429Poly(a-vinyl pyridine) $C_6H_8O$ 321 [7]343148166110990Poly(a-vinyl pyridine) $C_6H_8O$ 487 [7]492561212558093Poly(a-rolatam $C_6H_1OO_2$ 326 [7]525-1438-88513-13Poly(a-rolatam $C_6H_1OO_2$ 326 [7]736 [7]7388664176412-58Poly(a-rolathyl methacrylate) $C_6H_1OO_2$ 326 [7]73447399340-390Poly(a-rolathyl methacrylate) $C_6H_1OO_2$ 318 [7]47898646126<	Poly(tetrafluoroethylene) (PTFE)	$C_2F_4$	35 [7]	16	-19	36	1	50	15
Poly(methyl methacrylate) (PMMA) $C_3H_8O_2$ 461 [7]4862555392326-135Poly(thyl acrylate) $C_4H_8O_2$ 323 [7]4159248416139168Polymethacrylamide $C_4H_7NO_2$ 103 [7]180771989512623Polytyrene (PS) $C_8H_8$ 880 [7]90121554 $-373$ 313 $-614$ Poly(2-vinyl pyridine) $C_7H_7N$ 568 [7]580 $-32$ 590 $-22$ 568 $-44$ Poly(2-vinyl pyridine) $C_7H_7N$ 568 [7]313148166119429Poly(n-vinyl pyrolidone) $C_6H_9NO$ 332 [7]34513256 $-76$ 441109Polycaprolactam $C_6H_{11}NO$ 487 [7]492561212558093Polycaprolactam $C_6H_{10}O_2$ 380 [7]4788646176412 $-58$ Poly(chyl methacrylate) $C_6H_{10}O_2$ 380 [7]47898646166412 $-58$ Poly(2-6-dimethyl 1,4-ptenyleneoxide) (PPO) $C_8H_8O$ 261 [7]525 $-1$ 404 $-55$ Poly(4-vinyl phenol) $C_6H_{10}O_2$ 380 [7]4788646176412 $-58$ Poly(2-6-dimethyl 1,4-ptenyleneoxide) (PPO) $C_8H_8O$ 261 [7]52416331731348Poly(4-vinyl phenol) $C_6H_{10}O_2$ 138 [7]83 [7]83 [7]83 [7]	Poly(methyl methacrylate) (PMMA)	$C_5H_8O_2$	514 [7]	486	-28	553	39	326	-188
Poly(ethyl acrylate)C3H8O2323 [7]4159248416139168PolymethacrylamideC4H7NO2103 [7]1807719895512623Polystyrene (PS)C8H8927 [7]901-26554-373313-614Isotactic polystyrene (PS)C4H7N612 [7]580-22568-44Poly(2-vinyl pyridine)C7H7N568 [7]5801259022568-44Poly(4-vinyl pyridine)C7H7N568 [7]313148166119429Poly(1-phenylene sulfide) (PPS)C4H3N321 [7]345132 [56-76441109PolycaprolactamC4H1NO387 [7]492561212558093PolycaprolactamC4H1NO387 [7]492561212558093PolycaprolactamC4H1NO387 [7]4788646176412-58Poly(2-winyl pyrone)C6H100380 [7]73447999340-390Poly(2-winyl pyrone)C9H400316 [7]73447999340-390Poly(2-winyl pyrone)C9H403138 [7]17959246108244106Poly(2-winyl phenol)C8H60409 [7]42416343617531756Poly(2-winyl phenol)C8H60138 [7]7992246108244106 <trr< td=""><td>Poly(methyl methacrylate) (PMMA)</td><td><math>C_5H_8O_2</math></td><td>461 [7]</td><td>486</td><td>25</td><td>553</td><td>92</td><td>326</td><td>-135</td></trr<>	Poly(methyl methacrylate) (PMMA)	$C_5H_8O_2$	461 [7]	486	25	553	92	326	-135
Polymethacrylamide $C_4H_7NO_2$ 103[7]180771989512623Polystyrene (PS) $C_5H_8$ 927[7]901-26554-373313-614Isotactic polystyrene $C_9H_8N$ 880[7]90121554-326313-566Poly(2-vinyl pyridine) $C_7H_7N$ 612[7]580-32590-22568-44Poly(1,4-phenylene sulfide) (PPS) $C_6H_8N$ 165[7]313148166119429Poly(n-vinyl pyridino) $C_6H_8NO$ 332[7]34513256-76441109Polycaprolactam $C_6H_{11}NO$ 487[7]492561212558093Polycaprolactone $C_6H_{10}O_2$ 226[7]525-1438486164114929Poly(2-dimethyl styrene) $C_6H_{10}O_2$ 380[7]4789864626641232Poly(a-dimethyl J4-phenyleneoxide) (PPO) $C_8H_8O$ 261[7]424153999340-390Poly(4-vinyl phenol) $C_8H_8O$ 261[7]42416343617531756Poly(4-vinyl phenol) $C_8H_8O$ 261[7]824106108244106Poly(2-vinyl naphthalene) $C_1H_8O_3$ 138[7]19759246108244103Poly(di	Poly(ethyl acrylate)	$C_5H_8O_2$	323 [7]	415	92	484	161	391	68
Polystyrene (PS) $C_{4}H_{8}$ $927$ [7] $901$ $-26$ $554$ $-373$ $313$ $-614$ Isotactic polystyrene $C_{8}H_{8}$ $880$ [7] $901$ $21$ $554$ $-326$ $313$ $-567$ Poly(2-vinyl pyridine) $C_{7}H_{7}N$ $568$ [7] $580$ $-12$ $590$ $-22$ $568$ $-44$ Poly(1-vinyl pyridine) $C_{7}H_{7}N$ $568$ [7] $313$ $148$ $166$ $1$ $194$ $29$ Poly(n-vinyl pyridione) $C_{6}H_{9}O0$ $332$ [7] $345$ $13$ $256$ $-76$ $441$ $109$ Polycaprolactam $C_{6}H_{10}O_{2}$ $2526$ [7] $525$ $-1$ $438$ $-88$ $513$ $-13$ Poly(a-winyl pyrrolidone) $C_{6}H_{10}O_{2}$ $2501$ [7] $572$ $-1$ $438$ $-88$ $513$ $-13$ Poly(a-methyl methacrylate) $C_{6}H_{10}O_{2}$ $470$ [7] $478$ $8$ $646$ $176$ $412$ $-58$ Poly(2-dimethyl 1,4-phenyleneoxide) (PPO) $C_{7}H_{9}O$ $490$ [7] $424$ $15$ $398$ $-11$ $404$ $-5$ Poly(2-dimethyl 1,4-phenylene) $C_{6}H_{6}O_{3}$ $138$ [7] $831$ $-3$ $732$ $-102$ $835$ $1$ Poly(2-vinyl naphthalene) $C_{12}H_{10}O_{3}$ $806$ [7] $828$ $22$ $1027$ $221$ $813$ $7$ Poly(2-vinyl naphthalene) $C_{12}H_{10}O_{3}$ $217$ $331$ $-64$ $106$ $109$ $143$ $19$ $122$ $-2$ <td< td=""><td>Polymethacrylamide</td><td><math>C_4H_7NO_2</math></td><td>103 [7]</td><td>180</td><td>77</td><td>198</td><td>95</td><td>126</td><td>23</td></td<>	Polymethacrylamide	$C_4H_7NO_2$	103 [7]	180	77	198	95	126	23
