Lab Documentation

Student Instructions

I. Method 1 - Dibenzyl Terephthalate From PET

Week 1 - Dibenzyl Terephthalate From PET

Equipment/Glassware	Equipment/Glassware
• stirrer	• reflux condenser & rubber tubing
• thermowell	• stopcock grease
• 100 mL round bottom flask	• scissors
• cork ring	• 400 mL beaker
• magnetic stir bar	• powder funnel
• ring stand & clamp	• 50 mL graduated cylinder
• keck joint clip for 19/22 glassware	• spatula

Chemicals	Precautions
• PET (strips obtained from a 2-liter pop bottle)	• none
• benzyl alcohol	• irritant and hygroscopic
• zinc acetate	• toxic and irritant

Summary of procedure: PET is refluxed in an excess of benzyl alcohol in the presence of a metal catalyst (zinc acetate) for 24 hours. The product mixture is washed with water. With the addition of methanol and cooling the crude product precipitates. The product is recovered by filtration and purified by recrystallization from methanol.

1. Pre-weigh a 100 mL round bottom flask on the top-loading balance. Set the flask on the cork ring when doing this. Record the weight of the round bottom flask on the Data Sheet. Add between 2.5-3.0 g of PET to the 100 mL round bottom flask. Use the following procedure to accomplish this task. Return to your station. Place the 100 mL round bottom flask in a 400 mL beaker and place the neck of a powder funnel inside the neck of the round bottom flask. Obtain about eight strips of PET from the instructors desk. Prior to cutting these strips, place enough of them on the top-loading balance to reach between 2.5-3.0 g. Using a pair of scissors cut the strips of PET into squares (0.25 in. x 0.25 in.) while holding the strips over the mouth of the funnel. This way most of the squares will fall into the round bottom flask. Some PET squares will miss the flask and end up on the lab bench. These pieces can be gathered up and added to the round bottom flask as well. Determine the weight of the PET added to the round bottom flask on the top-loading balance and record the weight on the Data Sheet.

2. To the round bottom flask add a stir bar, 30 mL of benzyl alcohol, and 0.6 g zinc acetate. Measure out the benzyl alcohol using the 50 mL graduated cylinder. Weigh out zinc acetate on a weigh boat. Transfer these chemicals to the round bottom flask with the aid of the powder funnel. The round bottom flask should now contain, the PET squares, the stir bar, the benzyl alcohol and the zinc acetate.

3. Consult with your instructor as to which hood to use to run this reaction. Attach a reflux condenser to the round bottom flask. Be sure the two standard taper joints are properly greased. Secure the joints with a blue plastic clip. Place the round bottom flask and condenser assembly in the thermowell and the thermowell on top of the stirrer. Secure the assembly by positioning the clamp on the ring stand so that the neck of the round bottom can be clamped. Turn on the stirrer and adjust the speed of the stirrer so

the stir bar spins at a moderate rate. Wrap the exposed part of the round bottom flask with aluminum foil. Using marking tape, place a label near the top of the condenser identifying your group and lab section number.

4. Once the rubber tubing is properly connected and water is flowing through the condenser, turn the power on to the thermowell. A moderately high setting will be needed in order to get the benzyl alcohol to boil. Its boiling point is 205°C. The assembly should be checked before leaving lab to ensure the mixture is refluxing (boiling). This can be established by observing the benzyl alcohol vapors condensing an inch or two up the condenser. This reaction will be allowed to run for one day and then will be turned off for you. At the start of the second lab period, you will receive the round bottom flask back so that you may recover the product, dibenzyl terephthalate.

Week 2 - Dibenzyl Terephthalate From PET

Equipment/Glassware	Equipment/Glassware
• hot plate/stirrer	• neoprene cone
• 250 mL beaker	• 250 mL flask (3)
• stir bar (2)	• 100 mL beaker
• powder funnel	• spatula
• 50 mL graduated cylinder	• TLC developing jar
• weigh paper	• TLC strip
• 125 mL filter flask (3)	• 10 mL graduated cylinder
• Büchner funnel	• UV lamp

Chemicals	Precautions
• cyclohexane	• flammable liquid, irritant
• methanol	• flammable liquid, toxic, readily absorbed through the skin
• dichloromethane	• toxic, irritant
• acetone	• flammable liquid, irritant

1. Remove the stopper from the round bottom flask and then remove the grease from the inside neck of the flask. Use Kimwipes and a small amount of cyclohexane to accomplish this. Pour the product mixture into a 250 mL beaker. Add 100 mL of distilled water and place the beaker on a stirrer. Stir the two-phase mixture at a slow to moderate speed for 5-10 minutes. Caution: An emulsion may form especially if the stirring is vigorous. Decant off the benzyl alcohol product mixture into a clean 250 mL beaker. Discard the aqueous layer (the bottom layer).

