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EDAS and TOPSIS based Estimation of Oxidation of Methionine by Cr(VI) Reagents

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Abstract

Objectives: To find the suitable solvent for the oxidation of methionine by Cr(VI) reagents using EDAS and TOPSIS method. **Methods:** When methionine oxidized by Cr(VI) complexes i.e. tetrakis(pyridine)silver dichromate (TPSD), quinolinium bromochromate (QBC), tetraethylammonium chlorochromate (TEACC) and quonilinium chlorochromate (QCC) formation of corresponding sulfoxide take place. Reaction performed in chloroform (CF), 1,2-dichloroethane (DCE), dichloromethane (DCM), dimethylsulphoxide (DMSO) and acetone solvents. **Findings:** Reaction is fastest in DMSO and slowest in acetone for the oxidation of methionine in the following- DMSO, DCE, DCM, acetone, CF. **Novelty:** Solvent effect is investigated using the rate constant k_2, by EDAS and TOPSIS methods.

Keywords: Methionine; Oxidation; Solvent effect; EDAS; TOPSIS

1 Introduction

Oxidation reaction in non-aqueous conditions is a fundamental process in synthetic organic chemistry. Since metal ions are involved in so many biological processes, oxidation kinetics has gained a lot of attention. In redox reactions, chromium (VI) serves as an effective catalyst. A number of chromium(VI) oxidants, including pyridinium chlorochromate[1], tributylammonium chlorochromate[2], tripropylammonium fluorochromate[3], pyridinium fluorochromate[4], imidazolium fluorochromate[5], and isoquinolinium bromochromate[6], used for the oxidation process of various organic compounds. Several oxidants proposed as mechanistic studies for methionine oxidation[7–14]. Sulfur identified most vulnerable to attack by chromium(VI) and a low energy source for the electron transfer[15–17]. ATP and liver enzyme initiate the transfer of the methyl group of methionine[18]. Reactive oxygen species (ROS) can oxidise amino acids and the oxidation reaction can occur with one or two electron transfers[19–21]. Around the sulphide, amino and carboxyl groups control the redox process[22–24]. Methionine has a regulating role, based on potential reversion by the enzyme

methionine sulfoxide reductase (Msr)[25]. Methionine to methionine sulphur radical cation, oxidation can play an important role in protecting protein oxidation[26,27]. Many experiments conducted on the oxidation of methionine and methionine-containing peptides[28–31]. Met residue oxidation in vivo contributes to the formation of methionine sulfoxide, which can catalyse a thioredoxin-dependent decrease of methionine residue from sulfoxide, and the majority of the cells that produce methionine sulfoxidereductase[32]. Methionine oxidation is significant in physiology and pathology[33–37]. Solvent impact studies on acetaldehyde and benzaldehyde oxidation have been conducted[38,39]. A review of the literature shows that no research exists on the estimate of methionine oxidation by various Cr (VI) reagents using EDAS and TOPSIS. TOPSIS is a technique for evaluating performance on the basis of its resemblance to the ideal solution. Recently, it has been incorporated into renewable energy technologies[40–44]. Keshavarz Ghorabaee et al.[45] proposed the EDAS scheme, a contemporary and powerful technique. EDAS method applied to a variety of real-world problems[46–50]. The effect of solvent on the oxidation of methionine by Cr(VI) reagents is discussed in this paper. The assessment of solvent impact by EDAS and TOPSIS methods for the oxidation of methionine by Cr(VI) oxidizing agents is a significant achievement in this work.

2 Material and Methods

Material: The DL-methionine (Merck, Germany) is used exactly as prescribed. The stated methods are used to prepare TPSD[51], QCC[52], QBC[53], and TEACC[54], and purity is determined using an iodometric process. Solvents are purified using standard purification methods[55].

