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Frequency of Submission of Physical-Chemical Information on Premanufacture Notices

5. Frequency of Submission of Physical-Chemical Information on Premanufacture Notices

Many different types of information can be used to describe the physical and chemical properties of a substance. The most important for the Environmental Protection Agency (EPA) are those that describe or project the behavior of the chemical under normal environmental conditions. For instance, a chemical that is soluble in water presents problems different from those of a water-insoluble chemical.

OTA inspected premanufacture notices (PMNs) for the presence or absence of nine items of physical and chemical information. Those nine are listed in table **6** along with a short description of the use of each item. Table **6** also lists two other items that were checked by OTA. "Transportation" provides information about how the chemical is to be moved, and "emergency information" means that the submitter has developed methods to cleanup spills and decontaminate workers who come in contact with the substance.

Inspection of appendix A shows that EPA evaluated many of these items of information in evaluating PMNs. When an item was missing from the PMN file, and it was of value to the PMN review, EPA scientists had to estimate it. The items examined by OTA include seven (melting point, boiling point, density, vapor pressure, volubility in water, partition coefficient, and infrared spectra) identified by the Organization for Economic Cooperation and Development as useful in describing new chemicals, and, at one time, recommended for inclusion in PMNs by EPA **(46** F.R. **8986).**

Table 6.—items of Physical-Chemical Information That Were Scored on PMNs

Item/Usefulness in determining possible risks of chemicals
Purity. -Necessary to delineate final product composition and to know how much new chemical will be manufactured.
Infrared spectra.-Provides a "fingerprint" for identifying the chemical.
Analytical methods.—Provides information useful for identifying the chemical.
Melting point.- Provides information about the physical state (liquid or solid) of the chemical during use.
Boiling point.-Provides information about the physical state (liquid or gas) of the chemical during use and some information about volatility.
Density.—Provides information about whether the chemical will float or sink in water.
Vapor pressure. —Provides key information about potential for exposure through inhalation and escape of the substance into the atmosphere.
Water solubility.—Provides information about chemical behavior in water and an indication of the likelihood of chemical being taken up by animals and humans.
Partition coefficient.—This measurement reflects the relative affinity of a chemical for an aqueous versus an organic environment. It is important for making predictions about a substance's persistence in various environments.
Transportation. — Information about the method(s) used to move the chemical from site to site,
Emergency Information.—Warning of possible hazards of the chemical and methods to decontaminate people and areas.

SOURCE: In part from Mazza (1982); Office of Technology Assessment.

HOW MANY PHYSICAL-CHEMICAL DATA WERE SUBMITTED ON PMNs?

Data about the nine physical-chemical items listed in table **6** are collected by companies in the development and manufacture of at least some chemicals because such information is necessary or at least highly desirable to characterize the chemical and manage its manufacture. None of the items of physical-chemical data listed in table **6** is specified in the Toxic Substances Control Act

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(TSCA), but reporting of such data in "the possession or control" of the submitter is provided for by the general reporting requirements.

The data in table 7 show that none of the PMNs examined by OTA reported all the items of physical-chemical data listed there. Also shown is the fact that only 29 of the PMNs, 4 percent of the total, reported none of the physical-chemical items listed in the table.

There are, of course, several possible reasons for physical-chemical data not being present in the PMN. First, the submitter might not have the data because they have no value in the development or manufacture of the chemical. Second, the submitter might have some data, but, for one reason or another, not reported them. Third, data may have been lost from the file.

There was general agreement among reviewers of the first draft of this background paper that it would be unusual for a submitter to develop data about all items shown on table **6.** For instance, knowledge of the melting point is useful for a chemical that exists as a solid and a liquid under the conditions of manufacture and use; knowledge of the boiling point might be less important. Similarly, knowledge of the vapor pressure of a solid has little usefulness. Arguments like these certainly can be advanced to explain why none of the PMNs reported all the items and emphasize that submitters develop and collect data that are important to them. Since EPA is most interested in the properties of the chemicals under normal exposure conditions, the data collected by submitters should be useful to the Agency also.

One reviewer expressed the opinion that it is impossible to develop a chemical for manufacture without some physical-chemical data. The same reviewer also suggested that some submitters might elect not to report physical-chemical data because those items are not specified in TSCA.

Other reviewers emphasized that a new chemical that represents only a small change from an existing chemical may require few physical-chemical measurements to manage its development and manufacture. As an example, a reviewer suggested that a new polymer that differed from an existing polymer only in being somewhat longer might be produced without developing new physical-chemical data.

The physical-chemical datum most frequently reported was purity, followed by information about analytical methods. Those two items are especially important to the manufacturer. Knowledge of purity is necessary to any estimates of how much of the new chemical will be made, and analytical methods are necessary to locate and measure the substance.

