December 10, 2021

Mr. Nick Talken
Molecule Corp. Company
Henkel
5110 Port Chicago Highway
Concord, CA 94520

Reference No. 21-0089

Dear Mr. Talken:

This letter is in response to your August 23, 2021, letter requesting clarification of the Hazardous Materials Regulations (HMR; 49 CFR Parts 171-180) applicable to hazardous materials classification. You state that your company has developed a software data platform which provides—for any new chemical formulation—the appropriate hazard classification and description. The output includes the UN Identification Number (UNID), hazardous materials shipping description, hazard class, and packing group (PG) as appropriate. The automatic assignment of hazard classification and description information is based on historical company data (e.g., in-house testing data) and you provided further detail on how this function is performed by the software. You seek feedback from this Office on your company's software approach and technique for determination of hazard class and descriptions.

In accordance with § 173.22, it is the shipper's responsibility to properly classify and describe a hazardous material. There is no prohibition in the HMR against using a software approach as part of the process to perform the functions of classifying and describing a hazardous material; however, a software approach cannot act as a substitute for the performance of testing in determining a hazard classification, where it is required. It is our understanding that your software approach is an assistive tool and not a replacement for company testing in the absence of historical company test data that can be used as a comparison for a new formulation. Therefore, if your software approach—as described in your August 23, 2021, letter—provides the hazard classification and material description in compliance with the requirements of the HMR and international regulations for the transport of hazardous materials, then we see no issue with your company using this tool with regard to the shipper's responsibility.

Please note, this response letter is neither a validation nor a certification of your software approach.

I hope this information is helpful. Please contact us if we can be of further assistance.

Sincerely,

Dirk Der Kinderen
Chief, Standards Development Branch
Standards and Rulemaking Division

From:	Foster, Glenn (PHMSA)
To:	Dodd, Alice (PHMSA); Hillman, Kenetha CTR (PHMSA)
Subject:	FW: Henkel Company Correspondence
Date:	Monday, August 30, 2021 12:23:15 PM
Attachments:	EO - Kelley(Henkel) 30Aug21.pdf

Alice and Kenetha,

Please log this in as a request for a LOI and assign.

Thanks,
Glenn

From: Kelley, Shane (PHMSA) <shane.kelley@dot.gov>
Sent: Monday, August 30, 2021 12:20 PM
To: Foster, Glenn (PHMSA) <Glenn.Foster@dot.gov>
Subject: FW: Henkel Company Correspondence

Can we log this as an interp? I'd like to respond that we do not review software as a function of our Office, but that automated methods of classification are acceptable provided that the resulting classification is accurate and conforms to the requirements of the HMR. Something like that. Can be short and sweet.

From: Lisak, Frank (PHMSA) <frank.lisak@dot.gov>
Sent: Monday, August 30, 2021 12:00 PM
To: Kelley, Shane (PHMSA) <shane.kelley@dot.gov>
Subject: Henkel Company Correspondence

Hi, Shane:

The attachment is for your review.

I will keep the hardcopy in my locked cabinet until DOT resumes normal working hours.

Frank

Albert - Open Letter to Department of Transportation - United States of America

Date: August 23rd, 2021

Mr. Shane Kelley
Director, Standards and Rulemaking Division
U.S. DOT/PHMSA (PHH-10)
1200 New Jersey Avenue, SE East Building, 2nd Floor
Washington, DC 20590

Dear Mr. Kelley,

Over the past 4 years, we have been developing a software data platform (called Albert) which facilitates our ability to invent new chemical formulations and materials. Specifically, this data platform was built to capture structured data which can be used to accelerate innovation and enhance collaboration between chemists or laboratories. Albert has many capabilities and functions, include chemical inventory management, formulation and design of experiment, task management, reporting and visualization, and many more. However, the intent of this Open Letter is to describe a specific feature of Albert that is related to the shipment of Hazardous Materials (HM) / Dangerous Goods (DG).