Measurements: By holding an excess of methionine (X 10 or greater) over the oxidant, the reactions have been set up to operate under pseudo-first order conditions. The reactions take place at a steady temperature of 303 K. The reaction mixture is made by combining the required amounts of methionine and Solvent, etc., and then allowed to stand in a thermostatic bath for a suitable amount of time to allow the solution to reach the temperature of the bath. The reaction is started by pipetting in an oxidant solution that has previously been equilibrated in the thermostat. To blend the solution, the reaction flask was vigorously swirled. The reactions are then monitored spectro-photometrically for a decrease in [oxidant].

3 Results and Discussion

There are a variety of MCDM (multiple criteria decision making) approaches for selecting the optimal solvent among those available. We compare the value of the rate constant k_2 in five different solvents using the EDAS and TOPSIS methods.

3.1 Evaluation Based on Distance from Average Solution (EDAS) Method

Step-1 Identify the mean solution $(S\alpha_j)$

$$S\alpha_j = \frac{\sum_{i=1}^{n} A_{ij}}{n}$$

Step-2 Positive distances from mean
   If j^{th} criterion is beneficiary

$$PDM_{ij} = \frac{\text{Max}\left\{0, (A_{ij} - S\alpha_j)\right\}}{S\alpha_j}$$

If j^{th} criterion is non-beneficiary

$$PDM_{ij} = \frac{\text{Max}\left\{0, (S\alpha_j - A_{ij})\right\}}{S\alpha_j}$$

Step-3 Calculate negative distances from mean(NDM)
   If j^{th} criterion is beneficiary

$$NDM_{ij} = \frac{\text{Max}\left\{0, (S\alpha_j - A_{ij})\right\}}{S\alpha_j}$$

If j^{th} criterion is non-beneficiary

$$NDM_{ij} = \frac{\text{Max}\left\{0, (A_{ij} - S\alpha_j)\right\}}{S\alpha_j}$$

Step-4 Weighted addition of PDM

$$AP_i = \sum_{j=1}^{m} w_j PDM_{ij}$$

Step-5 Weighted addition of NDM

$$AN_i = \sum_{j=1}^{m} w_j NDM_{ij}$$

Step-6 Normalization of AP and AN

$$NMP_i = \frac{AP_i}{\text{Max}(AP_i)}$$

$$NMN_i = 1 - \frac{AN_i}{\text{Max}(AN_i)}$$

Step-7 Normalization of NMP and NMN

$$MX_i = (NMP_i + NMN_i)/2$$

In this study, we asserted the order of reactivity as acetone < DCE < DCM < CF < DMSO, when oxidants such as TPSD, QBC, TEACC, and QCC were used. This order corresponds to the best solvent claimed in earlier TOPSIS investigations [38].

3.2 Technique for Order of Preferences by Similarity to Ideal Solution (TOPSIS) Method

Step-1 Calculate the matrix's normalised value

$$A_{ij} = \frac{A_{ij}}{\sqrt{\sum_{i=1}^{n} A_{ij}^2}}$$

Step-2 Determine the weighted normalised matrix.

$$T_{ij} = A_{ij} \times W_j$$

Step-3 Calculate the best and worst ideal worth
　　Step-4 Calculate the Euclidean interval between the ideal best and the actual best.

$$D_i^+ = \left[\sum_{j=1}^{m} \left(T_{ij} - T_j^+\right)^2\right]^{0.5}$$

Step-5 Calculate the Euclidean interval between the ideal best and the actual worst.

$$D_i^- = \left[\sum_{j=1}^{m} \left(T_{ij} - T_j^-\right)^2\right]^{0.5}$$

Step-6 Determine the performance score

$$P_i = \frac{D_i^-}{D_i^+ + D_i^-}$$

In this analysis, we claimed the order of reactivity as acetone < DCM < DCE < CF < DMSO, when oxidants such as TPSD, QBC, TEACC and QCC are taken. This order is also satisfies with the best solvent claimed in previous studies using TOPSIS method [38].

