Supporting Information for How to estimate solid-electrolyte-interphase features when screening electrolyte materials

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1. Details on the redox fingerprint generation

a) Fragmentation of the molecule

The general organisation of this step is illustrated exemplarily in figure 1. The purpose of this program part is to generate all possible fragments of a molecule. The molecule, for which a redox



Figure 1: Exemplary fragmentation of ethylene carbonate.

fingerprint analysis (RFPA) is carried out, has to be supplied. The coordinates of the molecules are used to determine the bonds in a simple valence model approach. The program itself works with the heavy atom framework. All vectors are set up that contain the atoms between which the bond is allowed to break. Allowed bond cleavages are determined with heuristic rules. The rules have been deduced from bonds that 'usually' break in chemical reactions (textbook knowledge). Allowed bond cleavages are:

- Single bonds between a hetero atom with a coordination greater than one and an arbitrary heavy atom
- Single bonds between a cyanid group and an arbitrary heavy atom
- Single bonds in the neighborhood of carbonyl groups

• Single bonds between halogen atoms (coordination equals one) and an arbitrary heavy atom

The most likely bonds to break in 'usual' reactions are atoms in or in the neighborhood of functional groups. After a bond cleavage an atom cannot be left alone (coordination in the molecule has to be unequal to one) except for halogen atoms. It is highly unlikely that one atom other than halogens is left alone in a reaction and the option was excluded in this version of the program. This set of rules is not complete, but incorporates the most important possibilities for the treatment of 'usual' organic molecules. If a case is identified that has to be included, it can be easily implemented in the rule framework. The next necessary extensions of the rules would be the incorporation of the reactivity of double and triple bonds to account for addition reactions. From the number of the possible breaking points, hereon referred to as 'hetero bonds', the maximal number of possible fragments N_{frags} is identified.

$$N_{frags} = \sum_{i=1}^{N_{het}} \left(\binom{n}{i} \cdot (i+1) \right) = \sum_{i=1}^{N_{het}} \left(\frac{n!}{i!(n-i)!} \cdot (i+1) \right) \tag{1}$$

The number of the hetero bonds is denoted as N_{het}. All possible combinations without repetitions in equation 1 for each number i are determined that correspond to all possible bond breaking patterns. For each bond breaking pattern i+1 fragments originate. If a molecule contains four hetero bonds, one has first the possibility to break only one bond (i=1). There are four possibilities for the cleavage of one bond (hetero bond 1,2,3 or 4). When breaking one bond two fragments originate (1+1). Likewise the possibilities are determined if more than one bond is broken. At this step the upper limit is determined and no restrictions are made, if a cleavage is possible or not (e.g. one atom is left alone). For ethylene carbonate (four hetero bonds) the maximum number of possible fragments is 47. The molecule is fragmented in the next step. Initially, all possible bond breaking patterns are determined. While in equation 1 only the number of all possible combinations without repetitions is determined, a matrix is now written, in which the actual combinations are stored. These combinations, in which the numbers stand for the number of the hetero bond, are then resolved to the actual bonds that are broken. The molecule is then fragmented via its 'SMILES'. The abbreviation 'SMILES' stands for 'Simplified molecular-input line entry system.' It is a notation of the structure of a chemical species in a short string. The concept of SMILES was introduced in the 1980s by Weininger. [1, 2] Atoms are represented by the standard abbreviation of the chemical elements, for elements other than an organic subset (B, C, N, O, P, S, F, Cl, Br, I), the chemical elements are written in square brackets. When an atom is charged the charge is specified inside the brackets and possible hydrogens have to be included. Single bonds are assumed, if nothing else is specified or can be included as '-'. Double, triple and quadruple bonds are denoted as '=', '#', '\$' respectively. A ring closure is indicated by numbers on the non-adjacent atoms. The number increases for each ring. If the molecule is branched, the branches are indicated in parentheses. It is usually seen as a drawback that for a molecule various equally valid SMILES can be written. This is exploited in this program. Each atom number is associated with a partial SMILES string specifying the element of the heavy atom and the hydrogens bonded to it (e.q. [CH2]). It is necessary to specify the number of hydrogens here because the SMILES are later on converted into xyz-coordinates with the program OpenBabel. [3] If the number of hydrogens is not specified, OpenBabel adds hydrogens until the standard valence is reached, which is usually an utile feature. The valence on these atoms has to be specified as they deviate from the standard valence. For more convenience and unity the SMILES strings are generated for each heavy atom and not only for the atoms that deviate from the standard valence. The routine used to generate a SMILES string from the coordinates of the input molecule is illustrated graphically in figure 2. Starting from a specified atom, a chain of atoms bonded to the respective precurser



WHOLE SMILES: [CH2] -[CH2] -[O] -[C](=[O]) -[O]

Figure 2: Generation of a SMILES string from coordinates on the example of ethylene carbonate.

is identified (indicated in blue in figure 2). If a bond cleavage has been identified before, the bond between the two respective atoms is not classified as a bond and the chain generation does not propagate in this direction. The identified chain is taken as an input for the SMILES generation. The chain is paced out atom by atom. Each with an atom associated SMILES string is appended to the whole SMILES. If an atom is identified that is not part of the first chain, the chain generation is started again from this atom (indicated in orange in figure 2). The side-chain is appended to the