Within the Albert platform, any chemist who has created a formulation can automatically receive the appropriate HM / DG Shipping Classification for each relevant transportation regulation (49 CFR, IATA, IMDG). The output of this classification includes: UN Number, Hazard Materials Shipping Description, Hazard Class or Classes and Packing Group as appropriate. This automatic assignment of HM / DG shipping information is based on all historical data within Albert, where the newly created formulation is compared to historical formulations, to ensure compliance with the shipping regulations. The remaining content within this letter will describe in detail how this comparison and automatic assignment is done.
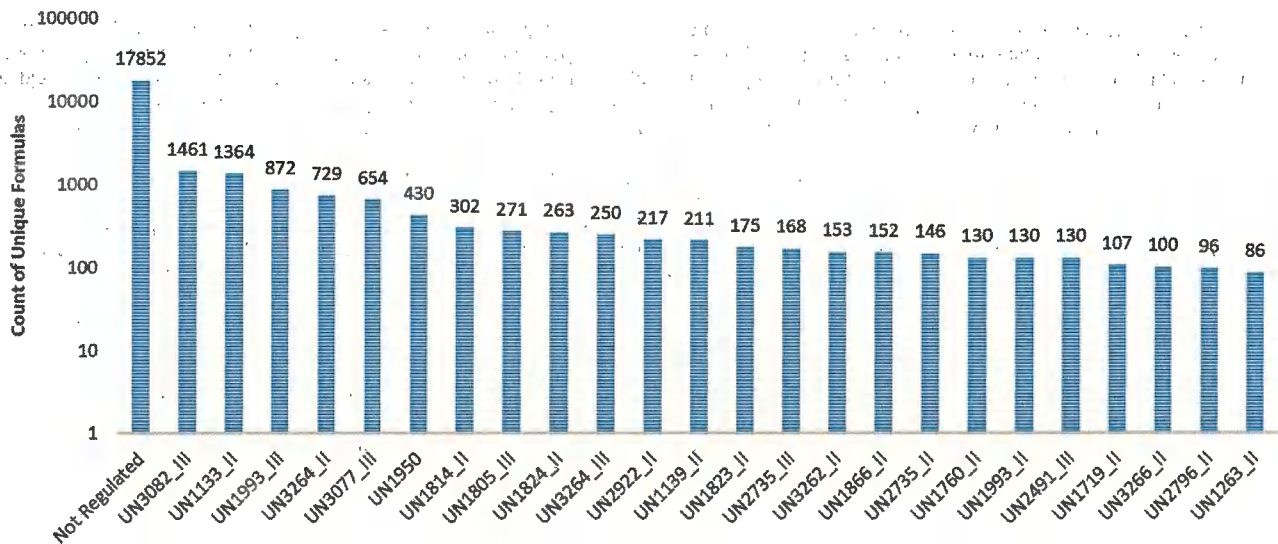
Historical Data:

Within Albert, we have over 20 years worth of historical formulas that have been commercialized and shipped within the USA. Below you can see the number of formulas which have been created, per Transportation method:

