Discussion

Within this lab, caffeine extraction was performed through liquid-liquid extraction (LLE) wherein a compound is separated into polar and non-polar components through dissolution in two immiscible solutions: in this case dichloromethane and aqueous sodium carbonate (Na_2CO_3). Non-polar components dissolve into the organic dichloromethane layer and polar components into the aqueous layer, allowing for separation of the constituents for further extraction and purification. Three of these extractions were performed to maximize separation of the impure compounds from the desired caffeine, as caffeine can dissolve within both organic and aqueous solutions. Re-extracting previously obtained aqueous solutions enables added caffeine to separate out and increase the overall yield of said product. The chemical property of pH was observed in these extractions as the addition of Na_2CO_3 to water in the aqueous solvent formed the strong base NaOH, allowing for neutralization reactions to form among components. Fatty esters in the binding material reacted to produce conjugate salts, allowing for the previously hydrophobic esters to bond with NaOH in the aqueous solvent. No organic solvents were discarded to alleviate possible error in the recrystallization process. An effective solvent, one which dissolves caffeine only at high temperatures as well as all impurities, must be determined within recrystallization to allow an effective purification process. Testing for such a solvent uses 'crude' caffeine – 'crude' due to trace impurities present - obtained from the evaporation of organic solvent. Hence, in case of an ineffective solvent, extra organic solvent allows additional crude product to be formed. Within recrystallization the chemical property of reactivity was emphasized, due to the dissolution of crude caffeine resulting in the breaking of bonds within the added acetone in the performance of a dissociation reaction. Following this dissociation, the cooling and formation of new bonds in a synthesis reaction occurred as to create caffeine crystals; cooling slowly to provide ample time for the maximum amount of bonds to form to produce large crystals. The final recrystallized product likely possesses a high purity, though not fully pure due to the sharpness of the purified caffeine's melting point (began at 231ºC, fully liquid at 234ºC), in contrast to the range of a highly pure substance (0.5-2 degrees difference). Such is likely due to human error, arising in an improper amount of drying agent used or an excess of trace impurities remaining in the final extracted organic solution, both resulting in the possible presence of impurities in the final product.