whole SMILES array in parentheses (branch). As this routine works recursively, the molecule can be branched arbitrarily often. After each addition to the whole SMILES the information of the bond order to the next atom in the chain is added. The generated SMILES string equals to the fragment resulting from the cleavage of the specified bonds. No rings are included in the generation of the SMILES. Information of rings is appended subsequently to the SMILES generation by comparision of the bond matrices of the original molecule and the generated fragment. The bond matrix of the fragment can be easily obtained in the chain generation, in which every bond is determined. If any bonds are not reproduced in the SMILES and are not the broken bonds, the ring is closed in the SMILES by appending ascending numbers to the connecting atoms. Currently, the SMILES generation is not fitted for annihilated rings and salts. Annihilated rings may be implemented by extending the matching approach. Salts are not included due to their bond type. To implement ionic bonds, bigger effort is needed, as the ionic bond is not directive and cannot just be replaced by an adding a new bond type into the SMILES. However, it is possible to neglect the ionic bond and treat the salt as a mixture of two molecules currently though the charge is not reproduced correctly. By specifying each atom explicitly with its hydrogens in square brackets, the routine is also applicable to any kind of element and does not have to be extended for the implementation of new elements. The atoms, on which the molecule has been broken, are stored in a logging file. The xyz-coordinates of the resulting fragments are determined in the next step. If not all atoms of the molecule are present in the fragment, the coordinates of the respective atoms in the input molecule can be adopted straightforwardly. If all atoms are part of the generated fragment, the adoption of the coordinates would not lead to a new fragment. This is for example the case if only one bond in a ring is broken, then all atoms are present in the SMILES, but bonded differently (chain instead of ring in example). In these cases the xyz-coordinates are created from the SMILES string with the program OpenBabel. The generation of the coordinates with Open-Babel is by far more time intensive than the adoption of the old coordinates. Auxiliary atoms are introduced to decrease the time effort and generate a realistic structure. These auxiliary atoms are appended to the positions in the SMILES, where the molecule was broken (valence deviates from standard valence). The denomination of the filenames is based on the number of atoms. If an atom is present in the fragment the number is one, otherwise zero (e.g. for the carbonate fragment: org001111.xyz). All generated fragments are then compared to each other and doubles

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are sorted out. The Tanimoto coefficient is used for sorting out of double entries. The Tanimoto coefficient (also known as Jaccard index) [4] was introduced in 1960 to compare the similarity of data sets. To calculate the Tanimoto coefficent the program OpenBabel is used. This program generates a fingerprint for each molecule. The molecule is characterised by its fingerprint, but the particular meaning of each bit of the fingerprint is not well defined just like in the analogy for a human fingerprint. The algorithm examines the molecule and generates a specific pattern for each atom, the nearest neighbours, each group of atoms and bonds connected by paths up to 2 bonds long, 3 bonds long and so on. A complete list of patterns is produced, *e.g.*, there is no cutoff limit. Each pattern than serves as a seed to a pseudo-random number generator that generates a corresponding set of bits, *i.e.* it is 'hashed'. The bits in these patterns are then used to calculate the Tanimoto coefficient. The Tanimoto coefficient is calculated from the sum of the counts of bits, wich both compared structures (X,Y) share. The numerator is divided by the sum of the bits that are in either of the structures.

$$T_s(X,Y) = \frac{\sum_i (X_i \wedge Y_i)}{X_i \vee Y_i} \tag{2}$$

The symbol \land denotes that the bit has to be present in both structures. The symbol \lor denotes that it has to be present in at least one of the structures. If the structures are identical the sums equal each other and the Tanimoto coefficient equals one. If the Tanimoto coefficient of two structures equals one, they are identical and doubles can be sorted out. In the pool of the final fragments each structure is unique. If more than one possibility exists to generate the same fragment, this information is stored in the logging file. At this point the fragmentation of the molecule is concluded. The originating eight fragments for ethylene carbonate can be seen in figure 1.

b) Generation of possible reactions

All generated fragments for the reactant molecule are then combined to reactions in a so-called 'backward decomposition'. The name 'backward decomposition' refers to the generation of the possible reactions starting from the fragments ('products') rather than the reactant. All possible reactions have to suffice the criterion of atom conservation. All atoms present in the reactant molecule(s) have to be conserved in the reaction to lead to a valid, balanced reaction. The generation of all possible reactions is not concluded yet after the backward decomposition, because reactions may not only lead to the complete fragmentation of the molecule, but as well to the formation of new products. New products are allowed to form from the combination of all frag-

ments to new molecules. The procedure to generate all possible reactions ties in directly with the generation of the fragments. It is illustrated in figure 3. All possible fragments (restricted by



Figure 3: Illustration of the backward recombination of fragments to possible reactions.

the bond-breaking rules) are needed as an input for this program part. The maximum number of reactant molecules has to be handed to the program (if differing from the default parameter) as an input parameter. The number of maximal involved molecules in one reaction is currently by default two. The number of possible backward decompositions is

$$N_{bd} = N_{molecules}^{N_{frags}}.$$
(3)

This equals to the possible number of permutations of the numbers of reactant molecules on N_{frags} positions. The number in the permutation on a certain position equals to the number of the fragment that this position was assigned to. The validity as a decomposition reaction is then checked for each permutation. A reaction in which all atoms are conserved is allowed. The number of atoms of the fragments contained in a permutation is counted. If this number can be divided by the number of atoms of the input molecule without remainder, then it is considered a possible reactions. But it has to meet further criteria. Not only the number of atoms has to

be conserved, but also the overall sumformula (equal amounts of atoms of the same elements). Multiple entries are then sorted out. These reactions do not correspond to all possible reactions yet. The generated fragments can form new compounds (reaction products) by being merged together. The considerations of the possible product formations are strictly combinatorial and not based on possible reaction mechanisms. The possible recombinations to new structures are determined for each valid decomposition. The information, which compounds (and their structure) are merged, together is stored in a so-called 'recombination file'. The generation is comparably laborious. For each reaction the products cannot only be all recombined to a product, but also only a certain amount of the fragments can be recombined, while the other fragments remain single. The combination starts with the combination of all fragments to one recombination file. The routine does not have to be called again, because no fragments remain. The number of combination is determined with

$$N_{comb} = \begin{pmatrix} N_{frags} \\ N_{tocombine} \end{pmatrix} = \frac{N_{frags}!}{N_{tocombine}!(N_{frags} - N_{tocombine})!}.$$
(4)

For the combination of $N_{frags} - 1$ numbers, one unpaired number remains. It is continued in the same way that every time numbers are still left after the formation of a combination, the routine is called again. This comparably complicated way was chosen to not limit the number of possible recombinations. The determination of all possible combinations of two fragments is evident, while it quickly becomes far more challenging with a larger number of fragments. All double entries for possible combinations are sorted out. For each possible combination all recombination files are then written as output. The denomination of the filenames results from the number of original fragments incorporated. If an original fragment is contained in the recombination fragment, its number differs from zero (*e.g.* rec11000000.xyz). The recombination to a single structure is carried out in the next part of the program. The final reactions are then written to an output file. All combinations are resolved to the actual recombination and original filenames. The output file contains how many educt files can be decomposed to which recombination and original files.