Isotactic polystyrene $C_8H_8$ 880 (7)90121554 $-326$ 313 $-567$ Poly(2-vinyl pyridine) $C_7H_7N$ 612 [7]580 $-32$ 590 $-22$ 568 $-44$ Poly(4-vinyl pyridine) $C_7H_7N$ 568 [7]5801259022568 $0$ Poly(4-vinyl pyridioe) $C_6H_8N$ 165 [7]313148166119429Poly(a-vinyl pyridione) $C_6H_1NO$ 332 [7]34513256 $-76$ 44110Polycaprolactam $C_6H_1NO$ 487 [7]492561212558093Polycaprolactone $C_6H_1O_2$ 326 [7]525 $-1$ 438 $-88$ 513 $-13$ Poly(dr.methacrylate) $C_6H_1O_2$ 370 [7]73447399340 $-390$ Poly(c/-methyl styrene) $C_9H_1O$ 730 [7]73447399340 $-390$ Poly(c/-methyl styrene) $C_6H_6O_3$ 138 [7]19759246106264Poly(e/vinyl phenol) $C_8H_8O$ 261 [7]42415391244106Poly(e/vinyl phenol) $C_6H_1O_2$ 806 [7]8282210272218137Poly(e/vinyl phenol) $C_8H_8O$ 411 [7]831 $-3$ 732 $-102$ 8351Poly(e/vinyl naphtalene) $C_{12}H_{10}O_3$ 279735 $-4$ 297187171Poly(benzo	Polystyrene (PS)	C <sub>8</sub> H <sub>8</sub>	927 [7]	901	-26	554	-373	313	-614
Poly(2-vinyl pyridine)C7H,N612 [7]580 $-32$ 590 $-22$ 568 $-44$ Poly(4-vinyl pyridine)C7H,N568 [7]58012590225680Poly(1,4-phenylene sulfide) (PPS)C6H,S165 [7]313148166119429Poly(n-vinyl pyrolidone)C6H,NO332 [7]34513256 $-76$ 441109PolycaprolactamC6H,1O2526 [7]525 $-1$ 438 $-88$ 513 $-13$ Poly(ethyl methacrylate)C6H,1O2526 [7]525 $-1$ 438 $-88$ 513 $-13$ Poly(ethyl methacrylate)C6H,1O2380 [7]478864626641232Poly(c-methyl styrene)C9H,0730 [7]73447399340 $-390$ Poly(-4-vinyl phenol)C6H,Q3138 [7]19759246108244106Poly(-vinyl phenol)C6H,Q3138 [7]19759246108244106Poly(-vinyl naphthalene)C1H0834 [7]831 $-3$ 732 $-102$ 8351Poly(chyl naphthalene)C1H0832 [7]35018 $-26$ $-358$ 10 $-192$ Poly(chylene terepthalate) (PET)C1H8Q41 [7]831 $-3$ 732 $-102$ 8351Poly(styrene maleic anhydride)C1H8Q21735018 $-26$ $-358$ 16 $-358$ 16	Isotactic polystyrene	C <sub>8</sub> H <sub>8</sub>	880 [7]	901	21	554	-326	313	-567
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly(2-vinyl pyridine)	C <sub>7</sub> H <sub>7</sub> N	612 [7]	580	-32	590	-22	568	-44
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly(4-vinyl pyridine)	C <sub>7</sub> H <sub>7</sub> N	568 [7]	580	12	590	22	568	0
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly(1,4-phenylene sulfide) (PPS)	C <sub>6</sub> H <sub>4</sub> S	165 [7]	313	148	166	1	194	29
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly( <i>n</i> -vinyl pyrrolidone)	C <sub>6</sub> H <sub>9</sub> NO	332 [7]	345	13	256	-76	441	109
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Polycaprolactam	C <sub>6</sub> H <sub>11</sub> NO	487 [7]	492	5	612	125	580	93
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Polycaprolactone	$C_6H_{10}O_2$	526 [7]	525	-1	438	-88	513	-13
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly(ethyl methacrylate)	$C_6H_{10}O_2$	470 [7]	478	8	646	176	412	-58
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly(ethyl methacrylate)	$C_6H_{10}O_2$	380 [7]	478	98	646	266	412	32
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly( $\alpha$ -methyl styrene)	$C_9H_{10}$	730 [7]	734	4	739	9	340	-390
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Poly(2.6-dimethyl 1.4-phenyleneoxide) (PPO)	C <sub>s</sub> H <sub>s</sub> O	409 [7]	424	15	398	-11	404	-5
Dy <td>Poly(4-vinyl phenol)</td> <td>C<sub>8</sub>H<sub>8</sub>O</td> <td>261 [7]</td> <td>424</td> <td>163</td> <td>436</td> <td>175</td> <td>317</td> <td>56</td>	Poly(4-vinyl phenol)	C <sub>8</sub> H <sub>8</sub> O	261 [7]	424	163	436	175	317	56
Poly(vinyl butyral) $C_8H_{14}O_2$ $806$ [7] $828$ $22$ $1027$ $221$ $813$ $7$ Poly(2-vinyl naphtalene) $C_{12}H_{10}$ $834$ [7] $831$ $-3$ $732$ $-102$ $835$ $1$ Poly(benzoyl 1,4-phenylene) $C_{13}H_8O$ $41$ [7] $83$ $42$ $153$ $112$ $144$ $103$ Poly(ethylene terephthalate) (PET) $C_{10}H_8O_4$ $332$ [7] $350$ $18$ $-26$ $-358$ $140$ $-192$ Poly(ether ketone) (PEK) $C_{13}H_8O_2$ $124$ [7] $143$ $19$ $122$ $-2$ $129$ $5$ Polylaurolactam $C_{12}H_{23}ON$ $743$ [7] $790$ $47$ $859$ $116$ $859$ $116$ Poly(styrene maleic anhydride) $C_{12}H_{10}O_3$ $279$ [7] $275$ $-4$ $297$ $18$ $171$ $-108$ (ABS) Poly(acrylonitrile butadiene styrene) $C_{15}H_{17}N$ $669$ [7] $674$ $5$ $827$ $158$ $267$ $-402$ Poly(hexamethylene adipamide) $C_{12}H_{12}O_4$ $474$ [7] $445$ $-29$ $340$ $-134$ $400$ $-74$ Poly(acrylonitrile butadiene styrene) $C_{12}H_{12}O_2N_2$ $615$ [7] $569$ $-46$ $612$ $-3$ $607$ $-8$ Poly(hexamethylene adipamide) $C_{12}H_8O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ </td <td>Poly(ethylene maleic anhydride)</td> <td>C<sub>6</sub>H<sub>6</sub>O<sub>3</sub></td> <td>138 [7]</td> <td>197</td> <td>59</td> <td>246</td> <td>108</td> <td>244</td> <td>106</td>	Poly(ethylene maleic anhydride)	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	138 [7]	197	59	246	108	244	106
