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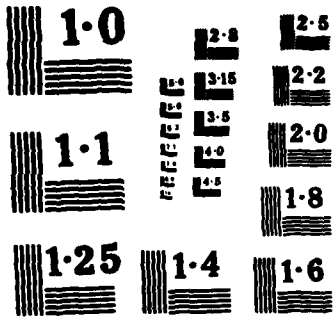
CALCULATION OF THE GLASS TRANSITION TEMPERATURES OF  
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November 1984

**CALCULATION OF THE GLASS  
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PART 1- RULES FOR HIERARCHICAL  
ORDERING OF THE DATA SET**

by

W. A. Lee

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CALCULATION OF THE GLASS TRANSITION TEMPERATURES  
OF LINEAR POLYMERS

PART 1 - RULES FOR HIERARCHICAL ORDERING  
OF THE DATA SET

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W. A. Lee

SUMMARY

The rational ordering of polymers in a large data set for the correlation of glass transition temperature ( $T_g$ ) with structure requires the establishment of seniority criteria. An extension of polymer nomenclature rules published by the International Union of Pure and Applied Chemistry is proposed and applied, with examples, to the groups in a large polymer data set. The rules can be extended to cover new polymers without upsetting the original order.

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## 1 INTRODUCTION

In a recent memorandum<sup>1</sup> the importance and significance of the transition temperatures of polymers was described and earlier papers concerned with the calculation of the glass transition temperature ( $T_g$ ) were listed. Many reasons were given to justify the  $T_g$  as one of the most important properties of a polymer especially in the sense that the practical role of a polymer depends to a great extent on the  $T_g$  value. With that in mind it is not surprising that the estimation of  $T_g$  in advance of synthesis has been a prime goal for many of the workers engaged in the synthesis, or development, of new useful polymers.

For the estimation of  $T_g$ , which is determined by the segmental relaxation rate of the constituent groups in polymers, it is highly desirable to base empirical calculations on as large a data set as practicable. It is hoped thereby to enhance the reliability of the data and, by increasing the number of different polymer environments in which constituent groups are represented, to increase confidence in the prediction of  $T_g$  values of polymers outside the data set. The data set in the series of calculations to be described comprises over 1100 polymers and is the largest set so far used in this type of work. In order to avoid duplication of structures in this set and to enable any particular polymer to be located as easily as possible, the set must be ordered. Thus, a set of criteria must be established which distinguishes between the structural characteristics of every polymer present. It is the object of this Report to define the criteria which have been employed.

## 2 SENIORITY CRITERIA FOR CONSTITUENT GROUPS

The seniority criteria for groups in polymers are based on rules described in an earlier report<sup>2</sup> with some enhancement and amendment. Thus, diradical seniority is basically determined according to the IUPAC tentative rules for systematic polymer nomenclature<sup>3</sup>. All the information necessary to extend the system is presented in this Report.

### 2.1 Criteria for all categories of groups

Polymer groups are divided into main-chain (MC) groups, which are most senior, and side-chain (SC) groups: amongst SC groups, a monoradical (terminal) group is subordinate to any multi-radical group. Each of these three categories are sub-divided into four further categories which, in decreasing order of seniority are:

- I containing a heterocyclic ring;
- II containing an element other than C (hydrogen being regarded as a substituent);
- III containing a carbocyclic ring;
- IV containing a carbon chain acyclic group.

Numbered criteria for determining seniorities within these classes are provided in three sets appropriate to categories I, II, III and IV. All the criteria could be combined into one system, but it is easier in practice to make the above subdivisions first and apply special criteria to the individual sets. A group which satisfies the criteria corresponding to the lowest criterion number has the highest seniority.

In the application of the criteria to SC groups which have branches, the SC groups are given the status of MC groups and the branch groups are regarded as side-chains to these "promoted" MC groups.

In the rules which follow, heteroatoms which are not actually in a ring, but are bonded to rings, are regarded as substituents, eg oxo substituents. When heteroatoms are bonded to acyclic structures they are also regarded as substituents to these structures, eg O bonded to S, or C is a substituent to the group containing S or C. Rings are numbered according to The Ring Index and otherwise according to IUPAC Nomenclature rules. In ring systems, it is assumed that groups and their mirror images have the same numbering.