The items that are most directly related to predicting the behavior of a chemical in the environment and its likelihood of being taken up by animals and humans—melting point, boiling point, density, volubility in water, and partition coefficient—were reported less frequently. Of these, sol-

Table 7.–Number of Physical-Chemical Data [terns Submitted on PMNs

	Manufactured		Nonmanufactured		June 1982		Regulated	Total	
	Number	Percent	Number	Percent	Number	Percent	Number	Number	Percent
PMNs	331	100	330	100	70	100	9	740	100
Infrared spectra	57	17	25	8	4	6	0	*86*	*12*
Purity	269	58	222	67	49	70	3	543	73
Analytical methods	191	58	176	53	39	56	8	414	56
Melting point	83	25	78	24	11	16	7	179	24
Boiling point	92	28	97	29	23	33	7	219	30
Density	61	18	63	19	9	13	7	140	19
Vapor pressure	83	25	73	22	18	26	6	180	24
Volubility (water)	149	45	129	39	27	39	3	308	42
Partition coefficient	15	5	11	3	0	—	1	*27*	4
Transportation	238	72	197	60	47	67	0	482	65
Emergency information	107	32	111	34	31	44	6	255	34
—all	0		0	—	o	—	o	0	—
—none	*9*	*' 3*	19	6	1	1	0	*29*	*4*

SOURCE: Office of Technology Assessment.

ubility in water was reported on 42 percent of all PMNs and melting point and boiling point on 24 and 30 percent respectively. Vapor pressure was reported on 24 percent and partition coefficient on 4 percent.

A reviewer pointed out that measurements such as melting points and boiling points are only possible on relatively pure substances. Many commercial chemicals are not so pure and such measurements, even if they were made, according to the reviewer, would be meaningless. Additionally, EPA reported that the majority of PMNs describe solid materials and that some measurements, especially vapor pressure, have little value for those substances.

The partition coefficient, which measures the relative affinity of a chemical for both aqueous and organic environments, is gaining wide acceptance as being especially useful in making predictions about possible bioaccumulation of a chemical. Its usefulness is limited to substances that are soluble in both octanol and water. Despite that limitation, EPA staff reported that partition coefficients are very important in making estimates of effects on the environment. It was often used in PMN reviews, and when it was not supplied on the PMN (it was absent from **96** percent), EPA reviewers estimated the partition coefficient based on knowledge of related chemicals.

An industry reviewer drew attention to an important piece of information that EPA often obtains on the PMN or subsequently requests. A simple "block diagram" of the process by which the chemical is to be made supplies much information about the temperatures and conditions of manufacture that is useful in assessing worker exposure and learning about the properties of the chemical. Another reviewer from an environmental organization also mentioned the block diagrams but characterized them as less valuable for risk assessment than are more detailed descriptions of the manufacturing processes. Unfortunately, OTA did not collect data about the frequency with which process descriptions were reported.

PHYSICAL-CHEMICAL DATA WERE REPORTED MORE FREQUENTLY ON MANUFACTURED PMNs

The data in table 7 show that PMNs that described manufactured chemicals were more complete in reporting physical-chemical data. An explanation for this observation could be that more data have been accumulated on chemicals that are *closer* to being manufactured. In other words, if a submitter waits to file a PMN until he is more nearly ready to produce the chemical, he may have accumulated more information about the chemical.

Table **8** reports an examination of the possibility that chemicals for which PMNs were submitted closer to the time of manufacture reported more information about physical-chemical properties of the substance. Manufactured chemicals were divided into eight groups-those for which notices of commencement of manufacture were filed before the end of the 90-day review period and those filed within 1 to **9** days, **10** to **29** days, **30** to **89** days, **90** to **119** days, 120 *to* **179** days, 180 to **365** days, and more than 1 year after the end of the review period. Inspection of table 8 does not reveal any consistent pattern in completeness of reporting and does not support the idea that the amount of physical-chemical information submitted on PMNs depends on the length of time between submission and manufacture.

The reason for more complete reporting on manufactured chemicals is not known, and further analysis would be necessary to find it. In absence of that knowledge, the apparent difference between manufactured and yet-to-be manufactured chemicals remain an interesting observation.

Table 8.—Completeness of PMNs for Physical-Chemical Information as a Function of the Time Between End of the Review Period and the Commencement of Manufacture

	Time to notice of commencement														
	<1 day	1-9 days		10-29 days		30-89 days		90-119 days		120-179 days		180-365 days		>365 days	
	No.	No.	Percent	No.	Percent	No.	Percent	No.	Percent	No.	Percent	No.	Percent	No.	Percent
PMNs	10	45	100	41	100	87	100	23	100	41	100	58	100	25	100
Infrared spectra	3	12	26	4	10	14	16	2	9	5	12	14	24	3	12
Purity	9	36	80	36	88	71	82	17	83	32	78	47	81	21	84
Analytical methods	7	30	67	20	49	55	63	9	39	22	54	34	59	13	52
Melting point	2	7	16	7	17	30	35	8	35	9	22	14	24	6	24
Boiling point	4	15	33	8	19	26	30	7	30	5	12	19	33	7	28
Density	5	11	24	7	17	15	17	4	17	3	7	9	16	6	24
Vapor pressure	5	13	29	7	17	26	30	4	17	4	10	17	29	6	24
Solubility water	4	21	47	18	44	43	49	11	48	18	44	26	45	7	28
Partition coefficient	1	1	2	0	—	3	3	0	—	2	5	7	12	1	4
Transportation	10	36	80	23	56	68	78	19	83	27	66	40	69	19	76
Emergency information	5	24	53	12	29	32	37	9	23	9	22	8	14	7	28

SOURCE: Office of Technology Assessment.