Poly(2-vinyl naphtalene) $C_{12}H_{10}$ $834$ [7] $831$ $-3$ $732$ $-102$ $835$ 1Poly(benzoyl 1,4-phenylene) $C_{13}H_8O$ 41 [7] $83$ 42 $153$ $112$ $144$ $103$ Poly(ethylene terephthalate) (PET) $C_{10}H_8O_4$ $332$ [7] $350$ $18$ $-26$ $-358$ $140$ $-192$ Poly(ether ketone) (PEK) $C_{13}H_8O_2$ $124$ [7] $143$ $19$ $122$ $-2$ $129$ $5$ Polylaurolactam $C_{12}H_{23}ON$ $743$ [7] $790$ $47$ $859$ $116$ $859$ $116$ Poly(styrene maleic anhydride) $C_{12}H_{10}O_3$ $279$ [7] $275$ $-4$ $297$ $18$ $171$ $-108$ (ABS) Poly(acrylonitrile butatiene styrene) $C_{15}H_{17}N$ $669$ [7] $674$ $5$ $827$ $158$ $267$ $-402$ Poly(1,4-butanediol terephthalate) (PBT) $C_{12}H_{12}O_2N_2$ $615$ [7] $569$ $-46$ $612$ $-3$ $607$ $-8$ Poly(1,4-phenylene adipamide) $C_{12}H_{8}O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ $0$ Poly(p-phenylene terephthalamide) $C_{14}H_{10}O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $52$ [7] $132$ $80$ $-5$ <t< td=""><td>Poly(vinyl butyral)</td><td><math>C_8H_{14}O_2</math></td><td>806 [7]</td><td>828</td><td>22</td><td>1027</td><td>221</td><td>813</td><td>7</td></t<>	Poly(vinyl butyral)	$C_8H_{14}O_2$	806 [7]	828	22	1027	221	813	7
Poly (benzoyl 1,4-phenylene) $C_{13}H_8O$ 41 [7]8342153112144103Poly (ethylene terephthalate) (PET) $C_{10}H_8O_4$ 332 [7]35018 $-26$ $-358$ 140 $-192$ Poly (ether ketone) (PEK) $C_{13}H_8O_2$ 124 [7]14319122 $-2$ 1295Polylaurolactam $C_{12}H_{23}ON$ 743 [7]79047859116859116Poly (styrene maleic anhydride) $C_{12}H_{10}O_3$ 279 [7]275 $-4$ 29718171 $-108$ (ABS) Poly (acrylonitrile butadiene styrene) $C_{15}H_{17}N$ 669 [7]6745827158267 $-402$ Poly (hexamethylene adipamide) $C_{12}H_{12}O_2N_2$ 615 [7]569 $-46$ 612 $-3$ 607 $-8$ Poly (1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ 115 [7]85 $-30$ 1161114 $-1$ Poly (p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ 42 [7]33 $-9$ 38 $-4$ 420Poly ( <i>n</i> -phenylene isophthalamide) $C_{14}H_10O_2N_2$ 52 [7]132 $-170$ 121 $-181$ 55 $-247$	Poly(2-vinyl naphthalene)	$C_{12}H_{10}$	834 [7]	831	-3	732	-102	835	1
Poly(ethylene terephthalate) (PET) $C_{10}H_8O_4$ $332$ [7] $350$ $18$ $-26$ $-358$ $140$ $-192$ Poly(ether ketone) (PEK) $C_{13}H_8O_2$ $124$ [7] $143$ $19$ $122$ $-2$ $129$ $5$ Polylaurolactam $C_{12}H_{23}ON$ $743$ [7] $790$ $47$ $859$ $116$ $859$ $116$ Poly(styrene maleic anhydride) $C_{12}H_{10}O_3$ $279$ [7] $275$ $-4$ $297$ $18$ $171$ $-108$ (ABS) Poly(acrylonitrile butadiene styrene) $C_{15}H_{17}N$ $669$ [7] $674$ $5$ $827$ $158$ $267$ $-402$ Poly(hexamethylene adipamide) $C_{12}H_{12}O_4$ $474$ [7] $445$ $-29$ $340$ $-134$ $400$ $-74$ Poly(nexamethylene adipamide) $C_{12}H_{12}O_2N_2$ $615$ [7] $569$ $-46$ $612$ $-3$ $607$ $-8$ Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ $0$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$	Poly(benzoyl 1,4-phenylene)	$C_{13}H_8O$	41 [7]	83	42	153	112	144	103
Poly(ether ketone) (PEK) $C_{13}H_8O_2$ 124 [7]14319122-21295Polylaurolactam $C_{12}H_{23}ON$ 743 [7]79047859116859116Poly(styrene maleic anhydride) $C_{12}H_{10}O_3$ 279 [7]275-429718171-108(ABS) Poly(acrylonitrile butadiene styrene) $C_{15}H_{17}N$ 669 [7]6745827158267-402Poly(1,4-butanediol terephthalate) (PBT) $C_{12}H_{12}O_4$ 474 [7]445-29340-134400-74Poly(hexamethylene adipamide) $C_{12}H_{12}O_2N_2$ 615 [7]569-46612-3607-8Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ 115 [7]85-301161114-1Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ 42 [7]33-938-4420Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ 52 [7]13280-5-57553	Poly(ethylene terephthalate) (PET)	$C_{10}H_8O_4$	332 [7]	350	18	-26	-358	140	-192
Polylaurolactam $C_{12}H_{23}ON$ 743 [7]79047859116859116Poly(styrene maleic anhydride) $C_{12}H_{10}O_3$ 279 [7]275-429718171-108(ABS) Poly(acrylonitrile butadiene styrene) $C_{15}H_{17}N$ 669 [7]6745827158267-402Poly(1,4-butanediol terephthalate) (PBT) $C_{12}H_{12}O_4$ 474 [7]445-29340-134400-74Poly(hexamethylene adipamide) $C_{12}H_{12}O_2N_2$ 615 [7]569-46612-3607-8Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ 115 [7]85-301161114-1Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ 42 [7]33-938-4420Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ 52 [7]13280-5-57553	Poly(ether ketone) (PEK)	$C_{13}H_8O_2$	124 [7]	143	19	122	-2	129	5