c) Recombination of fragments

The recombination files ('recfiles') have to been translated into an actual structure. Each recfile contains the coordinates of several original fragments. In this step the original fragments are merged into one structure. The merging occurs *via* their SMILES. An exemplary, schematic overview of this program part can be seen in figure 4. Figure 4 illustrates how three exemplary



Figure 4: Exemplary recombination of three fragments for one possible combination on the first hooks.

fragments are merged into one of the possible structures. The merging occurs for each recfile on its own. All possible combinations of the fragments contained in one recfile are determined by forming all possible permutations without repetitions. A total of N_{frags} ! is possible for each recfile. A permutation was chosen because the structure of the resulting molecule depends on the order in which the fragments are recombined. (Merging the first with the second and then the third differs from merging the first with third and then second). The merging itself occurs recursively. The first two fragments in the permutation are merged to one fragment. The resulting fragment is merged with the next fragment specified in the permutation, which is repeated until all fragments have been merged into one structure. The merging occurs independently for each possible permutation. At the start, each fragment in the recfile is given in xyz-coordinates. From the xyz-files the number of 'hooks' is determined. A 'hook' is defined as a spot at which fragments can be merged. They are determined by comparing the valence of each heavy atom to its standard valence. If they differ, the atom is classified as a hook. As can be seen in figure 4, it matters not only in which order fragments are merged, but as well on which hooks. To include all possibilities the merging is done $N_{hooks_1} \cdot N_{hooks_2}$ times in each recursive step. For each resulting fragment, the merging is continued individually. The positions of the hooks are passed to a routine that merges the fragments via their SMILES. In the first step (no merging occurred yet), the first fragment is given in xyz-coordinates and the SMILES is formed with the same routine introduced in section 1.1.1 (c.f. figure 2). In this section, the hooks are specified in the SMILES with a wild-card character ([*]) that is appended to the SMILES at each position that has been identified as a hook after the SMILES generation. An example for the resulting SMILES can be seen in figure 4. The SMILES of the second fragment is directly integrated into the SMILES of the first fragment to generate the SMILES of merged fragment (only for clarification in figure 4). The SMLES of the second fragment is appended in parentheses to the SMILES of the first fragment at the defined position of the hook. A wild-card character (former hook) is, therefore, replaced. The second SMILES string is determined beginning with the hook atom that has been passed with the above-mentioned routine. The SMILES of the merged fragments is saved as a temporary file and used as an input in the next step. Therefore, it is not necessary to perform a time-consuming conversion into xyz-coordinates and the re-conversion into a SMILES. The routine then directly resumes with going through the SMILES of the fragment and merging the next fragment to the passed hook. The hooks also do not have to be re-identified as they are stored implicitly in the number and positions of the wildcard symbol. The merging occurs for each possible combination of hooks (not only for starting fragments, but as well for intermediate steps). After all fragments have been merged to one SMILES, doubles are sorted out (only for one recfile). If no other SMILES is equal to the newly generated one, the SMILES is transformed into xyz-coordinates with OpenBabel. The structure of the originating compound is then compared to all previously generated structure and double entries are sorted out making use of the Tanimoto coefficient. If a full merging is not possible (no hooks left, e.g. after merging two methyl fragments to an ethylene molecule), the result is not saved as the atom conservation in the reactions of the reactions from the decomposition list would then be violated. Finally, the atoms on which the fragments have been merged are saved in logging files. A weakness of the program is the identification of the hooks. A hook currently is identified as an atom with a deviation from the standard valence. The definition excludes the possibility of hooking on mesomeric structures. Currently, no formation of rings is included in the code though it may be implemented. It has not been implemented yet because most reported compounds in the solid-electrolyte interphase do not undergo ring-closure reactions.

d) Determination of the charge for stable structures

All structures that have been generated up to this step (original fragments, recombined fragments) are checked for dangling bonds and their charges are determined. The determination of the charges of the structures is based on heuristic rules. It has to be rule-based, because the mechanism leading to a structure is not further specified. The set of rules may as well be expanded with an increasing knowledge. The charge is generally determined based on the deviation from the standard valence for each atom. If the valence of nitrogen, sulphur or oxygen is less than the standard valence, it is assumed that they are negatively charged with the deviation. If the valence of nitrogen is higher than the standard valence, but not higher than four, it is positively charged. A positive charge is not allowed for oxygen or sulphur. Halogens with the valence zero are assumed to have the charge minus one. For carbon atoms, different cases are determined on which the charge and the saturation differ. In general, no carbo-cations or anions are allowed. Sometimes a deviation from the standard valence originates from the simple underlying valence model that is only based on the bond lengths. If the valence is less than the standard valence, it is checked whether the carbon atom is sp2 or sp1 hybridised through the number of neighbours. If then no saturation is reached, the structure is discarded. If the valence is greater than the standard valence, the underlying structure is a carbon acid, for which the valence is not counted correctly (each carbon-oxygen bond is counted as a double bond). The number of oxygen and carbon atoms in the neighbourhood of the atom in guestion is counted. If it is a carbon acid (number of oxygens equals two) the structure is negatively charged. This checking is used to discard two undesired structures of the type $-CO_3$ or $-OCO_3$. Several other special cases are included, for which the charge is set instead of being determined through the valence: The charge for carbon monoxide and carbon dioxide is set to zero, the charge of cyanide to minus one. Structures with a peroxide bond or the sulphur analogue are excluded. For all other implemented elements, no rules have been specified, which forbids a deviation from the standard valence. The charge is determined with specified rules according to the products expected. While the rules are tailored to treat common electrolyte molecules well, they may not well-suited to describe other unknown

systems. On the other hand, additional rules can be easily included in the charge determination. Afterwards, all structures for which no charge could be assigned are discarded (dangling bonds, unwanted charge) The determined charge is included in the xyz-files of the structures. In the last step of this program, all fragments are checked for doubles.

e) Preparation of the data for subsequent calculations

This program part ties in with the second step of the program. In that step all combinatorially possible reactions with the conservation of the atom number (and sum-formula) are written as output. In these reactions the recfiles do not correspond yet to the actual merged structures. So for one initial reaction (backwards decomposition) several reactions may be possible. For the recfiles, all merging possibilities (merging in different orders, on different hooks) have to be taken into account. In the beginning for each entry, the original recfiles are substituted by all newly generated ones. If a reaction leads to more than one recombined reaction product, also all possible combinations of the recombination possibilities are included. It is then checked whether all files are reasonable structures (information from last step) for each reaction. In that case the charge of the files is read in. The sum of the charges of all reaction products has to equal the number of transferred electrons times the number of educts. Redox reactions are modelled in the program by the transfer of electrons. The number of these transferred electrons has to be conserved in the final reactions.

$$\sum_{i}^{N_{products}} q_i + N_{educts} \cdot q_{transfer} = 0 \tag{5}$$

The final output reactions equal to the redox fingerprint of the input molecule for the specific input parameters.

