

IR Identification of PC, ODA, and Their Reaction Products

Abbreviations for band assignments

v...stretching vibration
 δ ...deformation vibration
 ω ...wagging vibration
 ρ ...rocking vibration
 γ ...scissoring vibration
as...asymmetric
s...symmetric
o.o.p....out of plane
i.p....in plane

Abbreviations for band intensities

vw...very weak; w...weak; m...medium; strong; vs...very strong

Table S1. Assorted band assignments of Bisphenol-A based Polycarbonate (PC).

Wavenumber (cm ⁻¹)	Band assignment	Intensity	Molecular structure	References
3046	ν CH	w	aromatic ring (Ar)	[1,3]
2970	ν_{as} CH	m	CH ₃	[1,3]
2870	ν_s CH		CH ₃	[3]
1775 (dubl. 1785 trans-cis, 1767 trans-trans)	ν C=O	s	-O-(C=O)-O-, Ar-O-C(=O)-O-Ar	[2,4,6]
1600	δ_s CH, ν_{ip} CC ν CC	vw	aromatic ring	[3–5]
1505	ν C-C δ_{as} CH, Dublett, ν CC	s	aromatic ring	[2,3]
1462	δ CH, ν C=C, $\delta_{as, i.p.}$ CH	vw	CH ₃	[3,5]
1409	$\delta_{as, i.p.}$ C-H	vw	CH ₃	[3]
1388	δ_s CH, $\delta_{s, i.p.}$ CH	vw	CH ₃	[5,7]
1365	δ_{as} CH, Dublett, $\delta_{s, i.p.}$ CH	vw	CH ₃	[3,5]
1227	ν_{as} COC, δ C=O, ν O-C(O)-O	vs, broad	-O-(C=O)-O-, aromatic ring	[3,5,6]
1191	ν_{as} O-C(O)-O, $\omega_{i.p.}$ CH,	vs	-O-(C=O)-O-,	[3,5,6]
1168	ν O-(C=O)-O, ν COC, C-C, $\omega_{i.p.}$ CH	s	-O-(C=O)-O-, aromatic ring	[1,3,5,6]
1102	$\delta_{i.p.}$ CH	w	aromatic ring	[3]
1080	γ CCC, δ CH	m	aromatic ring	[2]

1009	ν_s OCO, ν OC	s	-O-(C=O)-O-, aromatic ring	[1-3,5]
884	ν C-C, $\delta_{o.o.p.}$ CH	w	C-CH ₃	[3,5]
830	$\delta_{o.o.p.}$ CH, ω CH, $\gamma_{o.o.p.}$ CH	m	aromatic ring	[2,3]

1. Dechant, J. *Ultrarotspektroskopische Untersuchungen an Polymeren*; Akademie-Verlag: Berlin, Germany, 1972.
2. Kraus, R.G.; Emmons, E.D.; Thompson, J.S.; Covington, A.M. *J. Polym. Sci Part P Polym. Phys.* **2008**, *46*, 734–742.
3. Asensio, R.C.; Moya, M.S.A.; de la Roja, J.M.; Gomez, M. *Anal. Bioanal. Chem.* **2009**, *395*, 2081–2096.
4. Heymans, N.; Dequenne, B. *Polymer* **2001**, *42*, 5337–5342.
5. Lee, S.-N.; Stolarski, V.; Letton, A.; Laane, J. *J. Mol. Struct.* **2000**, 52119–52123.
6. Sweileh, B.A.; Al-Hiari, Y.M.; Kailani, M.H.; Mohammad, H.A. *Molecules* **2010**, *15*, 3661–3682.
7. Abbate, M.; Martuscelli, E.; Musto, P.; Ragosta, G.; Scarinzi, G. *J. Polym. Sci Part B Polym. Phys.* **1994**, *32*, 395–408.

Table S2. Assorted band assignments of Octadecylamine (ODA).

Wavenumber (cm ⁻¹)	Band assignment	Intensity	Molecular structure	References
3331	ν_{as} NH	s	NH ₂	[1]
3255	ν_s NH	w	NH ₂	[1]
3173	2 δ NH overtone Amide II	m		[2]
2954	ν_{as} CH	m	CH ₃	
2917	ν_{as} CH	vs	CH ₂	[3]
2848	ν_s CH	s	CH ₂	[4]
1647		w		
1608		m		
1565	Amide II	m		[2,4]
1485	δ_{as} CH	m	CH ₃	[5]
1465	δ_{as} CH	m-s	CH ₂	
1437	δ_s CH	w-m	CH ₂	[3]
1380	δ_s NH	w	CH ₂	[3]
1307		w		
1150		w		
1113		w		
1060	ν CN	m		
1045		w		
894	ρ CH	m	CH ₂	[3]
719		w		

1. Sokoll, R.; Hobert, H. *J. Chem. Soc. Faraday Trans. I* **1986**, *82*, 1527–1535.
2. Spange, S.; Wolf, S.; Simon, F. *Progr. Colloid Polym. Sci.* **2006**, *132*, 110–116.
3. Rivas, B.L.; Seguel, G.V.; Geckeler, K.E. *Die angewandte Makromolekulare Chemie* **1997**, *251*, 97–106.
4. Das, P.K.; Ruzmaikina, I.; Belfiore, L.A. *J. Polym. Sci Part B: Polymer Phys.* **2000**, *38*, 1931–1938.
5. Kraus, R.G.; Emmons, E.D.; Thompson, J.S.; Covington, A.M. *J. Polym. Sci Part P Polym. Phys.* **2008**, *46*, 734–742.