## 2.2 Criteria for heterocyclic groups (categories I MC and I SC)

- (a) Containing nitrogen and a heteroatom other than nitrogen as high as possible in the descending order, O, S, Se, Te, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, and Hg, the positions of other atoms being determined within this order by their positions in the periodic table.
- (b) Containing nitrogen.
- (c) Containing a heteroatom other than nitrogen as high as possible in the descending order, O, S, Se, Te, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, and Hg: the positions of other atoms are determined within this order by their positions in the periodic table.
- (d) Having the largest number of rings which are fused (joined at more than one atom).
- (e) Having the largest number of the largest rings.
- (f) Having the largest number of heteroatoms (excluding substituents like F, oxo etc as noted above).
- (g) Having the greatest variety of heteroatoms.
- (h) Having the largest number of heteroatoms highest in the order of criterion(1).
- (j) Having the most unsaturated system (largest number of multiple bonds).
- (k) Having the lowest numbers for points of attachment between rings within the assembly consistent with the fixed numbering of the parent ring.
- (l) Having the lowest heteroatom locants.
- (m) Having the largest number of free (radical) bonds.
- (n) Having the largest number of heteroatom substituents.
- (o) Having the lowest MC free-bond locants.
- (p) Having the lowest SC free-bond locants.
- (q) Having the lowest substituent locants.
- (r) Having substituents whose names are highest in alphabetical order.
- (s) Having a cis configuration.

- (t) Having a trans configuration.
- (u) Having a specification other than cis or trans.

2.3 Criteria for carbocyclic groups (categories III MC and III SC)

- (a) Having the largest number of rings which are fused (joined at more than one atom).
- (b) Having the largest number of the largest rings.
- (c) Having the largest number of atoms common to rings.
- (d) Having the most unsaturated system (largest number of multiple bonds).
- (e) Having the largest number of free bonds.
- (f) Having the lowest locant numbers at the first point of difference for ring junctions.
- (g) Having the largest number of heteroatom substituents.
- (h) Having the lowest MC free-bond locants.
- (j) Having the lowest SC free-bond locants.
- (k) Having the lowest substituent locants.
- (l) Having substituents whose names are highest in alphabetical order.
- (m) Having a cis configuration
- (n) Having a trans configuration.
- (o) Having a specification other than cis or trans.

2.4 Criteria for acyclic groups (categories II MC, II SC, and IV SC)

- (a) Containing a heteroatom as high as possible in the descending order F, Cl, Br, I, O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B and Hg: the positions of other atoms being determined within this order by their positions in the periodic table.
- (b) Having the largest number of heteroatoms.
- (c) Having the greatest variety of heteroatoms.
- (d) Having the largest number of heteroatoms highest in the order of criterion (a).
- (e) Having the largest number of MC multiple bonds.
- (f) Having the largest number of multiple bonds between MC and SC or substituents.
- (g) Having the lowest heteroatom locants.
- (h) Having the largest number of free bonds.
- (j) Having a heteroatom substituent highest in the order of criterion (a).
- (k) Having the largest number of heteroatom substituents.
- (l) Having the greatest variety of heteroatom substituents.
- (m) Having the largest number of heteroatom substituents highest in the order of criterion (a).

- (n) Having the lowest MC free-bond locants.
- (o) Having the lowest SC free-bond locants.
- (p) Having a cis configuration.
- (q) Having a trans configuration.
- (r) Having an isotactic configuration.
- (s) Having a syndiotactic configuration.
- (t) Having a specification other than cis, trans, isotactic or syndiotactic.

The application of these seniority rules to the polymers in the present data set leads to the set of groups which are arranged in hierarchical order in Table 1. Within the calculations themselves, groups with fluorine substituents have been treated as though a fluorine substituents were part of the group to which it was attached rather than a separate group. Such combined groups have been included in Table 1 for the purpose of keeping all the group drawings together, but they have been given the same seniority as they would have had if the fluorine substituents were replaced by free bonds. Each group has been given an arbitrary number for reference purposes. It will be noticed that both asymmetric groups and their mirror images are shown, for example, the second and third groups denoted 170 and 167. These groups are, of course, identical and have the same seniority, but it is necessary to use both forms in order to discriminate between different points of attachment to them. This will be made clear in the numerical analysis of polymers which is described in a later report in this series. Main- and side-chain groups which belong to series of identical groups of general formula  $-(CX)_n$  have all been distinguished by different numbers for different values of  $n$ . In any particular series they have the same seniority, but in polymer situations, the rules for ordering polymers place the sequences in the order shown. This becomes apparent in detailed analysis studies. The drawings were plotted from a computer file of data used for drawing polymer structures in which some structures have lengthened bonds to avoid overlapping structures. For this reason some of the bonds on some drawings are shown to be longer than would be expected. All groups up to and including group 321 on page 5 of Table 1 are MC groups and all groups thereafter are SC groups, all groups after group 7 on page 6 are terminal SC groups. MC bonds are shown as horizontal lines up to group 321, bonds at any other angle denote SC attachments.