SUBMISSION OF PHYSICAL-CHEMICAL DATA ON PMNs OF DIFFERENT CLASSES

In general, less concern is attached to polymers (Class 3) substances than to other chemicals because their large size (high-molecular weight) tends to make them biologically inactive. Table 9 describes the number of polymer PMNs that contained physical-chemical data and compares that information to the same information submitted about nonpolymers (Classes 1 and 2).

As can be seen, there are few pronounced differences in reporting physical-chemical data between nonpolymers and polymers **(Class 3)** PMNs. For instance, the volubility of the chemical in water was more frequently reported for Classes 1 and 2 PMNs, probably because many polymers are water-insoluble. Although that could have been reported, it might have been left out of the submission as superfluous.

Class 2 submissions describe complex combinations of chemicals, and they less frequently report structures and formulae (see table 4) than do Class 1 submissions. However, PMNs for both Classes 1 and 2 report physical-chemical data with about the same frequencies. Therefore, despite the less frequent reporting of structure and formula for

Table 9.–Physical-Chemical Information on PMNs Describing Class 1, Class 2, and Class 3 Chemicals

	Class 1		Class 2		Class 3		Class 1 and Class 2	
	Number	Percent	Number	Percent	Number	Percent	Number	Percent
PMNs	293	100	73	100	374	100	366	100
Infrared spectra	32	11	12	16	42	11	44	12
Purity	233	80	59	81	253	67	292	80
Analytical methods	148	50	33	45	234	62	181	49
Melting point	110	36	17	23	52	14	127	35
Boiling point	69	24	31	42	119	32	100	27
Density	43	15	14	19	82	22	57	16
Vapor pressure	61	21	22	30	97	26	63	23
Volubility (water)	147	50	39	53	122	33	166	51
Partition coefficient	17	6	3	4	7	2	20	5
Transportation	155	53	45	62	283	75	200	55
Emergency information	87	30	29	40	140	37	116	32

SOURCE: Office of Technology Assessment.

Class 2 and 3 chemicals, EPA receives physical-chemical data useful for its analysis about equally for all classes of chemicals.

Transportation information was more frequently reported for polymers. The more frequent transportation information is consistent with the idea that polymers are end products of chemical production lines and moved to another manufacturing site to be incorporated into a final product. In contrast, Class 1 and 2 substances might more frequently be intermediates in production and not transported from the site of their manufacture.

The data in table 9 suggest that manufacturers develop and submit essentially the same amount of physical-chemical information about polymers and nonpolymers. At least some of the exceptions to this generalization are easily explainable given differences between the two kinds of chemicals.

SUMMARY OF FINDINGS ABOUT SUBMISSION OF PHYSICAL- CHEMICAL DATA

PMNs were inspected for the presence or absence of information about nine items concerning physical-chemical properties and whether or not emergency information and information about how the chemical was to be transported was submitted. Those items are listed and briefly described in table **6.**

None of the inspected PMNs reported all 11 items (table 7). Unlike the finding that TSCA-required information was reported equally frequently on manufactured and nonmanufactured PMNs, physical-chemical data were more frequent on manufactured PMNs.

A method was devised to investigate the possibility that manufacture of chemicals for which PMNs were prepared later in the development cycle contained more data. The idea was that a chemical that entered production very soon after submission of the PMN was further along in its development than a chemical that entered production after a longer delay. However, no consistent patterns were seen between frequencies of submission of physical-chemical data and the time between PMN submission and commencement of manufacture (table 8).

No other explanation for the dichotomy in reporting physical-chemical data on manufactured and nonmanufactured PMNs was investigated. However, there is at least one other possible explanation for the observation. Some EPA employees emphasized that the Agency does not require that the manufacturers notify the Agency of commencement of production of the chemical. Others were confident that those notices were nearly always submitted, and industry reviewers of the first draft of this report said that they understood submission of the commencement of manufacture notice was mandatory. Nevertheless, it is possible that some percentage of those PMNs listed as not manufactured do, in fact, describe chemicals that are now being produced. If that is true, the lower frequency of reporting physical-chemical data would parallel a lower frequency of notifying EPA of commencement of manufacture. This possibility was not examined, although calling submitters of nonmanufactured PMNs would be a way of exploring the possibility.