Transport Method	Count of Unique Formulas
49 CFR	26449
IATA	29699
IMDG	30147

For all of these historical formulations, a Risk Assessment and HM / DG Classification was performed by a certified expert within Henkel. Below you can see the specific UN Numbers and Packing groups that are contained within this dataset. These Classifications were all performed manually by a certified Risk Assessment expert team, primarily located in Dusseldorf, Germany.
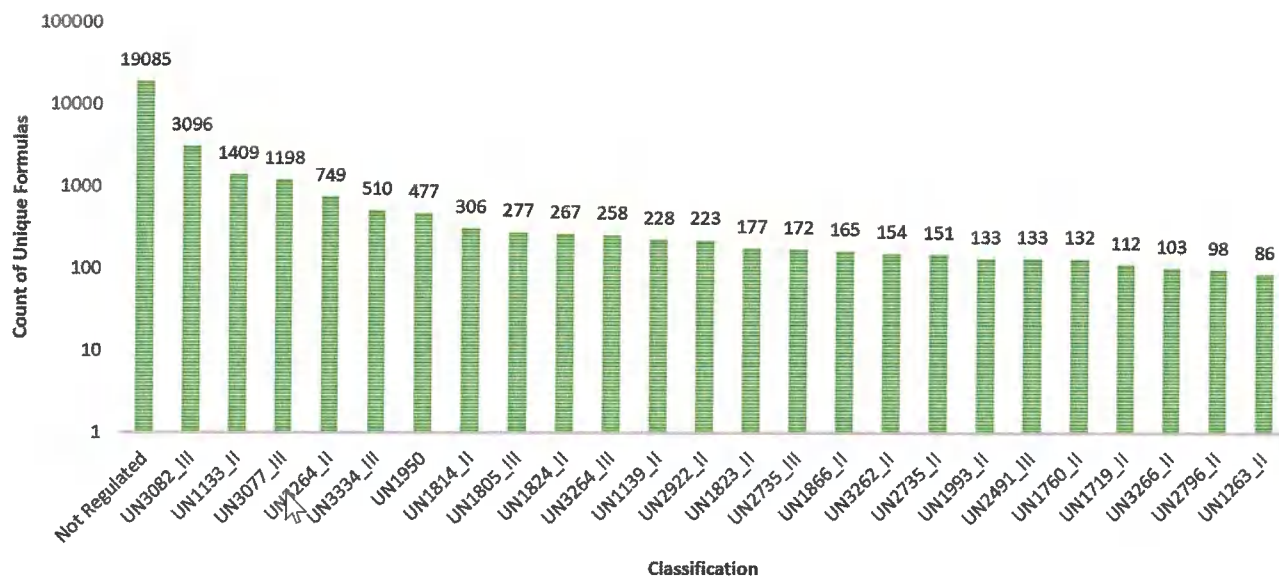
Classification Format: (UNnumber_PackingGroup)
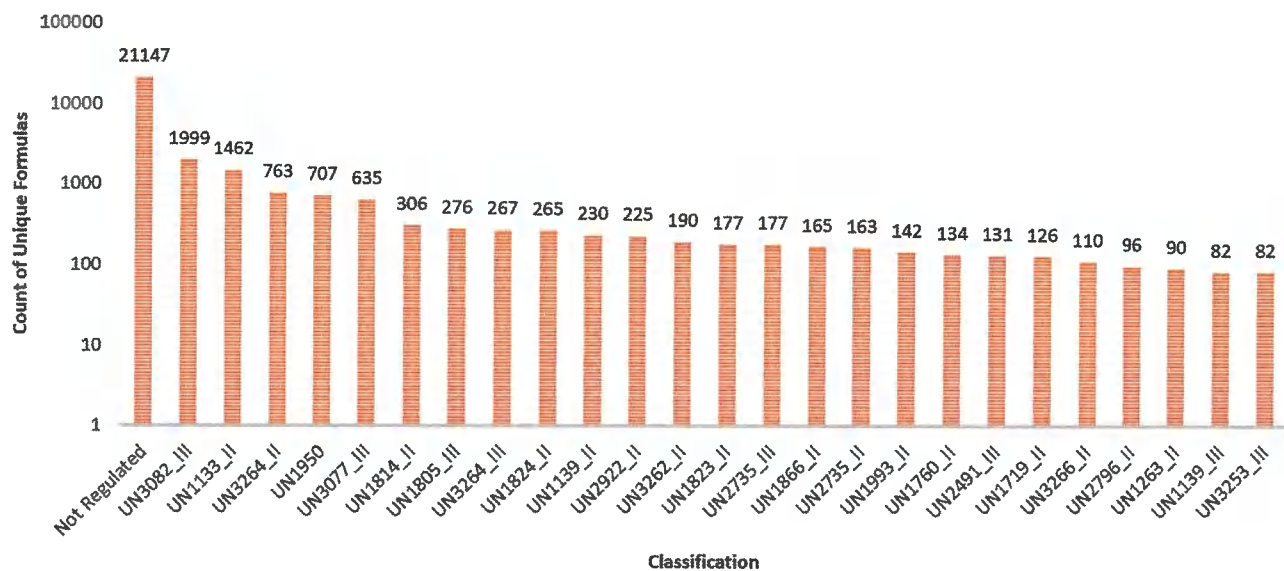