Poly(styrene maleic anhydride) $C_{12}H_{10}O_3$ $279$ [7] $275$ $-4$ $297$ $18$ $171$ $-108$ (ABS) Poly(acrylonitrile butadiene styrene) $C_{15}H_{17}N$ $669$ [7] $674$ $5$ $827$ $158$ $267$ $-402$ Poly(1,4-butanediol terephthalate) (PBT) $C_{12}H_{12}O_4$ $474$ [7] $445$ $-29$ $340$ $-134$ $400$ $-74$ Poly(hexamethylene adipamide) $C_{12}H_{12}O_2N_2$ $615$ [7] $569$ $-46$ $612$ $-3$ $607$ $-8$ Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ $0$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $52$ [7] $132$ $80$ $-5$ $-57$ $55$ $3$	Polylaurolactam	$C_{12}H_{23}ON$	743 [7]	790	47	859	116	859	116
(ABS) Poly(acrylonitrile butadiene styrene) $C_{15}H_{17}N$ $669$ [7] $674$ $5$ $827$ $158$ $267$ $-402$ Poly(1,4-butanediol terephthalate) (PBT) $C_{12}H_{12}O_4$ $474$ [7] $445$ $-29$ $340$ $-134$ $400$ $-74$ Poly(hexamethylene adipamide) $C_{12}H_{12}O_2N_2$ $615$ [7] $569$ $-46$ $612$ $-3$ $607$ $-8$ Poly(1,4-phenylene adipamide) $C_{12}H_9N_3$ $36$ [7] $97$ $61$ $225$ $189$ $120$ $84$ Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ $0$ Poly( <i>p</i> -phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$ Poly( <i>m</i> -phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $52$ [7] $132$ $80$ $-5$ $-57$ $55$ $3$	Poly(styrene maleic anhydride)	$C_{12}H_{10}O_3$	279 [7]	275	-4	297	18	171	-108
Poly(1,4-butanediol terephthalate) (PBT) $C_{12}H_{12}O_4$ $474$ [7] $445$ $-29$ $340$ $-134$ $400$ $-74$ Poly(hexamethylene adipamide) $C_{12}H_{12}O_2N_2$ $615$ [7] $569$ $-46$ $612$ $-3$ $607$ $-8$ Polyazomethine $C_{15}H_9N_3$ $36$ [7] $97$ $61$ $225$ $189$ $120$ $84$ Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ $0$ Poly(p-phenylene terephthalamide) $C_{14}H_{10}O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $52$ [7] $132$ $80$ $-5$ $-57$ $55$ $3$	(ABS) Poly(acrylonitrile butadiene styrene)	$C_{15}H_{17}N$	669 [7]	674	5	827	158	267	-402
Poly(hexamethylene adipamide) $C_{12}H_{12}O_2N_2$ $615$ [7] $569$ $-46$ $612$ $-3$ $607$ $-8$ Polyazomethine $C_{15}H_9N_3$ $36$ [7] $97$ $61$ $225$ $189$ $120$ $84$ Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ $0$ Poly(p-phenylene terephthalamide) $C_{14}H_1O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $52$ [7] $132$ $80$ $-5$ $-57$ $55$ $3$	Poly(1,4-butanediol terephthalate) (PBT)	$C_{12}H_{12}O_4$	474 [7]	445	-29	340	-134	400	-74
Polyazomethine $C_{15}H_9N_3$ $36$ [7] $97$ $61$ $225$ $189$ $120$ $84$ Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ $115$ [7] $85$ $-30$ $116$ $1$ $114$ $-1$ Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ $42$ [7] $33$ $-9$ $38$ $-4$ $42$ $0$ Poly(p-phenylene terephthalamide) $C_{14}H_1O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $52$ [7] $132$ $80$ $-5$ $-57$ $55$ $3$	Poly(hexamethylene adipamide)	$C_{12}H_{12}O_2N_2$	615 [7]	569	-46	612	-3	607	-8
Poly(1,4-phenylene ether sulfone) (PES) $C_{12}H_8O_3S$ 115 [7]85-301161114-1Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ 42 [7]33-938-4420Poly(p-phenylene terephthalamide) $C_{14}H_1O_2N_2$ 302 [7]132-170121-18155-247Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ 52 [7]13280-5-57553	Polyazomethine	$C_{15}H_9N_3$	36 [7]	97	61	225	189	120	84
Poly(p-phenylene benzobisoxazole) (PBO) $C_{14}H_6O_2N_2$ 42 [7]33-938-4420Poly(p-phenylene terephthalamide) $C_{14}H_1O_2N_2$ 302 [7]132-170121-18155-247Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ 52 [7]13280-5-57553	Poly(1,4-phenylene ether sulfone) (PES)	$C_{12}H_8O_3S$	115 [7]	85	-30	116	1	114	-1
Poly(p-phenylene terephthalamide) $C_{14}H_{10}O_2N_2$ $302$ [7] $132$ $-170$ $121$ $-181$ $55$ $-247$ Poly(m-phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ $52$ [7] $132$ $80$ $-5$ $-57$ $55$ $3$	Poly( <i>p</i> -phenylene benzobisoxazole) (PBO)	$C_{14}H_6O_2N_2$	42 [7]	33	-9	38	-4	42	0
Poly( <i>m</i> -phenylene isophthalamide) $C_{14}H_{10}O_2N_2$ 52 [7] 132 80 -5 -57 55 3	Poly( <i>p</i> -phenylene terephthalamide)	$C_{14}H_{10}O_2N_2$	302 [7]	132	-170	121	-181	55	-247
	Poly( <i>m</i> -phenylene isophthalamide)	$C_{14}H_{10}O_2N_2$	52 [7]	132	80	-5	-57	55	3