2. Add 50 mL of methanol to the beaker containing the product mixture and place the beaker in an ice bath. Upon cooling, a finely divided white powder should be suspended in the product mixture. Caution: Methanol is toxic and is readily absorbed through the skin. Wear gloves when handling it in this step and in all subsequent steps.

3. Using a 125 mL filter flask and a Büchner funnel recover the white solid (the crude dibenzyl terephthalate) by suction filtration. Be sure to wet the filter paper with a few milliliters of methanol and pull a vacuum to properly seat the filter paper before performing the suction filtration. Push down on the Büchner funnel and neoprene cone to ensure a tight seal and good vacuum. Be sure the crude

product is sufficiently free of benzyl alcohol and methanol before stopping the suction filtration.

4. Transfer the crude dibenzyl terephthalate to a clean, dry 250 mL Erlenmeyer flask. Do this by placing a sheet of paper on the lab bench with a sheet of weigh paper in the middle of the paper. Using a spatula, carefully scrape the crude product out of the Büchner funnel onto the weigh paper. Also grasp the edge of the filter paper and scrape the product off of it as well. Carefully transfer the crude product to the 250 mL Erlenmeyer flask. Add a stir bar.

5. Be sure to have a clean, dry suction filtration set up (a 125 mL filter flask and a Büchner funnel) ready to use for the last part of this step. To the flask containing the crude product add 100 mL of methanol. Place this flask on the hot plate/stirrer and while stirring, heat the methanol to its boiling point (65°C). Perform this operation in the hood. A small amount of the product may not dissolve in methanol (because it is an impurity). It may be necessary to add more methanol to get all the crude dibenzyl terephthalate to dissolve. Too much methanol is not a big problem - some of it will be boiled off in the last step. Perform a hot suction filtration on this methanol solution. Transfer the filtrate to a clean, dry 250 mL flask and add a stir bar to the flask. Place the flask on the hot plate and reduce the volume of methanol to half its present volume (- 40-50 mL). Set the flask aside and let it cool for 5-10 minutes and then place the flask in an ice bath for another ten minutes.

6. Using a 125 mL filter flask and a Büchner funnel recover the recrystallized dibenzyl terephthalate by suction filtration. Be sure to wet the filter paper with a few milliliters of methanol and pull a vacuum to properly seat the filter paper before performing the suction filtration. Push down on the Büchner funnel and neoprene cone to ensure a tight seal and good vacuum. Wash the product with a small amount of cold methanol. Pull a vacuum for another ten minutes. Be sure the product is sufficiently free of methanol before stopping the suction filtration. Carefully transfer the recrystallized dibenzyl terephthalate to a clean, dry, pre-weighed 100 mL beaker. Record the weight of the beaker on the Data Sheet. With the aid of a rubber band secure a Kimwipe over the mouth of the beaker. Label the beaker with your group and lab section number. Deliver the beaker to your instructor. The recrystallized product will be allowed to dry for a week.

7. Wash all glassware with soap and water. Use acetone to help dissolve any remaining residual dibenzyl terephthalate. Dispose of methanol and acetone in the organic waste container.

Week 3 - Dibenzyl Terephthalate From PET

1. After removing the rubber band and Kimwipe, weigh the beaker containing your product. Record the weight of the dried product on the Data Sheet.