TRANSPORT METHOD: CFR

TRANSPORT METHOD: IATA

Count of Unique Formulas (y-axis, logarithmic: 1, 10, 100, 1000, 10000, 100000)

Values by Classification (x-axis):
- Not Regulated: 19085
- UN3082_III: 3096
- UN1133_II: 1409
- UN3077_III: 1198
- UN1264_II: 749
- UN3334_III: 510
- UN1950: 477
- UN1814_II: 306
- UN1805_III: 277
- UN1824_II: 267
- UN3264_III: 258
- UN1139_II: 228
- UN2922_II: 223
- UN1823_II: 177
- UN2735_III: 172
- UN1866_II: 165
- UN3262_II: 154
- UN2735_II: 151
- UN1993_II: 133
- UN2491_III: 133
- UN1760_II: 132
- UN1719_II: 112
- UN3266_II: 103
- UN2796_II: 98
- UN1263_II: 86

Classification (x-axis label)

TRANSPORT METHOD: IMDG

Count of Unique Formulas (y-axis, logarithmic: 1, 10, 100, 1000, 10000, 100000)

Values by Classification (x-axis):
- Not Regulated: 21147
- UN3082_III: 1999
- UN1133_II: 1462
- UN3264_II: 763
- UN1950: 707
- UN3077_III: 635
- UN1814_II: 306
- UN1805_III: 276
- UN3264_III: 267
- UN1824_II: 265
- UN1139_II: 230
- UN2922_II: 225
- UN3262_II: 190
- UN1823_II: 177
- UN2735_III: 177
- UN1866_II: 165
- UN2735_II: 163
- UN1993_II: 142
- UN1760_II: 134
- UN2491_III: 131
- UN1719_II: 126
- UN3266_II: 110
- UN2796_II: 96
- UN1263_II: 90
- UN1139_III: 82
- UN3253_III: 82

Classification (x-axis label)

Automatic Generation of Classification for New Formulas:

Based on the Historical Data, whenever a new formula is created within the Albert Platform, Albert can lookup all similar formulas and determine the appropriate HM / DG classification, for each transportation method. This gives the chemist the ability to automatically determine the appropriate HM / DG classification. This is automatically done prior to shipping the chemical via a shipment method covered under 49 CFR, IATA or IMDG. This "lookup" algorithm was built by a team of chemists, engineers and data scientists, who are all Train-the-Trainer certified in DOT, IATA, IMDG as well as ADR Dangerous Goods regulations and associated shipments.

Algorithm Similarity:

It is very important to understand how the similarity is determined by the above mentioned Algorithm. This similarity is a combination of many factors, including GHS classification, Flash Point, Reaction Exotherm, Product Type, State of Matter, Chemical Composition, and others. The purpose of the Algorithm is to determine the best combination of factors (mentioned above) which allow for the closest formula comparison.

Validation of Algorithm:

In order to ensure this method of "lookup" is accurate for a wide variety of new potential formulas, we performed statistical testing on the historical data. First, we split the historical data into 2 partitions, with 80% in the "training set" and 20% in the "test set". For each of the transportation methods, we took the "test set" and used algorithm with the "training set" to determine the HM / DG classification. We then compared this HM / DG classification to the actual classification from the "test set". The results of this test ensures complete accuracy across all historical and new data.

We understand that compliance with these regulations is paramount at all times from the beginning to end of the classification and transport cycle.

Based on complete accuracy of this system information and the end result specifically (proper classification of the HM / DG) we believe that we can achieve compliance with the regulatory requirements pertaining to proper transport under 49 CFR, IATA and IMDG Standards.

Open Questions:

1. Based on the information provided, assuming the above information is accurate, we would like to solicit any input from the Department on our approach.
2. Please provide any other feedback on our software driven approach and techniques.
3. Please provide your position on our methods stated above, given that it has been shown to be more accurate than manual classification.

Thank you and we look forward to your response.

Sincerely,

Nick Talken

Head of Albert Data Platform

nick.talken@henkel.com

(925) 381-6796

Nick Talken

Ken Kisner

Head of Digital Innovation

ken.kisner@henkel.com

(925) 381-1253

Ken D. Kisner