## Table 1 continued

Name	Elemental composition in repeat unit composition	Exp.	New model	Dev	Walters– Lyon	Dev	Lyon et al.	Dev
Poly(ethylene naphthalate) (PEN)	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub>	309 [7]	215	-94	148	-161	321	12
Dicyclopentadienyl bisphenol cyanate ester	C <sub>17</sub> H <sub>17</sub> NO	493 [7]	393	-100	463	-30	_	_
Polycarbonate of bisphenol A (PC)	$C_{16}H_{14}O_3$	359 [7]	331	-28	176	-183	510	151
Polyphosphazene	C <sub>14</sub> H <sub>14</sub> PNO <sub>3</sub>	204 [7]	133	-71	262	58	_	_
Poly(dichloroethyl diphenyl ether)	$C_{14}H_8OC_{12}$	16 [ <b>7</b> ]	97	81	172	156	15	-1
Cyano-substituted Kevlar	$C_{15}H_9N_3O_2$	54 [ <b>7</b> ]	40	-14	116	62	94	40
Bisphenol E polycyanurate	$C_{16}H_{12}O_2N_2$	316 [7]	339	23	205	-111	222	-94
Bisphenol A polycyanurate	$C_{17}H_{14}O_2N_2$	283 [7]	377	94	123	-160	430	147
Poly(hexamethylene sebacamide)	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub> N <sub>2</sub>	878 [ <mark>7</mark> ]	919	41	727	-151	669	-209
Poly(ether ether ketone) (PEEK)	$C_{19}H_{12}O_3$	155 [7]	146	-9	143	-12	170	15
Poly(siloxytetraalkyl biphenylene oxide) (PSA)	$C_{18}H_{18}SiO_2$	119 [7]	119	0	293	174	121	2
Poly(ether ketoneketone) (PEKK)	$C_{20}H_{12}O_3$	96 [7]	140	44	103	7	84	-12
Tetramethyl bisphenol F polycyanurate	$C_{19}H_{18}O_{2}N_{2}$	280 [7]	277	-3	276	-4	390	110
Bisphenol C polycarbonate	$C_{15}H_8O_3Cl_2$	29 [7]	49	20	43	14	8	-21
Polybenzimidazole (PBI)	$C_{20}H_{12}N_4$	36 [7]	97	61	36	0	36	0
Poly(hexamethylene dodecane diamide)	$C_{18}H_{24}N_2O_2$	707 [7]	576	-131	769	62	701	-6
Bisphenol C. polycyanurate	$C_{14}H_{*}O_{2}C_{2}$	24 [7]	73	49	29	5	22	-2
Bisphenol A epoxy, catalytic cure phenoxy A	$C_{21}H_{24}O_4$	657 [7]	587	-70	473	-184	662	5
Phenolphthalein polycarbonate	C21H12O5	28 [7]	192	164	65	37	146	118
Poly(amide imide) (PAI)	$C_{22}H_{12}O_{3}N_{2}$	<u> </u>	56	23	20	-13	44	11
Novolac polycyanurate	$C_{22}H_{14}O_{3}N_{2}$	122 [7]	130	-20	31	-91	207	85
Polyimide (PI)	$C_{23}H_{13}O_{5}N_{2}$	25 [7]	60	35	39	14	25	0
Hexafluorobisphenol A polycyanurate	$C_{17}H_{10}O_{3}N_{2}F_{4}$	32 [7]	7	-25	10	-22	55	23
Bisphenol C epoxy		506 [7]	331	-175	332	_174	270	
Bisphenol M polycyanurate	$C_{20}H_{18}O_4O_2$	239 [7]	325	86	235	-4	552	313
Poly(phenyl sulfone)	$C_{26}H_{24}SO_{2}$	153 [7]	140	-13	182	29	159	6
Bisphenol C polyarylate	$C_{24}H_{16}O_4$	21 [7]	99	78	47	26	7	14
Bisphenol phthalonitrile	$C_{22}H_{12}O_4C_{12}$	21 [7] 15 [7]	90	75	84	20 69	, 241	226
Polysulfone of hisphenol A PSE	$C_{28}H_{14}H_{4}O_{2}$	345 [7]	320	_25	231	_114	241	-58
I appendix of displicitor A 131	$C_{27}H_{22}O_4S$	38 [7]	101	-23	_30	-114	207	-14
Enovy novolac, catalytic cure phenovy N	$C_{28}\Pi_{14}\Pi_{2}O_{6}$	246 [7]	101	237	230	-16	24	-14
Pierbanol A phthalonitrila	C H N O	240 [7] 40 [7]	465	123	128	-10	-	-
Tashnara	$C_{31}\Pi_{20}\Pi_4O_2$	40 [7]	105	123	110	90 10	120	1
Pierhanol A6E phthalonitrila	$C_{34}\Pi_{24}\Pi_{4}O_{5}$	0 [7]	10	24	61	-19 52	150	-1 150
Displicitor Aor philaioniune	$C_{31}\Pi_{14}\Pi_{4}O_{2}\Gamma_{6}$	9 [7] 121 [7]	100	1 70	61	52	155	24
Polyester of hydroxybenzoic and hydroxynapthoic acids	$C_{39}H_{22}O_{10}$	121 [7] 164 [7]	80	-84	350	-00 186	130	-34 -34
LaRC-TOR	C44H20N4O2P	135 [7]	208	73	136	1	_	_
LaRC-CP2	C27H18N2O6E6	14 [7]	52	38	31	17	-10	-24
LaRC-CP1	$C_{46}H_{22}N_2O_6F_{12}$	13 [7]	68	55	44	31	-23	-36
PHA-1	$C_{40}O_4N_2H_1A$	42 [24]	146	104	70	28	278	236
РНА-5	$C_{20}S_{4}C_{2}H_{14}$	8 [24]	35	27	-34	_42	_	_
PHA-7	$C_{23}N_2O_3M_{12}$	130 [24]	205	27 75	222	92	390	260
РНА-11	$C_{44}P_2O_4N_2H_{22}$	210 [24]	124	-86		_	_	
РНА-12	$C_{441} 2C_{61} 2132$	73 [24]	106	33	105	32	_	_
BEDB/4 4'-DDS	$C_{28}$ , $2120_{10}$ , $132$	420 [25]	260	_160	300	120	301	_110
BEDB/3 3'-DDS	$C_{341132112075}$	420 [25]	200 260	-160	300	120	1/15	-119 -294
BEDB/m-PDA	CacHaeNaO-	391 [25]	200	_01	295	96	223	_168
	~20**28**205	J I I I I I I I I I I I I I I I I I I I	500	71		20		100