Table 1. Rateconstants for the oxidation of methionine by various oxidants (k_2 $10^4 dm^3$/mol s)

Solvents	TPSD	QBC	TEACC	QCC
CF	77.6	50.1	35.8	75.9
DCE	87.1	41.7	29.3	67.6
DCM	72.4	42.6	34	63.1
DMSO	216	135	80.2	198
ACETONE	63.1	34.7	27	52.5

Table 2. Determination of meansolution

Solvents	TPSD	QBC	TEACC	QCC
CF	77.6	50.1	35.8	75.9
DCE	87.1	41.7	29.3	67.6
DCM	72.4	42.6	34	63.1
DMSO	216	135	80.2	198
ACETONE	63.1	34.7	27	52.5
	103.24	60.82	41.26	91.42

Table 3. PositiveDistance from Mean (PDM)

Solvents	TPSD	QBC	TEACC	QCC
CF	0.24835335	0	0	0
DCE	0.15633475	0	0	0
DCM	0.29872143	0	0	0
DMSO	0	1.219664584	0.943771	1.165828
ACETONE	0.38880279	0	0	0

Table 4. Negative Distance from Mean (NDM)

Solvents	TPSD	QBC	TEACC	QCC
CF	0	0.17625781	0.132332	0.169766
DCE	0	0.314370273	0.289869	0.260556
DCM	0	0.299572509	0.175957	0.309779
DMSO	1.09221232	0	0	0
ACETONE	0	0.429463992	0.345613	0.425727

Table 5. Weightedsum of PDM

TPSD	QBC	TEACC	QCC	SPi
0.06208834	0	0	0	0.062088
0.03908369	0	0	0	0.039084
0.07468036	0	0	0	0.07468
0	0.30491615	0.235943	0.291457	0.832316
0.0972007	0	0	0	0.097201

Table 6. Weightedsum of NDM

TPSD	QBC	TEACC	QCC	SNi
0	0.04406445	0.033083	0.042441	0.119589
0	0.07859257	0.072467	0.065139	0.216199
0	0.07489313	0.043989	0.077445	0.196327
0.27305308	0	0	0	0.273053
0	0.107366	0.086403	0.106432	0.300201

Table 7. Rank the order with normalised criterion

Solvents	APi	ANi	NAPi	NANi	MXi	Rank
CF	0.06209	0.11959	0.299745	0.334731	0.31724	2
DCE	0.03908	0.2162	0.188662	-0.2027	-0.007	4
DCM	0.07468	0.19633	0.360524	-0.09217	0.13418	3
DMSO	0.83232	0.27305	4.018094	-0.51895	1.74957	1
ACETONE	0.0972	0.3002	0.469241	-0.66999	-0.1004	5

Table 8. Normalized matrix

Solvents	TPSD	QBC	TEACC	QCC
CF	0.29438	0.31378	0.3501	0.32
DCE	0.330419	0.26117	0.2865	0.285
DCM	0.274653	0.26681	0.3325	0.266
DMSO	0.819408	0.84552	0.7843	0.835
ACETONE	0.239373	0.21733	0.264	0.221

Table 9. Weighted normalized matrix

Solvents	TPSD	QBC	TEACC	QCC
CF	0.073595	0.07845	0.0875	0.08
DCE	0.082605	0.06529	0.0716	0.071
DCM	0.068663	0.0667	0.0831	0.066
DMSO	0.204852	0.21138	0.1961	0.209
ACETONE	0.059843	0.05433	0.066	0.055