2. Analysis of the redox fingerprint - used methods

The analysis of the redox fingerprint consists of several independent steps that are brought together to get final estimates of what components the SEI may consist. Throughout the course of the analysis various programs are used ranging from quantum chemistry programs to chemo informatics. The generated structures are converted from SMILES to xyz-structures, optimised on force field level, with Openbabel. [3] OpenBabel is as well used to determine the tanimoto coefficient (measure for similarity) of two structures. [3]. We use the Tanimoto coefficient as one of the kinetic estimates. The reason, why some thermodynamically preferred reaction products are not encountered, most likely traces back to the exact reaction mechanisms. These cannot be retraced with the program, as the products are formed based on purely combinatorial (and heuristic) considerations. The explicit of the kinetics of each reaction is not feasible as illustrated by the fact that after several years of research no agreement was reached yet on even the most basic reactions in the SEI. [5] To take the kinetics nevertheless into account, we have to rely on simpler estimators. A first estimate is the degree to which the compounds have to transform in a reaction, which can be measured with the Tanimoto coefficient. If the reaction product is more similar (but not identical) to the educt molecule, it can be taken as a first indication that no unlikely transitions have to be made to form this molecule. In this work, the energy of the structures is determined with a semi-empirical method, PM6-DH+ [6, 7], using MOPAC2012 [8]. We determined the correlation with BP86 and B3LYP DFT calculations [9, 10, 11, 12] with TURBOMOLE 6.4 [13] unsing D2 dispersion corrections [14] and the RI approximation for two-electron integrals [15, 16] and TZVP AO basis sets. [17] Solubilities have been determined with COSMOtherm [18] on top of the SQM and DFT calculations.

3. Table: Complete redox fingerprint of ethylene carbonate

The following table contains the whole redox fingerprint of ethylene carbonate for the default input of the transfer of one and two electrons and the reduction of a maximum of two reactant molecules.

Transfer of 1 electron			Transfer of 2 electrons			
	Input	Output	ΔE	Input	Output	ΔE
1	$2 \text{ EC} \longrightarrow$		-71.79	$2 \text{ EC} \longrightarrow$	° + ° , °	-126.10
2	2 EC \rightarrow	°, ^L o~o~, °	-57.34	1 EC \longrightarrow	о 0 + H ₂ C=CH ₂	-55.87

Table 1: Output for ethylene carbonate

	Transfer of 1 electron				Transfer of 2 electrons		
	Input	Output	ΔE	Input	Output	ΔE	
3	$2 \text{ EC} \longrightarrow$		-43.97	$2 \text{ EC} \longrightarrow$	° ° [⊥] ° + ° [⊥] ° +	-111.74	
4	2 EC \rightarrow	° °	-34.51	2 EC \rightarrow	$H_2C=CH_2 + H_2C=CH_2$ $ \bigcirc O \longrightarrow O O O O O O O O O O O O O O O O O$	-102.58	
5	2 EC \longrightarrow	$\circ \sim \circ \sim \circ \sim \circ \circ$	-33.98	$2 \text{ EC} \longrightarrow$		-93.42	
6	$2 \text{ EC} \longrightarrow$		-33.16	1 EC \longrightarrow	$\odot \sim \sim 0 \odot \odot$	-46.71	
7	$2 \text{ EC} \longrightarrow$	$\circ \sim \circ \circ$	-30.09	$2 \text{ EC} \longrightarrow$		-93.16	
8	2 EC \longrightarrow	$\circ \overset{\circ}{\longrightarrow} \circ \overset{\circ}{\to} \circ \circ$	-28.18	2 EC \rightarrow		-89.43	
9	2 EC \longrightarrow	$\circ \circ $	-24.04	$2 \text{ EC} \longrightarrow$	°°, + °°, ↓°°	-84.62	
10	2 EC \longrightarrow	°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°	-21.43	$2 \text{ EC} \longrightarrow$	$\overset{\circ}{\circ}$ + $\overset{\circ}{\overset{\circ}{\sim}}$ +	-64.06	
11	2 EC \rightarrow	°~~°~~°~~°	-11.34	2 EC \rightarrow	°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°	-59.11	
12	2 EC \rightarrow	0 0 0 0 0 0 0 0 0 0 0 0 0 0	-9.24	2 EC \longrightarrow	°~~~~°~~°	-42.10	
13	2 EC \rightarrow	o [⊕] o d o d o + H₂C=CH₂	-7.43	2 EC \rightarrow	° + ° + ° + ° ~ °	-38.55	
14	2 EC \rightarrow		0.66	2 EC \rightarrow	+ $H_{0}C=CH_{2}$ $O \longrightarrow O O O O O O O O O O O O O O O O O O$	-29.39	
15	$2 \text{ EC} \longrightarrow$	°, °, °, °, °, °, °, °, °, °, °, °, °, °	3.71	$2 \text{ EC} \longrightarrow$	$\Big\ + \circ^{\Theta} \circ^{\Theta} + \circ^{\Theta} \circ^{\Theta} \circ^{\Theta} + \circ^{\Theta} \circ^{O} \circ^{O} \circ$	34.17	
16	2 EC \longrightarrow	$\overset{\Theta}{\overset{\Theta}{\overset{\Theta}{\overset{\Theta}{\overset{\Theta}{\overset{\Theta}{\overset{\Theta}{\overset{\Theta}$	5.42	$2 \text{ EC} \longrightarrow$	$\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}$	34.64	
					°, °, °, °, °, °, °, °,		
17	$2 \text{ EC} \longrightarrow$	$\overset{\odot}{_{\rm O}} \sim \overset{\circ}{_{\rm O}} \overset{\circ}{_{\rm O}} \overset{\circ}{_{\rm O}} \sim \overset{\circ}{_{\rm O}}$	9.23				