Name	Elemental composition in repeat unit composition	Exp.	New model	Dev	Walters– Lyon	Dev	Lyon et al.	Dev
BEDB/2,4-DT	$C_{27}H_{30}N_2O_5$	372 [ <mark>25</mark> ]	320	-52	367	5	428	56
BEDB/2,6-DT	$C_{27}H_{30}N_2O_5$	530 [ <b>25</b> ]	320	-210	460	70	428	-102
BEDB/2,3-DT	$C_{27}H_{30}N_2O_5$	326 [ <mark>25</mark> ]	320	-6	460	-134	428	102
BEDB/3,4-DT	$C_{27}H_{30}N_2O_5$	415 [ <b>25</b> ]	320	-95	367	48	428	13
BEDB/4-CmP	$C_{26}H_{27}N_2O_5Cl$	169 [ <mark>25</mark> ]	221	52	157	12	181	12
BEDB/5-CmP	$C_{26}H_{27}N_2O_5Cl$	292 [ <mark>25</mark> ]	221	-71	157	135	181	-111
BEDB/4-CoP	$C_{26}H_{27}N_2O_5Cl$	389 [ <mark>25</mark> ]	221	-168	157	232	216	-173
BEDB/3-3'-DMB	$C_{30}H_{36}N_2O_5$	400 [25]	371	-29	423	-23	369	-31
BEDB/3-3'-DMoB	$C_{30}H_{36}N_2O_7$	288 [ <mark>25</mark> ]	326	38	334	-46	394	106
EBPA/DDM	$C_{34}H_{38}N_2O_4$	737 [ <mark>25</mark> ]	554	-183	485	252	241	-496
EBPA/DDS	$C_{33}H_{36}N_2O_6S$	513 [ <mark>25</mark> ]	484	-29	309	204	149	-364
EBPA/m-PDA	$C_{27}H_{35}N_2O_4$	761 [ <mark>25</mark> ]	572	-189	408	353	214	-547
ETBBA/DDM	$C_{34}H_{34}N_2O_4Br_4$	308 [25]	254	-54	177	131	_	_
ETBBA/DDS	$C_{33}H_{32}N_2O_6Br_4S$	443 [ <mark>25</mark> ]	215	-228	88	355	_	_
ETBBA/m-PMA	$C_{27}H_{24}Br_4N_4$	238 [25]	226	-12	79	159	_	_
BPA Polyarylate	C <sub>22</sub> O <sub>5</sub> Cl <sub>2</sub> H <sub>12</sub>	360 [ <mark>26</mark> ]	342	-18	68	-292	29	-331
Chalcone II	$C_{25}O_6H_{18}$	110 [ <mark>26</mark> ]	91	-19	105	-5	286	176

 Table 1
 continued

atoms is important for prediction of the HRC of a desired polymer. Since the presence of the other elements cannot improve the coefficient of determination  $(R^2)$  [14] value, their contributions are zero. Magnitude of  $R^2$  is important for validation of the new correlation because it determines that whether regression accounts for the variation or not. For the value of  $R^2$  equals 1.0, the regression accounts for all of the variations and that the correlation is deterministic. Meanwhile, the value of  $R^2$  equals zero means that the regression accounts for none of the variations [15]. Beside the contribution of the above-mentioned elemental composition, repeat units containing molecular moieties - $(CH_2)_{n>1}-C(X)(Y)-Z-$  or -X-Ar-Y- with specific X, Y and Z groups can increase the value of the HRC on the basis of elemental composition. Moreover, the presence of oxygen and carbonyl groups between two aromatic rings as well as -O-P or >CHCO and -OC(O)- in repeat units can decrease the value of the HRC on the basis of elemental composition. Halogen-containing polymers can also act as heat-resistant polymers with the discovery that some chlorinated organic compounds were highly toxic and/or persistent in the environment. Since the contribution of specific groups in molecular moieties depends on the kind of these groups, different values may be considered, which are given in Table 2. On the basis of the training data set, the correlation of the HRC of a desired polymer can be obtained as follows:

HRC = 97.00

$$+\frac{5850n_{\rm H}-17532n_{\rm N}-7495n_{\rm O}-19601n_{\rm Cl}-83828n_{\rm S}}{\rm MW_{\rm repeat\ unit}}$$

$$+\ 236.5 {\rm HRC}_{\rm (CH_2)_n CXYZ, XArY}-116.2 {\rm HRC}_{\rm YXArZ, Hal}$$
(4)

where HRC is in J  $g^{-1}$  K<sup>-1</sup>;  $n_{\rm H}$ ,  $n_{\rm N}$ ,  $n_{\rm O}$ ,  $n_{\rm Cl}$  and  $n_{\rm Si}$  are the number of moles of hydrogen, nitrogen, oxygen, chlorine, and silicon atoms per mole of repeat unit, respectively; MW<sub>repeat unit</sub> is the molecular weight of repeat unit in g mol<sup>-1</sup>; and HRC<sub>(CH<sub>2</sub>)<sub>n</sub>CXYZ,XArY</sub> and HRC<sub>YXArZ,Hal</sub> are two correcting functions in  $J g^{-1} K^{-1}$  for the presence of molecular fragments  $-(CH_2)_{n>1}-C(X)(Y)-Z-$  or -X-Ar-Y- and Y-X-Ar-Z or halogens (fluorine) in repeat units. The numerical coefficients for  $n_{\rm H}$ ,  $n_{\rm N}$ ,  $n_{\rm O}$ ,  $n_{\rm Cl}$  and  $n_{\rm Si}$  have units of  $J \mod^{-1} K^{-1}$ . Since aliphatic polymers such as vinyl-based polymers have higher energy gap than aromatic or unsaturated polymers containing nitrogen and oxygen, the contribution of molecular fragment  $-(CH_2)_{n \geq 1} - C(X)(Y) - Z - \mbox{ in these polymers can increase}$ significantly the value of HRC(CH2)\_CXYZ,XArY. As seen in Eq. (1), all coefficients of the number of atoms are negative except the coefficient of  $n_{\rm H}$ , which indicate that increasing the values of  $n_{\rm N}$ ,  $n_{\rm O}$ ,  $n_{\rm Cl}$  and  $n_{\rm Si}$  in a desired polymer can decrease the value of the HRC. Since the value of the coefficient  $n_{\rm H}$  is smaller than the coefficients of  $n_{\rm N}$ ,  $n_{\rm O}$ ,  $n_{\rm Cl}$ 

Molecular fragment in repeat unit	X		Y		Ζ		HRC <sub>(CH<sub>2</sub>)<sub>n</sub>CX<sup>*</sup></sub>	YZ,XArY	Example
Predicting HRC <sub>(CH<sub>2</sub>)<sub>n</sub>CXYZ,XA</sub>	rY								
$-(CH_2)_{n>1} - C(X)(Y) - Z -$	–H		-H		-CH <sub>2</sub> -	-	3.3		Polyethylene (PE)
_			–R				2.9		Polypropylene (PP)
			Carbocyclic aroma without substitue	atic ent			1.5		Polystyrene (PS)
			Pyridine				1.1		Poly(2-vinyl pyridine)
			–OH				0.4		Poly(vinyl alcohol) (99%; PVOH)
			Cyclic ether				1.1		Poly(vinyl butyral)
			CN				0.8		Poly(acrylonitrile butadiene styrene) (ABS)
			-H		-OCH	[ <sub>2</sub> -	0.9		Poly(ethylene oxide)
					-C(O) C(O)	–NH– or – )O–	0.2		Polycaprolactam
					-OC(0	D)Ar-O-	0.7		Poly(ethylene terephthalate) (PET)
					-NH- C(O	$C(O)-(CH_2)_m$ )- where $m \leq 1$	- 1.6 8		Poly(hexamethylene adipamide)
	–R		–R		CH <sub>2</sub> -	-	0.4		Polyisobutylene
			-COOH				0.6		Poly(methacrylic acid)
			-COOCH <sub>3</sub>				0.3		Poly(methyl methacrylate) (PMMA)
			Carbocyclic aroma without substitue	atic ent			0.6		Poly(\alpha-methyl styrene)
-X-Ar-Y-	-C(=	=CCl <sub>2</sub> )–	-OC(O)-		-		1.1		BPA Polyarylate
	–CR	R'-	-O-CH <sub>2</sub> - or -O-C	C=N	-		0.6		EBPA/DDM
Molecular moiety in repeat u	nit	X		Y		Ζ	HRC <sub>YXArZ,Hal</sub>	Exar	nple
Estimating HRC <sub>YXArZ,Hal</sub>									
Y–X–Ar–Z		-CO-		Ar		-	2.0	Poly	(benzoyl 1,4-phenylene)
		-O- or simult -O- a SO2- -Ar-C	the presence aneously of both nd $-CO-$ (or $-$ or $-SO-$ ) without $C(CH_3)_2-Ar-$			_	1.0	Poly	(ether ketone) (PEK)
		-О-Р		Ar	or R	-	1.0	Poly	phosphazene
		-		>0	CHCO	-OC(O)-	1.3	Chal	con II
$-CF_3$ or more than one $-CF_2$	2	-		-		-	0.7	Poly (P1	(tetrafluoroethylene) IFE)