Table 10. Best and worst ideal values

V+	0.204852	0.21138	0.1961	0.209
V-	0.059843	0.05433	0.066	0.055

Table 11. Euclideandistances, Performance scores and ranks

Solvents	D_i^+	D_i^-	Pi	Rank
CF	0.251	0.043	0.146	2
DCE	0.266	0.03	0.103	3
DCM	0.269	0.025	0.086	4
DMSO	0	0.293	1	1
ACETONE	0.293	0	0	5
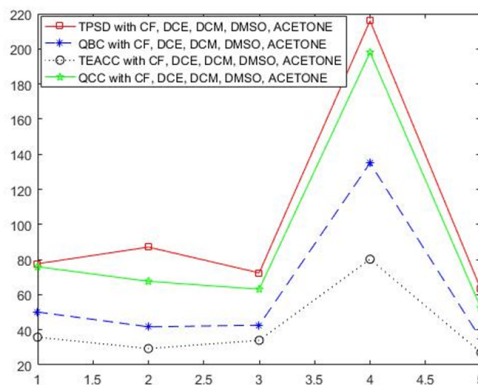
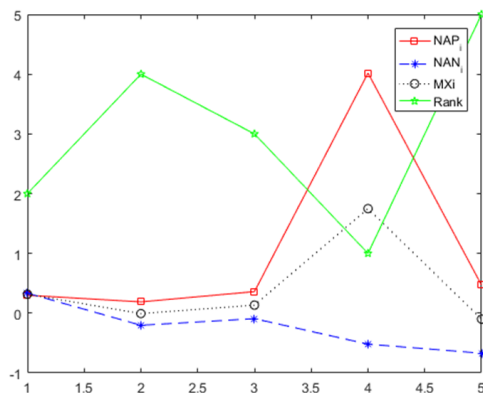**Fig 1.** Distribution of rateconstants by various oxidants

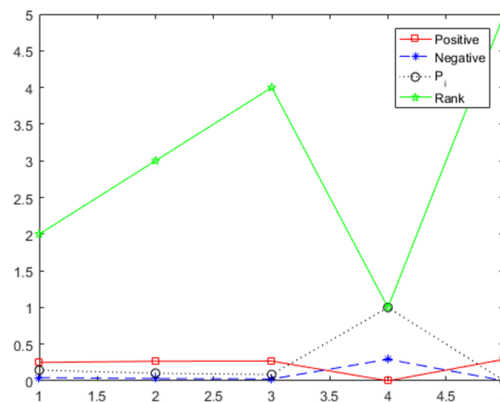**Fig 2.** Sensitivity analysisof optimal values in EDAS

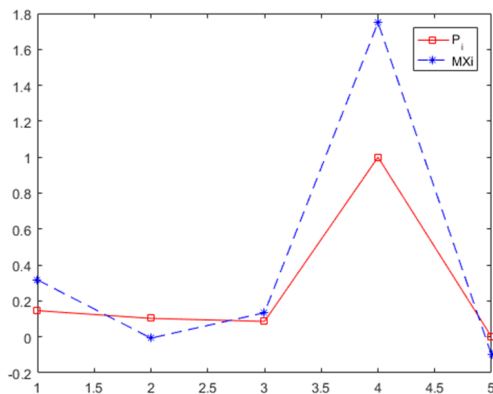**Fig 3.** Sensitivity analysis of optimal values in TOPSIS

Fig 4. Comparative study of EDAS and TOPSIS

4 Conclusion

Comparative solvent effect analysis is a critical concept of physical organic chemistry. EDAS and TOPSIS are decision-making algorithms that are used in various decisions. In this analysis, we discovered the following solvent preference order for methionine oxidation:

- Making use of EDAS technique obtained as acetone < DCE < DCM < CF < DMSO.
- Making use of TOPSIS technique obtained as acetone < DCM < DCE < CF < DMSO.

The reaction occurs most rapidly in DMSO and most slowly in acetone. Oxidation of methionine by Cr(VI) reagents using EDAS and TOPSIS methods is the new work in the field and is very applicable to choose the best alternative from the available solvents for more reactivity. The current study was limited to a crisp scenario of available data, but in real-world circumstances, there are many uncertainties in data that cannot be addressed with the evaluated methodologies. So, in the future, our primary focus will be on dealing with uncertainty through the use of probability ideas and fuzzy mathematical methodologies.

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