Table 1: Output for ethylene carbonate

	Transfer of 1 electron				Transfer of 2 elect	trons
	Input	Output	ΔE	Input	Output	ΔE
18	$2 \text{ EC} \longrightarrow$	$\overset{\odot}{\underset{0}{\circ}} \sim \overset{\circ}{\underset{0}{\circ}} \overset{\circ}{\underset{0}{\circ}} \overset{\circ}{\underset{0}{\circ}} \sim \overset{\circ}{\underset{0}{\circ}}$	25.08			
19	2 EC \longrightarrow	$\stackrel{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{\overset{\circ}{$	30.94			
		H ₂ C=CH ₂				
20	2 EC \longrightarrow	°, °, °, °, °, °, °, °, °, °, °, °, °, °	35.90			
21	$2 \text{ EC} \longrightarrow$	°~~°~~°° + °° +	39.62			
		O C				
22	$2 \text{ EC} \longrightarrow$	$\overset{\circ}{\to}\overset{\circ}{\to}\overset{\circ}{\to}^{\circ}$ + $\overset{\circ}{\to}\overset{\circ}{\to}^{\circ}$	103.34			

Table 1: Output for ethylene carbonate

5. Methodological considerations for the redox fingerprint analysis

The redox fingerprint can be analysed on a desired level of theory. We decided on PM6-DH+ calculations. To evaluated if the properties in question can be described acceptably well on this level of theory, we look at the correlation values with B3LYP/TZVP hybrid DFT calculations. For the energies of the products as well as for the reaction energies of ethylene carbonate a very high correlation is observed. The correlations are tabulated below. We can conclude that the inclusion

Table 2: Correlations (Pearson R values) for energies at different theoretical levels						
	R for absolute energies	R for reaction energies				
	Transfer of one electron					
$E(SQM)/E(SQM+Li^+)$	1.00	0.98				
E(DFT)/E(SQM)	0.91	0.98				
$E(DFT)/E(DFT+Li^+)$	1.00	0.99				
	Transfer of two electrons					
$E(SQM)/E(SQM+Li^+)$	0.99	1.00				
E(DFT)/E(SQM)	0.92	0.99				
$E(DFT)/E(DFT+Li^+)$	1.00	0.97				

of Li^+ can be neglected for the ranking of the compounds with overall very high correlations. The B3LYP/TZVP calculations correlate well with the PM6-DH+ calculations. It is reasonable to carry out the redox fingerprint analysis on the basis of fast PM6-DH+ calculations which makes it suitable for the incorporation in a screening approach. However, the redox fingerprint analysis can be executed on a desired level of approximation. Similar conclusions were reached for the evaluation of the chosen descriptors.

The solubility is investigated as a first probability estimate in the spirit of Balbuena and coworkers. [19] Balbuena found LBDC to be more stable than LEDC in static electronic structure calculations, though LEDC was found to be the main component of the SEI. In her work, she argued that the solubility of LBDC is higher than LEDC and it therefore does not stay in the SEI, but is dissolved in the electrolyte and cannot be observed experimentally. We calculated the solubility and the chemical potential of each product in EC using COSMOtherm on top of SQM and BP86 DFT calculations. On the one hand the solubilities of the free species was calculated, on the other hand the solubilites of the lithiated compounds because Balbuena referred to the lithiated species. The results for EC can be seen in table 3.

> Table 3: Solubility of the reaction products of the thermodynamically most favorable reactions.

	PM6-DH+		PM6-DH+	- with Li^+	BP86/	TZVP
Compound	$Log10(x_{Sol})$	μ [kcal/mol]	$Log10(x_{Sol})$	μ [kcal/mol]	$Log10(x_{Sol})$	μ [kcal/mol]
	Transt	er of one elec	tron			
H ₂ C=CH ₂	-0.87	-2.03	-0.87	-2.03	-0.50	-2.05
EC^{-}	0.00	8.41	0.00	8.41	0.00	5.30
$O_{O_{O_{O}}}^{\Theta} O_{O_{O}} O_{O_{O}}^{\Theta} O_{O}^{\Theta} O_{O}^{O} O_{O}^{\Theta} O_{O}^{O} O_$	0.00	11.87	-3.65	4.35	0.00	9.11
	0.00	12.97	-3.73	4.13	0.00	9.20
	0.00	13.48	-3.16	2.57	0.00	9.37
Transfer of two electrons						
H ₂ C=CH ₂	-0.87	-2.03	-0.87	-2.03	-0.50	-2.05
0 II C	-0.37	-1.36	-0.37	-1.36	-0.63	-1.44
	0.00	17.15	-3.74	2.17	0.00 12.54	

Table 3: Solubility of the reaction products of the thermody-

	PM6-DH+		PM6-DH+	- with Li^+	BP86/	TZVP
Compound	$Log10(x_{Sol})$	μ [kcal/mol]	$Log10(x_{Sol})$	μ [kcal/mol]	$Log10(x_{Sol})$	μ [kcal/mol]
	0.00	17.72	-4.10	3.90	0.00	15.21
	0.00	25.41	-5.31	3.56	0.00	14.77
$^{\ominus}_{0}$	0.00	28.34	-5.14	3.47	0.00 18.80	
	0.00	29.98	-4.74	4.77	0.00	27.20
°⊖∽∽⊖ °	0.00	33.99	-5.48	4.35	0.00	24.93
EC^{-2}	0.00	34.10	0.00	34.10	0.00	16.79

namically most favorable reactions.

A solubility of zero indicates a high solubility in the solvent. Without the coordination of Li^+ cations, the solubility of all charges species is high in the solvent. This can be expected because the polar solvent interacts favourably with the charged species. In turn, uncharged species are rather poorly soluble, the solubility remains the same when taking Li^+ into account because Li^+ ions are assumed to be only coordinated to charged compounds. When adding Li^+ to the charged compound, the solubility decreases significantly. The decrease arises from the fact that the Li^+ is not allowed to detach from the compound in a COSMOtherm calculation. It would be expected that in the solution the lithiated compound is not coordinated to each other, but is dissolved. Therefore, when calculating the solubility of the compound, the free species should be investigated. The chemical potential is an indicator how good the solubility is, which is especially important when the solubility is zero. Compounds with a higher the chemical potential are more soluble. In contrast to the reasoning of Balbuena, who did not perform explicit calculations of the solubility, we observe a nearly equal solubility of LEDC and LBDC on top of both, SQM and DFT, calculations. In fact, LBDC is even slightly better soluble than LEDC, when examining the free species. The solubility of a charged compound therefore can hardly be taken as an estimate for the probability to encounter it in the SEI formed from a polar solvent.