2. Determine the melting point of the recrystallized dibenzyl terephthalate.

3. Measure the R_f value of the recrystallized dibenzyl terephthalate. Use a 3:1 dichloromethane (also called methylene chloride)/cyclohexane mixture to develop the TLC strip. Place a total of 12 mL of the solvent mixture in the TLC jar. Add a spatula-tip full of the recrystallized dibenzyl terephthalate to a small test tube and add 0.5 mL of dichloromethane to the test tube. Use this solution to spot the TLC plate. Using a pencil, lightly draw a straight line across the bottom (½" from the bottom) of the TLC strip before spotting the plate. Use the especially drawn glass capillary tubes located at the instructor's desk to spot the TLC plate. Develop the TLC strip in the 3:1 mixture of dichloromethane/cyclohexane. Remove the strip when the solvent front advances to ¼ inch from the top of the strip. Mark the position of the solvent front immediately after removing the strip from the jar. Let the strip air dry and then view it under a UV lamp. Circle any spots that show up under the UV light. The most intense spot is that corresponding to the recrystallized dibenzyl terephthalate. Determine the R_f value of your recrystallized dibenzyl terephthalate in this solvent system. Show your work on the Data Sheet.

4. To obtain an IR spectrum of your recrystallized dibenzyl terephthalate, make a concentrated solution of

dibenzyl terephthalate in CH_2Cl_2. Use 1 mL of CH_2Cl_2 in a disposable test tube. Using a disposable pipet and bulb place one or two drops of the CH_2Cl_2 solution on the face of a NaCl plate. After the CH_2Cl_2 has dried, repeat the process several more times. Record the IR spectrum of your product. If the intensity of the peaks in the IR spectrum is too weak (consult your instructor) increase the thickness of the film and rerecord the IR spectrum.

II. Method 2 - Dibenzyl Terephthalate From Terephthaloyl Chloride

Week 1 - Dibenzyl Terephthalate From Terephthaloyl Chloride

Equipment/Glassware	Equipment/Glassware
• hot plate/stirrer • 15 cm test tube & No. 2 stopper • 10 mL graduated cylinders (2) • glass stirring rod • thermometer • Vortex-Genie	• 125 mL filter flask (2) • Büchner funnel & neoprene cone • 250 mL flask • stir bar (2) • 100 mL beaker (2) • 25 mL graduated cylinder

Chemicals	Precautions
• terephthaloyl chloride • benzyl alcohol • pyridine • methanol	• corrosive, lachrymator • irritant, hygroscopic • flammable liquid, irritant • flammable liquid, toxic, readily absorbed through the skin

Summary of procedure: Dibenzyl terephthalate is prepared by briefly heating terephthaloyl chloride in an excess of benzyl alcohol in the presence of pyridine. The crude product is recovered by filtration and recrystallized from methanol.

1. Caution: Because terephthaloyl chloride is corrosive and a lachrymator (a tear gas) and because pyridine has a very unpleasant odor, the synthesis of dibenzyl terephthalate must be performed in the hood. Wear gloves when performing manipulations involving these chemicals.

2. The terephthaloyl chloride has been pre-weighed for you. It has been placed in a test tube and the test tube sealed with a rubber stopper. Do not remove this stopper from the test tube until the test tube is in the hood. Obtain the test tube from your instructor and record the weight of the terephthaloyl chloride (which is marked on the test tube) on the Data Sheet.

3. Using the 10 mL graduated cylinders provided, measure out 10 mL of benzyl alcohol and add it to the test tube containing the terephthaloyl chloride. Two mL of pyridine has been measured out for you and placed in test tube which is sealed with a rubber stopper. This test tube is located in your hood. Add the 2 mL of pyridine to the test tube containing the terephthaloyl chloride and benzyl alcohol. Using a glass stirring rod, stir the three-component mixture. Caution: the reaction is very exothermic. After mixing, return the stopper to the test tube. Place the test tube containing the reaction mixture in a hot water bath held at 85°C for 15 minutes. At five minute intervals remove the test tube from the hot water bath and agitate the mixture using a Vortex-Genie. At the end of the 15 minutes allow the test tube to cool back down to room temperature. At this point, the product mixture will appear as a white milky

gel.

4. Add 10 mL of methanol to the product mixture in the test tube and cool the test tube in an ice bath. Caution: Methanol is toxic and is readily absorbed through the skin. Wear gloves when handling it in this step and in all subsequent steps. At this point the product mixture should be safe to handle outside the hood. Stir the contents of the test tube and using a 125 mL filter flask and a Büchner funnel recover the white solid (the crude dibenzyl terephthalate) by suction filtration. Be sure to wet the filter paper with a few milliliters of methanol and pull a vacuum to properly seat the filter paper before performing the suction filtration. Push down on the Büchner funnel and neoprene cone to ensure a tight seal and good vacuum. Use a wash bottle filled with methanol to help you rinse the remaining product out of the test tube and into the Büchner funnel. Try to minimize the amount of methanol that is used in this process. Be sure the crude product is sufficiently free of benzyl alcohol and methanol before stopping the suction filtration.