Table 2 Values of two correcting functions HRC(CH2), CXYZ, XArY and HRCYXArZ, Hal

and  $n_{\rm Si}$ , its contribution in lowering the HRC is minor. The coefficients of electronegative elements  $n_{\rm N}$  and  $n_{\rm Cl}$  as well as  $n_{\rm Si}$  are much higher than the coefficient of  $n_{\rm O}$ , which indicates increasing  $n_{\rm N}$ ,  $n_{\rm Cl}$  and  $n_{\rm Si}$  is more effective than  $n_{\rm O}$  for reduction in the HRC. Increasing of unsaturation in a new designed heat resistance polymer is one of the appropriate ways for decreasing the value of the HRC because it reduces the value of  $n_{\rm H}$ . Since the addition of relatively small amounts of silicon compounds to various

polymeric materials can improve their flame retardancy [16–18], the coefficient of  $n_{Si}$  in Eq. (4) has the largest negative value with respect to the coefficients of the other atoms. Thus, introducing silicon element and its groups into monomers of suitable polymers such as epoxy can also improve some other properties of the epoxy resins, such as thermal stability, high resistance to thermal oxidation, low surface energy and low toxicity [19, 20]. It was found that phosphorus-containing compounds or resins have been

demonstrated as effective flame retardants for epoxy resins. As indicated in Table 2, this situation has been considered in the new correlation because the presence of -O-P can decrease the value of the HRC through the contribution of the HRC<sub>YXArZ,Hal</sub>. As indicated in Eq. (4), the effects of halogens for decreasing the value of the HRC appear in two terms: (a)  $n_{Cl}$  for chlorine as additive term and (b) HRC<sub>YXArZ,Hal</sub> for fluorine as non-additive contribution. For those polymers such as biphenol phthalonitrile where HRC<sub>(CH<sub>2</sub>)<sub>n</sub>CXYZ,XArY</sub> and HRC<sub>YXArZ,Hal</sub> have no contribution and  $\frac{5850n_{H}-17532n_{N}-7495n_{O}-19601n_{Cl}-83828n_{Si}}{MW_{repeat unit}} < 97$ , the value of the HRC should be taken 20 J g<sup>-1</sup> K<sup>-1</sup>.

The last column of Table 2 indicates the use of two correcting functions in Eq. (4). For example, the value of HRC for poly(2-vinyl naphthalene) is calculated as follows:

#### **Repeating unit:**



Elemental composition and  $MW_{repeat unit}$ :  $n_{\rm H} = 10$ ,  $n_{\rm N} = n_{\rm O} = n_{\rm Cl} = n_{\rm Si} = 0$  and  $MW_{\rm repeat unit} = 154.22 \text{ g mol}^{-1}$ .

The various parameters for repeating unit with general molecular fragment  $-(CH_2)_{n \ge 1}-C(X)(Y)-Z-n = 1$ , X = -H, Y = carbocyclic aromatic without substituent and  $Z = -CH_2-$  where as given in Table 2, the value of  $HRC_{(CH_2)_nCXYZ,XArY}$  is 1.5 J g<sup>-1</sup> K<sup>-1</sup>. Since there is no contribution of  $HRC_{YXArZ,Hal}$ , the value of  $HRC_{YXArZ,Hal} = 0$ . Thus, Eq. (4) gives the value of the HRC as:

$$HRC = 97.00 + \frac{5850(10)}{154.22} + 236.5(1.5) = 831 \text{ J g}^{-1} \text{ K}^{-1}$$

# Statistical parameters in new model and their significance

Table 3 shows important statistical parameters of the new model including regression coefficients, standard errors, t statistics, P values, as well as the upper and lower bounds of a 95% confidence interval. The statistical significance of the regression coefficients in predicting the HRC values can be evaluated on the basis of the above-mentioned statistical parameters as: (1) standard error-if the standard error is small relative to each coefficient, its variable is significant; (2) t statistic—since it is the ratio of coefficients to their standard errors, higher t statistic values correspond to the more significant coefficients [21, 22]; (3) *P* value—it shows the probability that a parameter estimated from the measured data should have the value which was determined. However, the effect of variable is significant and the observed effect is not due to random variations for P value of <0.05 [15]. As seen in Table 3, all statistical parameters show that the proposed nine descriptors in Eq. (4) have a highly significant ability to predict the HRC. As shown in Table 1, the predicted results of the new model, Walters and Lyon [6] and Lyon et al. [8], have been compared with experimental data. For several polymers, the group additivity methods of Walters and Lyon [6] and Lyon et al. [8] cannot be used because some particular functional groups in these polymers are absent for these methods. The predictive reliability of the new method has been tested for some new polymers, which are given in Table 4. As seen in Table 4, the results of the model as well as two group additivity

Table 3 Regression coefficients, standard errors, t statistics, P values and confidence intervals for new model

Variable	Coefficient	SE	t statistic	P value <sup>a</sup>	Lower bound <sup>b</sup> /95%	Upper bound <sup>c</sup> /95%
Intercept	97.00	31.45	3.08	0.00262	34.62	159.38
n <sub>H</sub> /MW <sub>repeat unit</sub>	5850	383	15.29	2.98E-28	5091	6609
n <sub>N</sub> /MW <sub>repeat unit</sub>	-17,532	2490	-7.04	2.21E-10	-22,471	-12,593
n <sub>O</sub> /MW <sub>repeat unit</sub>	-7495	1352	-5.55	2.28E-07	-10,176	-4815
n <sub>Cl</sub> MW <sub>repeat unit</sub>	-19,601	3960	-4.95	2.92E-06	-27,455	-11,746
n <sub>Si</sub> /MW <sub>repeat unit</sub>	-83,828	24,909	-3.37	0.00108	-133,229	-34,427
HRC <sub>(CH2)<sub>n</sub>CXYZ,XArY</sub>	236.5	17.6	13.45	2.05E-24	201.6	271.3
HRC <sub>YXArZ,Hal</sub>	-116.2	24.5	-4.75	6.68E-06	-164.8	-67.7

<sup>a</sup> P value = probability of rejecting a true null hypothesis

<sup>b</sup> Lower bound (95%) = lower bond of a 95% confidence interval

<sup>c</sup> Upper bound (95%) = upper bond of a 95% confidence interval

methods of Walters and Lyon [6] and Lyon et al. [8] have also been compared with experimental data. Among eleven polymers given in Table 4, two group additivity methods can be applied only for seven polymers because these methods do not contain some particular functional groups.