The energies of the highest occupied molecular orbitals as an indicator for the oxidative stability are tabulated below.

	PM6-DH+		B3LYP/TZVP		
Compound	E_{HOMO} [eV]	E_{HOMO} [eV] + Li^+	E_{HOMO} [eV]	E_{HOMO} [eV] + Li^+	
		Transfer of one elect	tron		
	-11.21	-11.09	-6.47	-7.30	
${}^{O}\!$	-11.20	-11.30	-6.51	-7.31	
$H_2C = CH_2$	-10.79	-10.79	-7.57	-7.57	
	-10.42	-10.42	-6.31	-6.58	
		Transfer of two election	rons		
0 = C	-12.02	-12.02	-10.36	-10.36	
	-11.29	-10.95	-6.82	-6.82	
	-11.10	-10.41	-6.01	-6.01	
$H_2C = CH_2$	-10.79	-10.79	-7.57	-7.57	
	-10.46	-9.82	-5.55	-5.55	
	-9.64	-9.27	-4.91	-4.91	
	-9.46	-9.05	-4.57	-4.57	
o⊖∽∽⊖ 0	-9.38	-8.59	-4.04	-4.04	

Table 4: HOMO values of the reaction products of the ther-

modynamically most favorable reactions.

The oxidative stability is again highly correlated with R >= 0.95. The other chosen descriptors are not depended on the level of theory as they are determined from the chemical structure of the resulting compound (number of necessary fragmentations, recombinations and the tanimoto coefficient. Similarly high correlations can be observed for all selected standard electrolyte molecules.

6. Table: Redox fingerprints of selected standard electrolyte molecules

The following table contains a detailed redox fingerprint of the other selected standard electrolyte solvents: propylene carbonate (PC), dimethyl carbonate (DMC), dimethoxy methane (DMM), 1,3-dioxolane (1,3-DL) and tetrahydrofuran (THF).

Solvent	Thermodynamically favourable	Lowest	Minimal Num-	Minimal Num-	Tanimoto coeffi-
Name	reaction products	HOMO	ber of Fragmen-	ber of Recombi-	cient
(e^-)			tations	nations	
PC (1e)	1) ° , , , , , , , , , , , , , , , , , ,	8)	1), 2), 3)	1), 2), 3), 8)	8)
$\sum 63$	2) °°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°				
	3) ^{oo} ^o ^o ^o ^o ^o ^o ^o ^o ^o				
	4) [°]				
	5) ^{°, , , , , , , , , , , , , , , , , , ,}				
	7) ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° °				
	8) + -				
PC (2e)		16)	1), 2), 3), 4), 5),	3)	10)
			6), 8, 10), 11), 12), 14), 15)		
$\sum 30$	2) ° · · · · · · · · · · · · · · · · · ·				
	3) ⋻ੈ⊥ੈ⊖ + ⋻ੈ⊥ੈ⊖ + ∖_ + ∖_				
	4) [⊥] [⊥] [⊥] [⊗] [⊥] [⊗] [⊥] [⊗] [⊥] [⊗]				
	5) [°] + '⊨ + [°] [⊥] [°]				
	12) 🖕 + 🗍				

Table 5: Redox fingerprint analysis of selected standard electrolyte solvents.

Solvent	Thermodynamically favourable	Lowest	Minimal Num-	Minimal Num-	Tanimoto coeffi-
Name	reaction products	HOMO	ber of Fragmen-	ber of Recombi-	cient
(e ⁻)			tations	nations	
	14) <u> </u>				
	15) °~ + ° °				
	16) [°] + [°] + [°]				
DMC	1) \ + \ + H_3C-CH3	1)	1)	1)	1), 2)
(1e)		,			
$\sum 19$	2) **** + *				
	3) 4 + ~ + 848				
	ولارة الم				
	4) + ··· + ···				
	5) — + `o — в + нас-ё о				
DMC	1) нэс-сн, + 이사이	1), 3)	1), 2), 3) 4) 5)	1), 3), 5)	1), 2), 5)
(2e)	0 9				
$\sum 7$	2) $\overset{\mu}{\longrightarrow}$ + $\overset{\mu}{\otimes}\overset{\mu}{\longleftarrow}$ + $\overset{\mu}{\otimes}\overset{\mu}{\circ}$ + $\overset{\mu}{\circ}\overset{\sigma}{\circ}$ + $\overset{\mu}{\circ}\overset{\sigma}{\circ}$				
	3) ⁽¹⁾ ₀ + ^{H₃C₁₀}				
	4) 0 + H_SC-CH_S + H_SC 0 + H_SC 0				
	, 5) н₅с-сн₅ + с + с + с + с + с + с + с + с + с +				
	H _s C _{io}				
DMM	1) ~ ~ ~ ~ ~ + Hsc-cHs + 0	1)	4)	3)	3)
(1e)	-,	-)	-)	-,	-,
$\sum 7$	2) ~~ + ~~ + ~~				
	3) ∽°∽ + `⊙∽ [⊕] + ^{CH} ₃				
	, 4) ∽₀∽◦ + ∞ + ⇔				
	5) - + + + +				
DMM	1) нус-сну + ⁸ ~ ⁹	1)	1), 2)	1)	1), 2)
(2e)	-,	-)	.,, _,	- ,	-,, _,
$\sum 10$	2) _ + $^{\circ}_{\sim \circ}^{\circ}$ + $^{\circ}_{\circ}$ + $^{\circ}_{\circ}$ + $^{\circ}_{\circ}$				
1,3-DL	1) °~o~~°~°	7), 8)	1), 6)	1), 6), 7), 8)	7)
(1e)	,		,, ,		,
$\sum 10$	2) ిాంాం				
	3)				
	4) °~~~~°~~~°				
	5) °~~°~~°				
	6) ୖୢୣୣୣୣୣୖୣୣୢୖୖୢୣୣୣୣ				
	7) °°_o				
	8) ° ° ° ° ° + H₂C=CH₂				

Table F. Daday financy wint analysis of calented standard clasticity is achieved.
Table 5: Redox ingerprint analysis of selected standard electrolyte solvents.