### 3 SENIORITY CRITERIA FOR POLYMERS

The following rules are in priority order. The most senior polymer is that containing in the chemical repeating unit (CRU) the:-

- (1) Most senior group (see seniority rules for atoms and groups) which is placed at the extreme left hand end of a graphical representation.
- (2) Shortest bridge (number of atoms in the MC) from the first group (the most senior) to the next occurrence of this group in the infinite polymer (not in the CRU, which may contain only one such group). The shortest bridge is placed at the extreme left hand end of the graphical representation.

(3) Shortest sequence of bridges in the infinite polymer between the most senior group and the next occurrences of groups which are identical with the most senior group. A bridge sequence of 1,1,4,9 is senior to a bridge sequence of 1,3,1,5. (At the first point of difference 1,1,4,9 has the shortest bridge.) Note, therefore, that the most senior bridge is not necessarily that with the most senior group in it.

(4) Most senior group at the first point of difference proceeding from left to right through the CRU regardless of the seniority of the groups which occur in the bridge(s) beyond the first point of difference.

(5) Most senior SC, which is that with the most senior group in the first SC from the left, at the first point of difference travelling away from the MC and proceeding if necessary, down any branch. If, in two polymers being compared, the first SC from the left are identical, the second then the third, etc, SC are compared until the first point of difference is reached.

(Asymmetrical groups and their mirror images are regarded as having the same seniority.)

Table 2 has been constructed to illustrate the application of the seniority criteria described in this section. The polymers are in decreasing seniority order from left to right and from top to bottom. Rule 1 applies to all polymers. Rule 2 places Polymer 849 senior to Polymer 271 because in the former the first bridge between the first group (-O-) and the next occurrence of this group consists of a -CH<sub>2</sub>- group whereas the comparative bridge in Polymer 271 comprises two groups (-CO-CO-) which is longer. Rule 3 places Polymer 1157 senior to Polymer 1162 because although a g-phenylene group is senior to a -CF<sub>2</sub>- group, the sequence of bridges in the respective polymers is 3, 9 and 3, 12 which makes the former sequence senior. Rule 4 places Polymer 1250 senior to Polymer 1248 because the polymers have the same bridge sequence, that is 0, 15 and at the first point of difference from the left the group -O- is senior to the group -NH. Rule 5 places the next four polymers in the order 27, 34, 29, 15. Polymer 27 is senior to Polymer 34 because in the SC the second group in the horizontal branch from the first branch point is senior to its comparable group in Polymer 34 at the same atom-distance from the MC. (-CH- is senior to -CH<sub>3</sub> and also -CH<sub>2</sub>- is senior to -CH<sub>3</sub> in the vertical branch.) Polymer 34 is senior to Polymer 29 because the nearest group to the horizontal SC branch point (-CH<sub>2</sub>-) is senior to the group (-CH<sub>3</sub>) in the corresponding position in Polymer 29. Polymer 29 is senior to Polymer 15 because at the first point of difference, which occurs at the second branch point in the SC of Polymer 29, the group -CH- is senior to -CH<sub>2</sub>-) which is the corresponding group in Polymer 15.

#### 4 CONCLUSIONS

A system is proposed for the unambiguous classification of single-strand organic polymers in hierarchical order. The system greatly facilitates the location of polymers within classified lists and eliminates the need for multiple naming and indexing: it is therefore particularly appropriate for polymer data handbooks and like publications. The system can readily be extended by the application of rules of nomenclature in current use, without upsetting the existing order.