Table 5 shows a comparison between further statistical parameters of Eq. (4) and two group additivity methods for model building and the test dataset. Root-mean-squared (RMS) error provides a reliable indication of the fitness of the model, which is independent of the distribution of data points. RMS values should be low and as similar as possible to ensure both the predictive ability (low values) and generalizability (similar values) [23]. Mean absolute deviation (MAD) is also a linear measure of errors that assesses the average size of errors when negative signs are ignored. Statistical parameters RMS, MAD and maximum of errors of these data for different models are given in Table 5. These parameters for new polymers are close to those obtained for training set. Low values of these statistical parameters confirm high reliability of the new model as compared to two available group additivity methods of Walters and Lyon [6] and Lyon et al. [8].

It should also be mentioned that derivation of Eq. (4) was done from an examination of the HRC of different types of polymers given in Table 1 where their repeat units containing chemical groups/moieties by two principal steps as:

- 1. *Elemental composition:* It was found that the ratios of the number of moles of some atoms ( $n_{\rm H}$ ,  $n_{\rm N}$ ,  $n_{\rm O}$ ,  $n_{\rm Cl}$  and  $n_{\rm Si}$ ) to MW<sub>repeat unit</sub> have important contribution because *P* values of corresponding coefficients are <0.05 [14].
- The presence of some specific molecular fragments: It is possible to correct large deviations of the predicted results of step 1 through introducing two correcting functions HRC<sub>(CH2)<sub>n</sub>CXYZ,XArY</sub> and HRC<sub>YXArZ,Hal</sub> as well as adjusting their coefficients by minimizing RMS error [14].

Figure 1 shows a graphical comparison between the new model and the group additivity methods for all data. As indicated, the predictions of the new model methods exhibit a lower dispersion with respect to both group additivity methods. This is consistent with the fact that the new method has lower RMS values for model building and testing data as compared to group additivity methods. Figure 2 shows the range of absolute errors of the new model (AE =  $|\text{HRC}_{\text{exp.}} - \text{HRC}_{\text{pred.}}|$ ) for all 122 data points given in Tables 1 and 4, which indicate high reliability of the new method.

**Table 4** Comparison of the predicted results of HRC in J  $g^{-1} K^{-1}$  of the new model as well as two molar group contributions of Walters and Lyon [6] and Lyon et al. [8] for some new polymers with the measured values

Name	Elemental composition in repeat unit composition	Exp.	New model	Dev	Walters– Lyon	Dev	Lyon et al.	Dev
BHDB-sulfone (1)	C <sub>26</sub> H <sub>18</sub> O <sub>5</sub> S	120 [27]	134	14	218	98	108	-12
BHDB-sulfoxide (2)	$C_{26}H_{18}O_4S$	66 [27]	157	91	210	144	182	116
BHDB/biphenyl (9)	C <sub>25</sub> H <sub>17</sub> O <sub>4.5</sub> S	86 [ <b>27</b> ]	137	51	333	247	265	179
BHDB/sulfide (10)	$C_{25}H_{17}O_{4.5}S_{1.5}$	138.5 [27]	131	-8	333	195	265	126
PPSU	$C_{24}H_{16}O_4S$	228 [28]	140	-88	182	-46	159	-69
BDHB acrylate	$C_{22}H_{14}O_5$	65 [28]	70	5	39	-26	39	-26
BDHB phosphinate	$C_{20}H_{14}O_4P$	65 [28]	129	64	_	-	_	-
BHDB poly(arylate-co-phosphonate) (1:1)	$C_{42}H_{28}O_9P$	35 [28]	1	-34	_	-	_	-
Polyester carbonate (white)	$C_{37}H_{26}O_{10}$	213 [28]	219	6	126	-87	293	80
Polyester carbonate (gray)	$C_{37}H_{26}O_{10}$	192 [28]	219	27	_	-	_	_
Polyester carbonate (clear)	$C_{37}H_{26}O_{10}$	168 [28]	219	51	-	-	-	-

**Table 5** Statistical parameters of the predicted results of HRC in J  $g^{-1} K^{-1}$  of the new model as well as two molar group contributions of Walters and Lyon [6] and Lyon et al. [8] for model building and testing

	RMS			MAD			Maximum of	Maximum of errors			
	Equation (4)	Walters– Lyon	Lyon et al.	Equation (4)	Walters– Lyon	Lyon et al.	Equation (4)	Walters– Lyon	Lyon et al.		
Model building	80	147	208	58	100	129	237	605	681		
Testing	50	141	102	40	120	87	91	247	179		



Fig. 1 Predicted results of HRC in J  $g^{-1}$  K<sup>-1</sup> for the new model (122 data) as well as two molar group contributions of Walters and Lyon [6] (117 data) and Lyon et al. [8] (108 data) versus experimental data



Fig. 2 Range of absolute errors of the new model for all data points (122 data)

## Conclusions

A simple and accurate model was developed for prediction of the HRC values of different polymers with their repeat units that are comprised of chemical groups/moieties such as methyl, phenyl, carbonyl, ether, amide and ester. The model is based on the contribution of  $n_{\rm H}$ ,  $n_{\rm N}$ ,  $n_{\rm O}$ ,  $n_{\rm Cl}$  and  $n_{\rm Si}$  divided by MW<sub>repeat</sub> unit as well as two correcting functions of HRC<sub>(CH<sub>2</sub>)<sub>n</sub>CXYZ,XArY</sub> and HRC<sub>YXArZ,Hal</sub>. The predicted results of the new model were compared with the calculated data of two group additivity methods, which confirm higher reliability of the new correlation. The values of  $HRC_{(CH_2)_nCXYZ,XArY}$  and  $HRC_{YXArZ,Hal}$  beside elemental composition and  $MW_{repeat unit}$  can be easily obtained from repeat units of polymers.

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