5. Transfer the crude dibenzyl terephthalate to a clean, dry 250 mL Erlenmeyer flask. Do this by placing a sheet of paper on the lab bench with a sheet of weigh paper in the middle of the paper. Using a spatula, carefully scrape the crude product out of the Büchner funnel onto the weigh paper. Also grasp the edge of the filter paper and scrape the product off of it as well. Carefully transfer the crude product to the 250 mL Erlenmeyer flask. Add a stir bar.

6. Be sure to have a clean, dry suction filtration set up (a 125 mL filter flask and a Büchner funnel) ready to use for the last part of this step. To the flask containing the crude product add 100 mL of methanol. Place this flask on the hot plate/stirrer and while stirring, heat the methanol to its boiling point (65°C). Perform this operation in the hood. A small amount of the product may not dissolve in methanol (because it is an impurity). It may be necessary to add more methanol to get all the crude dibenzyl terephthalate to dissolve. Too much methanol is not a big problem - some of it will be boiled off in the last step. Perform a hot suction filtration on this methanol solution. Transfer the filtrate to a clean, dry 250 mL flask and add a stir bar to the flask. Place the flask on the hot plate and reduce the volume of methanol to half its present volume (- 40-50 mL). Set the flask aside and let it cool for 5-10 minutes and then place the flask in an ice bath for another ten minutes.

7. Using a 125 mL filter flask and a Büchner funnel recover the recrystallized dibenzyl terephthalate by suction filtration. Be sure to wet the filter paper with a few milliliters of methanol and pull a vacuum to properly seat the filter paper before performing the suction filtration. Push down on the Büchner funnel and neoprene cone to ensure a tight seal and good vacuum. Wash the product with a small amount of cold methanol. Pull a vacuum for another ten minutes. Be sure the product is sufficiently free of methanol before stopping the suction filtration. Carefully transfer the recrystallized dibenzyl terephthalate to a clean, dry, pre-weighed 100 mL beaker. Record the weight of the beaker on the Data Sheet. With the aid of a rubber band secure a Kimwipe over the mouth of the beaker. Label the beaker with your group and lab section number. Deliver the beaker to your instructor. The recrystallized product will be allowed to dry for a week.

8. Wash all glassware with soap and water. Use acetone to help dissolve any remaining residual dibenzyl terephthalate. Dispose of methanol and acetone in the organic waste container.

Week 2 - Dibenzyl Terephthalate From Terephthaloyl Chloride

1. After removing the rubber band and Kimwipe, weigh the beaker containing your product. Record the weight of the dried product on the Data Sheet.

2. Determine the melting point of the recrystallized dibenzyl terephthalate.

3. Measure the R_f value of the recrystallized dibenzyl terephthalate. Use a 3:1 dichloromethane (also called methylene chloride)/cyclohexane mixture to develop the TLC strip. Place a total of 12 mL of the

solvent mixture in the TLC jar. Add a spatula-tip full of the recrystallized dibenzyl terephthalate to a small test tube and add 0.5 mL of dichloromethane to the test tube. Use this solution to spot the TLC plate. Using a pencil, lightly draw a straight line across the bottom (½" from the bottom) of the TLC strip before spotting the plate. Use the especially drawn glass capillary tubes located at the instructors desk to spot the TLC plate. Develop the TLC strip in the 3:1 mixture of dichloromethane/cyclohexane. Remove the strip when the solvent front advances to ¼ inch from the top of the strip. Mark the position of the solvent front immediately after removing the strip from the jar. Let the strip air dry and then view it under a UV lamp. Circle any spots that show up under the UV light. The most intense spot is that corresponding to the recrystallized dibenzyl terephthalate. Determine the R_f value of your recrystallized dibenzyl terephthalate in this solvent system. Show your work on the Data Sheet.

4. To obtain an IR spectrum of your recrystallized dibenzyl terephthalate, make a concentrated solution of dibenzyl terephthalate in CH_2Cl_2. Use 1 mL of CH_2Cl_2 in a disposable test tube. Using a disposable pipet and bulb place one or two drops of the CH_2Cl_2 solution on the face of a NaCl plate. After the CH_2Cl_2 has dried, repeat the process several more times. Record the IR spectrum of your product. If the intensity of the peaks in the IR spectrum is too weak (consult your instructor) increase the thickness of the film and rerecord the IR spectrum.