Solvent	Thermodynamically favourable	Lowest	Minimal Num-	Minimal Num-	Tanimoto coeffi-
Name	reaction products	HOMO	ber of Fragmen-	ber of Recombi-	cient
(e^-)			tations	nations	
1,3-DL	1) ° · · · · · · · · · · · · · · · · · ·	4), 5)	1), 2), 3), 4), 5)	5)	3)
(2e)					
$\sum 10$	2) ° · · · · · · · · · · · · · · · · · ·				
	3) ° · · · · · · · · · · · · · · · · · ·				
	4) _{H₂C=CH₂} + [©] _O ^O → ^O ^O ^O ^O				
	5) H₂C=CH₂ + 0 [⊗] [∞] + H₂C=CH₂ + 0 [⊗] [∞]				
THF (1e)	1) 🖏	1)	1)	1)	1)
$\sum 1$					
THF (2e)	-				

Table 5: Redox fingerprint analysis of selected standard electrolyte solvents.

7. Graphite Intercalation Compounds

Several different settings have been evaluated to determine the stability of graphite intercalation compounds (GICs). Example compounds for the different settings are shown below. The Small GIC denotes a coronen sandwich, the large GIC a C150-Sandwich. The setting large-side refers to a large GIC with the compound located on the edge of the sheat rather than the middle. The images below clearify the approach. The C150-Sandwiches are formed in the same manner, just with a bigger graphene sheat.

 Table 6: Different settings for the calculation of the graphite intercalation compound stability

 Small
 Standard (Small Double)





The different settings were tested for ethylene carbonate and propylene carbonate. The results were found to be in reasonable agreement with the results of Tasaki and Winter [20, 21]. The results are most consistent for the standard and large-side double settings. The standard setting

Ι	LD (Max/Avg) [Å] (EC)	ILD (Max/Avg) [Å] (PC)
	6.29/6.25	7.45/7.32
	6.77/6.63	6.87/6.77
	6.55/6.15	6.92/6.43
ble	6.48/6.29	6.92/6.61
	6.60/6.15	6.85/6.41
Double	6.61/6.27	6.77/6.58
	I ble Double	$\begin{array}{c c} \text{ILD (Max/Avg) [Å] (EC)} \\ \hline 6.29/6.25 \\ 6.77/6.63 \\ 6.55/6.15 \\ \hline ble & 6.48/6.29 \\ 6.60/6.15 \\ \hline Double & 6.61/6.27 \\ \end{array}$

Table 7: Evaluation of different settings for the determination of the stability of a graphite intercalation compound.

was chosen, because it requires less computational effort.

8. Table: Graphite intercalation compound analysis for all predicted compounds

The following table contains the interlayer distance (ILD) and the heat of formation (HOF) of all by the redox fingerprint analysis predicted products for the reduction of ethylene carbonate and propylene carbonate.

Compound	ILD (Max/Avg) [Å]	HOF [kcal/mol]
	Ethylene Carbona	te
, end of the second sec	6.41/6.28	-75.93
O H C	6.34/6.20	0.28
0 = C = 0	6.36/6.34	-2.59
H ₂ C=CH ₂	6.24/6.22	-4.01
8/ 6	7.03/6.95	6.36
$\overset{\otimes}{_{O}} \sim \overset{\circ}{_{O}} \overset{\circ}{_{O}} \sim \overset{\otimes}{_{O}}$	6.45/6.17	8.87
°	6.82/6.70	-3.17
° Correction of	7.51/7.34	-11.18
$\circ \overset{\circ}{\sim} \sim \overset{\circ}{\leftarrow} \circ \circ$	6.93/6.84	-9.41
ୢୖୄୣୣୣୖୖୄୣୣୢୖୄ	7.10/6.87	5.07
$\operatorname{e}_{o} \operatorname{e}_{o} \operatorname{e}_{o} \operatorname{e}_{o} \operatorname{e}_{o}$	7.09/6.99	5.01

Compound	ILD (Max/Avg) [Å]	HOF [kcal/mol]
$\circ^{\Theta}_{\mathrm{constraint}} \circ^{\Theta}_{\mathrm{constraint}} \circ^{O}_{\mathrm{constraint}} \circ^{O}_{\mathrm{constraint}$	6.93/6.66	-8.35
00000000000000000000000000000000000000	6.98/6.92	-1.58
ë~~~~ [⊖]	6.94/6.89	-2.81
° Contraction of the contraction	7.36/6.84	8.45
	7.21/6.83	-12.18
°, °, °, °, °, °, °, °, °, °, °, °, °, °	6.99/6.70	-2.80
$\circ^{\ominus} \frown \circ \frown \circ \frown \overset{\circ} \smile \overset{\circ} \circ \circ \overset{\circ} \smile \overset{\circ} \smile \overset{\circ} \circ \circ \overset{\circ} \smile \overset{\circ} \circ \circ \overset{\circ} \smile \overset{\circ} \circ \circ \circ \overset{\circ} \smile \overset{\circ} \circ \circ \circ \overset{\circ} \circ \overset{\circ} \circ \circ \circ \circ \overset{\circ} \circ \overset{\circ} \circ \circ \circ \circ \circ \circ \overset{\circ} \circ $	7.45/7.33	-1.53
ୢୖୄୖୖୖୖୢୄୢୄୖୖୖୖ	8.49/8.03	-15.55
$\circ \sim \circ \sim \circ \sim \circ \circ$	6.97/6.80	-10.16
$\operatorname{e}_{0}^{\circ}\operatorname{h}_{0}^{\circ}\operatorname{h}_{0}^{\circ}\operatorname{h}_{0}^{\circ}\operatorname{h}_{0}^{\circ}$	7.52/7.20	-7.62
$\circ \overset{\circ}{\longrightarrow} \circ \overset{\circ}{\to} \circ \circ$	7.18/7.01	0.84
°, do the second	7.31/7.01	2.37
$\circ^{\ominus}_{\sim} \sim \circ^{\ominus}_{\circ} \circ^{\ominus}_{\circ}$	6.68/6.55	2.48
$\circ \overset{\circ}{\longrightarrow} \circ \overset{\circ}{\to} \circ \circ$	6.76/6.62	36.74
° o o o	7.59/7.29	-302.31
¢	6.64/6.47	-8.95
O II C	0.00/0.00	0.00
e e He	0.00/0.00	0.00
${\rm H_2C}\!=\!{\rm CH_2}$	0.00/0.00	0.00
°⊖∽∽⊖ 0	0.00/0.00	0.00
	6.94/6.92	-2.32
	5.94/5.73	41.32
8~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	7.02/6.85	-5.74
	6.69/6.54	15.86
	6.73/6.70	-3.16
\odot	7.39/7.10	-5.79