Table 1  
GROUPS IN HIERARCHY ORDER

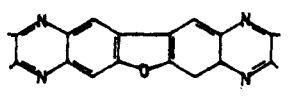
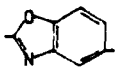
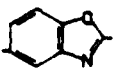
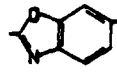
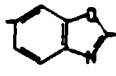



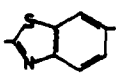
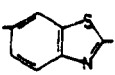


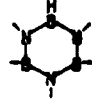
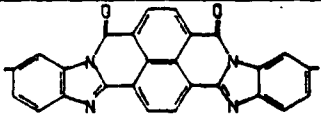
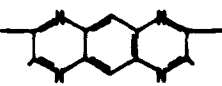
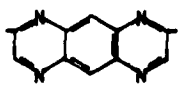
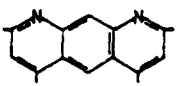
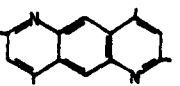
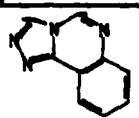
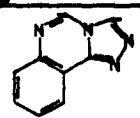
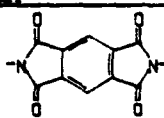
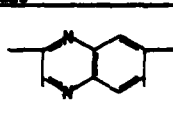
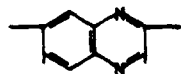
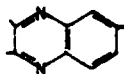
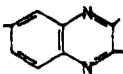
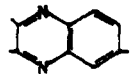
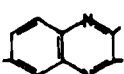
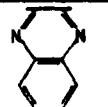
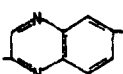
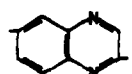
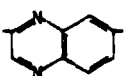
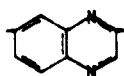
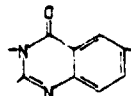
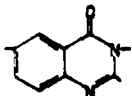
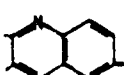
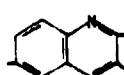
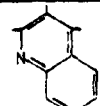
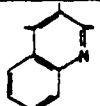
			
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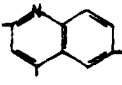
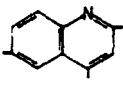
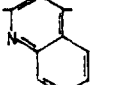
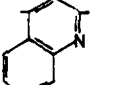
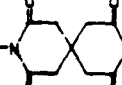
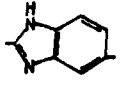
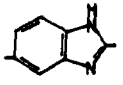
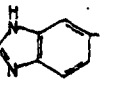
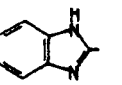
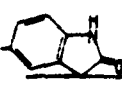
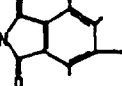
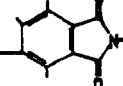
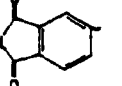
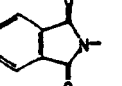
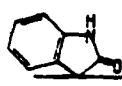
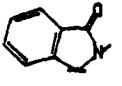
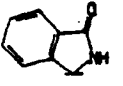
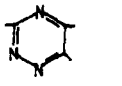




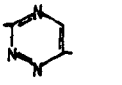
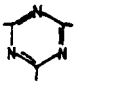

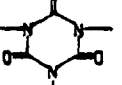
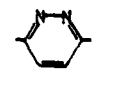

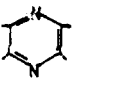
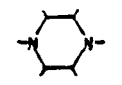
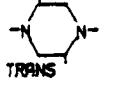
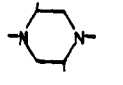
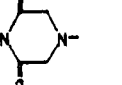
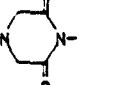
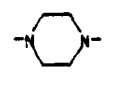







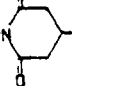
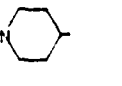
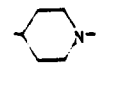



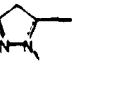

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 256	 90	 257	 89	 226
 260	 261	 243	 84	 80
 82	 81	 285	 285	 287
 284	 283	 288	 100	 258
 289	 99	 143	 202	 278
 205 TRANS	 270	 278	 275	 72
 144	 145	 182	 152	 279
 280	 231	 291	 203	 204
 273	 274	 92	 282	 283

Table 1 (Continued)



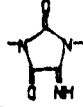
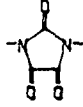
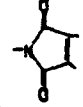
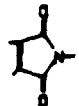
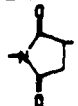