Weight PET Used			Weight DBT Recovered	
wt. flask, cork ring and PET			wt. vial, cap and DBT	
wt. flask and cork ring			wt. vial and cap	
wt. PET			wt. DBT	

Data for Recrystallized Dibenzyl Terephthalate (DBT)		
% Yield =	m.p. =	R_f =

Calculation of % Yield of DBT	Sketch of TLC

Data Sheet for Method 2

Weight Terephthaloyl Chloride Used			Weight DBT Recovered	
wt. test tube, stopper, terephthaloyl chloride			wt. vial, cap and DBT	
wt. test tube, stopper			wt. vial and cap	
wt. terephthaloyl chloride			wt. DBT	

Data for Recrystallized Dibenzyl Terephthalate (DBT)		
% Yield =	m.p. =	R_f =

Calculation of % Yield of DBT	Sketch of TLC

Instructors Notes

I. CAS Registry Numbers for Compounds Used in Methods 1 and 2

Compound	Precaution(s)	Registry No.
benzyl alcohol	irritant, hygroscopic	[100-51-6]
cyclohexane	flammable liquid, irritant	[110-82-7]
dichloromethane	toxic, irritant	[75-09-2]
methyl alcohol	flammable liquid, toxic	[67-56-1]
polyethylene terephthalate	none	[25038-59-9]
pyridine	flammable liquid, irritant	[110-86-1]
terephthaloyl chloride	corrosive, lachrymator	[100-20-9]
zinc acetate dihydrate	toxic	[5970-45-6]

II. Hazards

1. Although PET is safe to handle without gloves and safety goggles, the rest of chemicals in this lab are not. All the manipulations involving the organic compounds should be performed in a well-ventilated hood. If the terephthaloyl chloride and pyridine are measured out for the students in advance, this will simplify working with the organic compounds considerably.

2. Special care should be taken in handling methanol. Since methanol is toxic and readily absorbed through the skin, gloves should be worn whenever it is handled. The operation of heating methanol should only be performed in a well-ventilated hood. A steam bath is an excellent heat source! If steam is not available use a hot plate - do not use a flame.

III. Method 1 - Dibenzyl Terephthalate From PET

1. The PET for this experiment is obtained from clear, 2-liter pop bottles. The students are supplied long narrow (¼ ") strips cut from the body of the bottle. We do not use the base or neck of the bottle and we also avoid those portions of the bottle that have glue (which was used to hold the label to the bottle) on the outside surface . A large paper cutter comes in handy when its comes to cutting the strips from the panel you cut from the body of the bottle. These strips are then set out for the students. They then take a pair of scissors and cut the strips into small squares (¼" x ¼") as described in the *Student Instructions* section (Part A. Week 1, #1).

2. The benzyl alcohol used in this reaction serves as both a reactant and the solvent and is present in excess. Because it takes at least several hours to break down the PET and definitely longer than a typical lab period, we allow the reaction to proceed for approximately one day. A shorter time period would probably suffice. Upon cooling the round bottom flask after the reaction is complete, the product mixture often has a yellow cast to it and contains a small amount of white solid. Provided the PET squares have been in contact with the hot benzyl alcohol (and don't cling to the inside wall of the round bottom flask or condenser) there is never a trace of PET left at the end of the reaction. Because of the long reaction period, the reaction is performed in a hood outside the General Chemistry lab. In our situation, we have five lab sections per week using our one General Chemistry lab room. So as to not tie up the hood space in that room this reaction is run in a different location. At the beginning of Week

2, the students are handed the round bottom flask (stoppered) with their product mixture inside (minus the condenser, thermowell, etc.).