Compound	ILD (Max/Avg) [Å]	HOF [kcal/mol]
	6.39/6.20	-0.98
0	6.34/6.30	-6.54
	Propylene Carbona	ate
o II	6.33/6.20	0.21
0	6.36/6.34	-2.57
\	6.75/6.54	-6.52
8-6	7.09/6.97	6.08
	7.41/7.11	-89.47
° Contraction of the second se	8.22/8.10	5.41
${\rm e}_{\rm o}^{\rm e} {\rm i}_{\rm o} {\rm e}_{\rm o}^{\rm e} {\rm e}_{\rm o}^{\rm e}$	8.36/8.07	-2.03
$\operatorname{Sec}_{\mathrm{s}} \operatorname{Sec}_{\mathrm{s}} $	9.64/9.33	-13.12
	8.31/8.25	-3.26
°	7.46/7.22	-4.51
°y°yyyyyo Lo	8.59/8.44	-15.13
	7.76/7.37	-9.43
	8.37/8.33	-7.77
° jo jo jo	8.25/8.02	-13.83
	8.35/8.22	-8.48
°	7.73/7.45	-12.47
° Lo Lo C	8.01/7.70	-3.32
$\operatorname{end}_{o}^{o} \operatorname{end}_{o}^{o} \operatorname{end}_{o}^{o}$	7.92/7.70	-11.62
	7.89/7.82	-8.78
° °	9.37/9.17	-9.50
	8.18/8.06	-7.31

Compound	ILD (Max/Avg) [Å]	HOF [kcal/mol]
	8.07/7.73	-9.82
	8.00/7.71	-10.94
$\operatorname{res}_{\operatorname{O}}^{\operatorname{O}}$	8.40/8.11	-11.16
° LoLo	8.17/8.01	10.22
	7.89/7.78	-3.68
	7.62/7.60	0.03
, ,	8.32/8.19	-2.55
°~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	7.20/7.13	-4.98
erter e	7.96/7.83	-8.16
°	8.28/8.07	-13.40
o⊖↓_o↓ o	8.27/8.11	-7.11
	8.23/8.03	-6.71
°~°	7.74/7.52	-7.23
°J°+~°Å°	7.46/7.32	-0.86
o [©] , ↓ _o ↓ _o ↓ _e	7.82/7.65	-14.32
ૻ૾૾૾ૢૢૢૢૢૢૢૢૢૢૢૢૢૺ૾ૡ	8.09/7.86	10.36
	7.42/7.11	-3.47
o [⊕] , ↓ o ⁰ , ⊕ o	6.90/6.83	12.14
°LoLoque e	8.22/7.98	-7.98
	8.43/8.24	-7.16
	9.05/8.69	-4.94
	7.56/7.30	-5.15
Å Å	7.55/7.29	-4.34

Table 8: Interlayer distances and head of formations of theby the redox fingerprint analysis predicted products.

Compound	ILD (Max/Avg) [Å]	HOF [kcal/mol]
$\operatorname{res}_{\operatorname{s}}^{\operatorname{o}} \operatorname{res}_{\operatorname{o}}^{\operatorname{o}} \operatorname{res}_{\operatorname{o}}^{\operatorname{o}}$	7.97/7.89	-2.35
$\mathcal{L}_{\mathcal{A}}^{\mathbb{O}}$	7.86/7.64	-3.26
	8.26/8.15	-6.14
°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°°	8.12/8.01	-9.09
$\bigvee_{0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0$	8.54/8.19	-4.70
	8.34/7.96	-1.33
	7.64/7.43	-1.45
${\rm e}_{\rm e}^{\rm e}$	8.55/8.23	-13.31
$\circ = \circ \circ$	8.80/8.55	-8.31
$\operatorname{c}_{\mathrm{O}}^{\otimes} \xrightarrow{O}_{\mathrm{O}}^{\otimes} \operatorname{c}_{\mathrm{O}}^{\otimes} \xrightarrow{O}_{\mathrm{O}}^{\otimes} \operatorname{c}_{\mathrm{O}}^{\otimes}$	7.68/7.38	-13.46
	7.60/7.18	-2.03
°	7.89/7.67	-14.43
:~~i	8.33/7.98	-5.64
°, to to	8.11/7.90	-6.04
° y ° y ° y ° y ° y ° y ° y ° y ° y ° y	8.79/8.57	-9.01
	8.04/7.87	-5.66
	7.52/7.28	0.40
° ,	7.68/7.36	-3.48
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	7.56/7.43	-10.46
	7.62/7.32	-8.56
${}_{0}^{\otimes} \not \downarrow_{0} \not \downarrow_{0}^{\otimes} \not \downarrow_{0}^{\otimes}$	7.67/7.25	-11.42
	7.47/7.39	-9.14
¢, Love	7.45/7.05	-11.20
o II	6.36/6.20	0.19

Compound	ILD (Max/Avg) [Å]	HOF [kcal/mol]
e e	6.03/5.77	10.35
\	6.77/6.55	-6.48
<u>}</u>	7.58/7.53	-7.87
	7.05/6.82	-16.53
°	7.49/7.43	4.53
	8.20/8.04	-3.80
°~~↓~°	8.24/8.04	-10.12
	7.62/7.30	0.24
	7.57/7.44	-2.37
	8.12/7.76	-0.57
8~ <u>_</u> 8	7.96/7.85	-5.87
	6.69/6.54	15.88
	8.39/8.12	-5.75
° Lo Co	7.70/7.26	-4.26
	8.35/8.12	-8.86
	8.28/8.07	-9.45
	8.32/8.01	-8.41
	7.41/7.14	-1.97
	7.84/7.67	-7.00
00	6.38/6.34	-6.61

Table 8: Interlayer distances and head of formations of theby the redox fingerprint analysis predicted products.

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