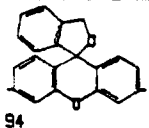
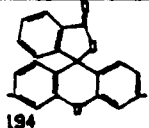
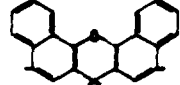
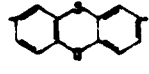

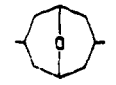
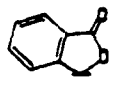










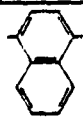
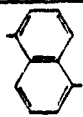
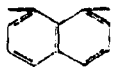
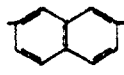
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 288	 289	 282	 94	 194
 3	 283	 4	 277	 83
 78	 185	 78	 86	 33
$\text{-C}_{10}\text{H}_{10}\text{C-}$ METR 101	$\text{-C}_{10}\text{H}_{10}\text{C-}$ PRRN 18	$\text{-C}_8\text{H}_8\text{C-}$ 128	$\text{-O-}$ 108	$\text{-N-}$ 108
 120	 148	 118	$\text{-S-}$ 118	$\text{-N-}$ 151
$\text{-NPF}_2$ 134	$\text{-N=N-}$ 110	$\text{-N=}$ 217	$\text{-N-}$ 104	$\text{-N-}$ 192
$\text{-NH-}$ 102	$\text{-P-}$ 113	$\text{-S-}$ 115	$\text{-P-}$ 112	$\text{-A-}$ 212
$\text{-S-}$ 172	$\text{-S-}$ 215	$\text{-S-}$ 121	$\text{-S-}$ 173	 223
 89	 62	 84	 57	 68

Table 1 (Continued)

65	222	69	186	154	199	224	58
141	190	163	53	55	140	147	165
47	49	51	189	166	41	40	39
38	37	8	9	34	184	183	43
TRNS	-C=C-						
42	29	28	191	25	150	176	148
149	28	31	5	219	22	23	19
138	132	402	403	404	405	408	407
408	409	410	411	412	413	414	415
416	417	418	419	420	421	18	17
14	129	6	302	303	304	305	306

Table 1 (Continued)


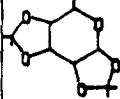
























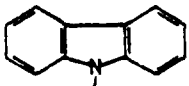







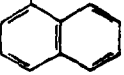
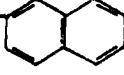




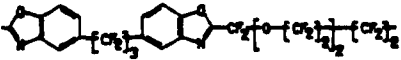
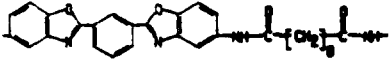
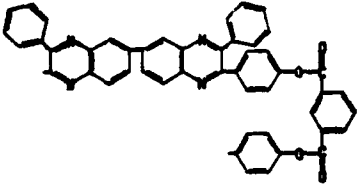
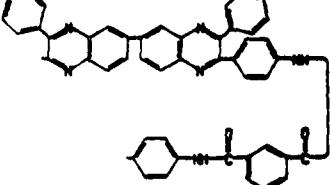
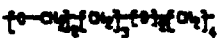
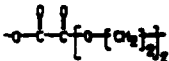
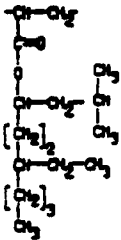
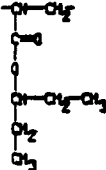
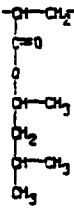
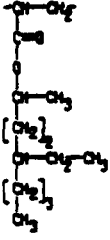
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307	308	309	310	311	312	313	314
$[\text{CH}_2]_{15}$	$[\text{CH}_2]_{16}$	$[\text{CH}_2]_{17}$	$[\text{CH}_2]_{18}$	$[\text{CH}_2]_{19}$	$[\text{CH}_2]_{20}$	$[\text{CH}_2]_n$	
315	316	317	318	319	320	321	210
			$\text{O}=\text{S}=\text{O}$	$\text{S}=\text{O}$	$\text{S}$	$\text{N}^+$	$\text{N}^-$
207	158	109	211	119	117	218	105
$\text{NH}$		$\text{P}$	$\text{As}$	$\text{Sb}$	$\text{Bi}$	$\text{At}$	$\text{Sn}$
103	114	213	171	214	173	122	135
							