3. The product mixture is first extracted with water. The students are instructed to stir the product mixture at a slow to moderate speed with 100 mL of water in a 250 mL beaker. An emulsion of sorts is likely to occur at this stage. We have tried using a separatory funnel and performing a liquid-liquid extraction, but this turns out to be a very messy process in most cases. Thus, we have resorted to this cruder approach. Typically it is not possible to free the product mixture from all the water. However, this is not a serious problem. When the first bit of methanol is added to the product mixture (after washing it with water) an oil sometimes forms. However, if enough methanol is added to the mixture and it is cooled a white solid (the crude product) always forms. Enough methanol needs to be added to the mixture to get the product to fall out of solution. Too much alcohol may dissolve a significant amount of the product. The 50 mL the students are instructed to add to the water washed product mixture is thus a rough guideline. If the water extraction step is omitted, the crude product will contain a significant amount of methanol-insoluble residue (off-white in color). We believe the water extraction takes up the zinc acetate catalyst and the ethylene glycol and possibly other impurities/side products. We believe the extraction with water is a necessary step in the recovery dibenzyl terephthalate, albeit a messy one.

4. After the crude product is collected by suction filtration, it is recrystallized from hot methanol. This process includes a hot filtration. There are few or no insoluble impurities in the product. However, the hot (boiling) methanol solution containing the crude product typically has a cloudy white appearance. The hot filtration is done as a suction filtration which is perhaps unorthodox, but it typically runs smoothly if the solution is hot, contains an excess of methanol, and you work fast. We supply the students with insulated gloves so they can handle the hot flask and immediately after removing it from the hot plate commence with the hot, suction filtration. If the Büchner funnel clogs, running hot methanol through it eliminates the problem. Often some of the product crystallizes out in the filter flask with the filtrate. This problem is remedied by heating the filtrate. The volume of the filtrate is reduced to 40-50 mL. This yields a moderately large amount of product on cooling. The product is recovered by suction filtration, washed with small amounts of cold methanol and air dried for one week.

IV. Method 2 - Dibenzyl Terephthalate From Terephthaloyl Chloride

1. Users of this experiment who wish to showcase the depolymerization of PET by benzyl alcohol can skip Method 2 altogether.

2. For those individuals who decide to employ Method 2, precautions should be taken in handling both the terephthaloyl chloride and the pyridine. We have opted to weigh/measure out these reactants for the students. This greatly minimizes any potential handling problems with these chemicals. We have had no problems with either one of these substances.

3. The reaction is run in the test tube (6" x 1") that the students receive the terephthaloyl chloride in. The benzyl alcohol and pyridine are just added to the terephthaloyl chloride. To get these materials intimately mixed they must be stirred with a stirring rod. A stir bar doesn't work. The reaction between benzyl alcohol and terephthaloyl chloride in the presence of pyridine is very exothermic. Next, to insure completeness of reaction the reaction mixture is placed in a hot water bath at 85°C for 15 minutes. Upon cooling, the white product mixture has a gel-like consistency. Methanol is added to make the mixture less viscous, to facilitate the transfer of the mixture into the Büchner funnel, and to speed up the filtration process.

4. Neither the odor of terephthaloyl chloride or pyridine was detectable in any of the crude DBT samples made by Method 2. Thus, once the reaction is over, the subsequent steps can be performed outside the hood.

5. Once the crude product is recovered, the work up of the dibenzyl terephthalate is identical to that outlined in Method 1.

V. Lab Write Up

1. Before the students write up and turn in their lab report, the melting points, R_f values, and the key IR stretches obtained by their classmates are tabulated and distributed to the class as a whole. They are also given the ^{13}C NMR spectrum of DBT. When asked to compare the physical properties of the different DBT samples, the students conclude that they have all made the same compound.

2. To determine the percent yield of product made by Method 1, it is assumed that the molecular weight of the PET is the molecular weight of the repeat unit, 192.0 g/mol.

3. The complete set of ^{13}C NMR chemical shift values (in ppm) for DBT in $CDCl_3$ is: 165.37, 135.53, 133.80, 129.51, 128.49, 128.25, 128.11 and 66.95.

4. The students are encouraged to go to the *Aldrich Library of IR Spectra* and the *Aldrich Library of ^{13}C and ^{1}H NMR Spectra* and search for a compound similar to dibenzyl terephthalate. The better students find benzyl benzoate. Listed below is a comparison of some of the key assignments for DBT and benzyl benzoate.

Method	IR	^{13}C NMR	
Compound	< (C=O)	$-CH_2-$	C=O
benzyl benzoate	1719.3 cm^{-1}	66.61 ppm	166.27 ppm
DBT (from PET)	1718.5 $\pm$ 1 cm^{-1}	66.95 ppm	165.37 ppm