Stoichiometry rules for common classes of reagents/catalysts not used at single equivalent amounts, applied each time these species are encountered

- Carbonate, phosphate, acetate: 3 equivalents
- Organic bases: 3 equivalents
- Alkoxides: 2 equivalents
- Phosphine ligand: 0.2 equivalents
- Palladium, other transition metal catalysts: 0.1 equivalents
- Strong acids: 5% of solvent

Reaction classification dictionary:

- **Template_ID: { }** ASKCOS reaction classifier name (str)

Augmented context dictionary:

- **reaction_smiles:** str: reaction smiles
- **reactant:** [[str: smiles, float: mols],]: a list of lists containing smiles and mol amounts
- **reagent:** [[str: smiles, float: mols],]: a list of lists containing smiles and mol amounts
- **catalyst:** [[str, float],]: a list of lists containing smiles and mol amounts
- **solvent:** [[str, float],]: list of lists containing smiles and volumetric percent
- **temperature:** float: reaction temperature
- **probability:** float: forward predictor probability of forming desired product
- **order:** [[str,],]: list of lists of smiles grouping reactants/reagents into well addition order
- **air_free:** bool: true/false whether or not the reaction should be conducted air free

Reaction Rules dictionary:
Key:

- **reaction_name: { }** Name as given by ASKCOS reaction classifier
  Values:
  - **template_IDs: [ ]** ASKCOS template IDs matching the reaction name [str]
  - **default_context: { }** a default augmented context dictionary based on the reaction class, not currently used, only use (modified) predicted contexts
  - **reaction_sets : [{ }]** list of set of conditions that appear in literature for specified reaction (e.g. one oxidation may be conducted in the range of 0-20 °C with mCPBA or in the range of 80-100 °C with H2O2, but not at 0-20 °C with H2O2)
    - **reactants:** { reactant_substruct_smarts: str, [reactant_equivs=1.0: float, order=1: int]}
      - Dictionary of reactants and their amounts in equivalents to the first entry in the list (therefore Reactants[0][1] = 1.0 always). Reactants are usually delivered in stoichiometric amounts (Reactants[i][1] = 1.0)
    - **reagents:** [{ reagent_smiles: str, [reagent_equivs=1.0: float, order=1:int] }]
      - List: context must contain at least one reagent from each entry in list, list will typically have a length = 1
      - Dictionary: key=reagent_smiles, value=[reagent_equivalents w.r.t first reactant, default value of 1.0, order in which chemicals are to be added, default value of 1]
    - **catalysts:** [{ catalyst_smiles: str, [catalyst_equivs=0.1: float, order=1:int }]
      - Same as reagents but with different default amount
    - **solvents:** [{ solvent_smiles: str, solvent_percent=1/len(Solvents): float }]
      - Same as reagents but amounts are defined as volumetric ratios with default solutions of equal %v/v
    - **temperature:** [lower_bound: float, upper_bound: float]
      - An upper and lower bound for temperatures
    - **air_free:** =False: bool
    - **template_IDs:** [ ]
      - A list of templates that correspond to that reaction set. Not necessarily a 1-to-1 mapping. This field is for reaction analysis when doing manual inspection of reaction outcomes