70	80	187	142	58	57	54	181
							
201	138	56	164	139	169	48	50
				$\text{C}$	$\text{CH TRANS}$	$\text{CH}$	$\text{O}$
52	137	153	160	21	182	27	32
$\text{N}^-$	$[\text{CH}_2]$	$\text{C}^-$	$\text{CF}^-$	$[\text{CF}_2]_n$	$[\text{CF}_2]_{20}$	$[\text{CF}_2]_{19}$	$[\text{CF}_2]_{18}$
157	180	20	158	471	470	469	468
$[\text{CF}_2]_{17}$	$[\text{CF}_2]_{16}$	$[\text{CF}_2]_{15}$	$[\text{CF}_2]_{14}$	$[\text{CF}_2]_{13}$	$[\text{CF}_2]_{12}$	$[\text{CF}_2]_{11}$	$[\text{CF}_2]_{10}$
487	488	485	484	483	482	481	480
$[\text{CF}_2]_9$	$[\text{CF}_2]_8$	$[\text{CF}_2]_7$	$[\text{CF}_2]_6$	$[\text{CF}_2]_5$	$[\text{CF}_2]_4$	$[\text{CF}_2]_3$	$[\text{CF}_2]_2$
459	458	457	456	455	454	453	452

Table 1 (Concluded)

$\overset{ }{\text{CF}}_2$	$\overset{ }{\text{CF}}_3$	$\overset{ }{\text{CH}}^-$	$\overset{ }{\text{FCH}}$	$\overset{ }{\text{CHF}}_2$	$\overset{ }{\text{CH}_2}_n$
133	131	15	130	200	371
$\overset{ }{\text{CH}_2}_{20}$	$\overset{ }{\text{CH}_2}_{19}$	$\overset{ }{\text{CH}_2}_{18}$	$\overset{ }{\text{CH}_2}_{17}$	$\overset{ }{\text{CH}_2}_{16}$	$\overset{ }{\text{CH}_2}_{15}$
370	369	368	367	366	365
$\overset{ }{\text{CH}_2}_{14}$	$\overset{ }{\text{CH}_2}_{13}$	$\overset{ }{\text{CH}_2}_{12}$	$\overset{ }{\text{CH}_2}_{11}$	$\overset{ }{\text{CH}_2}_{10}$	$\overset{ }{\text{CH}_2}_9$
364	363	362	361	360	359
$\overset{ }{\text{CH}_2}_8$	$\overset{ }{\text{CH}_2}_7$	$\overset{ }{\text{CH}_2}_6$	$\overset{ }{\text{CH}_2}_5$	$\overset{ }{\text{CH}_2}_4$	$\overset{ }{\text{CH}_2}_3$
358	357	356	355	354	353
$\overset{ }{\text{CH}_2}_2$	$\overset{ }{\text{CH}_2}$	$\overset{ }{\text{CH}_2}\text{F}$			
352	7	129	178	79	
					
99	95	96	177	75	74
	$\overset{ }{\text{Cl}}^-$	$\overset{ }{\text{Cl}}$	$\overset{ }{\text{Br}}$	$\overset{ }{\text{I}}$	$\overset{ }{\text{NO}_2}$
73	218	125	124	127	111
$\overset{ }{\text{CH}}\text{O}$	$\overset{ }{\text{OH}}$	$\overset{ }{\text{CH}}\text{N}$	$\overset{ }{\text{NH}_2}$		
30	107	24	174	61	62
				$\overset{ }{\text{CH}}\text{CH}_2$	$\overset{ }{\text{CH}_3}$
ISOTACTIC 46	45	36	44	25	1

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Table 2  
ILLUSTRATIONS OF SENIORITY CRITERIA

 <p>POLYMER 1187</p>	 <p>POLYMER 1182</p>		
 <p>POLYMER 1288</p>	 <p>POLYMER 1248</p>		
 <p>POLYMER 848</p>	 <p>POLYMER 271</p>		
 <p>POLYMER 27</p>	 <p>POLYMER 34</p>	 <p>POLYMER 29</p>	 <p>POLYMER 15</p>

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<u>No.</u>	<u>Author</u>	<u>Title, etc</u>
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**REPORT DOCUMENTATION PAGE**

Overall security classification of this page

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