Table S3. Assorted band assignments of Bisphenol-A (BPA).

Wavenumber (cm ⁻¹)	Band assignment	Intensity	Molecular structure	References
3350	ν_{as} OH	s, broad	associated, H-bond	[1]
3065	ν CH	w	aromatic ring	[2]
3029	ν CH	w	aromatic ring	[1]
2966	ν_{as} CH	s	CH ₃	[1]
2871	ν_s CH	s	CH ₃	[1]
1612		s-m	p-substituted aromat	[1]
1598		s-m	p-substituted aromat	[1]
1511		s		[1]
1455		s-m		
1363		m	C-CH ₃	[1]
1178		s		[1]
826		m		[1]

1. Fei, B.; Chen, C.; Peng, S.; Zhao, X.; Wang, X.; Dong, L. *Polymer Int.* **2004**, *53*, 2092–2098.
2. Abbate, M.; Martuscelli, E.; Musto, P.; Ragosta, G.; Scarinzi, G. *J. Polym. Sci Part B Polym. Phys.* **1994**, *32*, 395–408.

Table S4. Assorted band assignments of urethane.

Wavenumber (cm ⁻¹)	Band assignment	Intensity	Molecular structure	References
3453	v NH	w	non H-bonded	[1]
3381	v NH, Ar-O-C(=O)-NH-R	m	H-bonded	[2,3]
3330-3320	v NH	w	H-bonded	[1]
3280	v NH	sh, w	H-bonded	[1]
3060	v CH	vw	aromatic ring	
1715-1690	v C=O	s	aliphatic-aromatic H-bond, non H-bond	[1,4,5,8–11]
1530	γ N-H+v C-N, Ar-O-C(=O)-NH-R	s-m	secondary urethanes	[1,4,6,13]
1506	v C-C, ring	m	secondary urethanes, associated or in solid phase	[4]
1470	γ NH + v CN, γ CH aliphatic, Ar-O-C(=O)-NH-R	m	γ CH ₂ + ω CH ₂	[7]
1387	δ _s CH, δ _{s, i.p.} CH	vw	CH ₃ , compare to Polycarbonate	
1220	v CN, v CO	s-m	secondary urethanes, associated or in solid phase	[7,12,13]
1170	v as COC	s		[7,13]
1080	v COC	m	v s C-O-C aliphatic,	[7,13]
1020	v COC, v CN, aliphatic, Ar-O-C(=O)-NH-R	m		[7,13]

1. McCarthy, S.J.; Meijs, G.F.; Mitchell, N.; Guntillake, P.A.; Heath, G.; Brandwood, A.; Schindhelm, K. *Biomaterials* **1997**, *18*, 1387–1409.
2. Yu, S.; Ma, M.; Liu, J.; Tao, J.; Liu M.; Gao, C. *J. Membr. Sci.* **2011**, *379*, 164–173.
3. Li, M.-S.; Ma, C.-C.M.; Lin, M.-L.; Lu, M.-S.; Chen, J.-L.; Chang, F.-C. *Polymer* **1997**, *38*, 845–853.
4. Lin, M.-L.; Chang, K.-H.; Chang, F.-C.; Li, M.-S.; Ma, C.-C.A. *J. Polym. Sci. Part B Polym. Phys.* **1997**, *35*, 2183–2191.
5. Günzler, H.; Gremlich, H.-U. *IR-Spektroskopie - Eine Einführung*; Wiley-VCH: Weinheim, Germany, 2000.
6. Lee, S.-N.; Stolarski, V.; Letton, A.; Laane, J. *J. Mol. Struct.* **2000**, *521*, 19–23.
7. Mendoza-Payan, J.G.; Gallardo, S.F.; Marquez-Lucero, A. *Sens. Actuators B* **2009**, *142*, 130–140.
8. Coleman, M.M.; Lee, K.H.; Skrovanek, D.J.; Painter, P.C. *Macromolecules* **1986**, *19*, 2149–2157.
9. Corcuera, M.A.; Rueda, L.; Fernandez d'Arlas, B.; Arbelaiz, A.; Marieta, C.; Mondragon, I.; Ecaiza, A. *Polym. Degrad. Stab.* **2010**, *95*, 2175–2184.
10. Coleman, M.M.; Skrovanek, D.J.; Hu, J.; Painter, P.C. *Macromolecules* **1988**, *21*, 59–65.
11. Dechant, J. *Ultrarotspektroskopische Untersuchungen an Polymeren*; Akademie-Verlag: Berlin, Germany, 1972.
12. Nyquist, R.A.; Potts, W.J. *Spectrochim. Acta* **1961**, *17*, 679–697.
13. Socrates, G. *Infrared and Raman Characteristic Group Frequencies*, 3rd Ed.; Wiley: Hoboken, NJ, USA, 2001.