

Table 1. Effect of substituents in benzene ring

Substituent	Charge* withdrawal (+) from ring	Charge* on atom next to ring	δC^*	δH^*	Conju- gation with ring	Orien- tation effect
O ⁻	-0.627	-0.373	-0.084	-0.025	None	o,p
Si(CH ₃) ₃	-0.241	0.289	-0.049	0.011	None	o,p(weak)
C(CH ₃) ₃	-0.085	-0.035	-0.035	0.025	None	o,p
CH ₃	-0.052	-0.032	-0.032	0.028	None	o,p
H	-0.030	0.030	-0.030	0.030	None	
C ₆ H ₅	0	-0.027	-0.027	0.033	Possible	o,p
NH ₂	0.092	-0.176	-0.019	0.042	None	o,p
CH ₂ Cl	0.171	-0.012	-0.012	0.049	None	o,p
OCH ₃	0.174	-0.309	-0.012	0.049	None	o,p
CN	0.180	-0.011	-0.011	0.050	Possible	m
COCH ₃	0.181	-0.011	-0.011	0.050	Possible	m
OH	0.247	-0.303	-0.005	0.056	None	o,p
Cl	0.251	-0.251	-0.005	0.056	None	o,p
CHO	0.252	-0.005	-0.005	0.056	Possible	m
CHCl ₂	0.400	0.008	0.008	0.070	None	o,p
N(CH ₃) ₃ ⁺	0.446	-0.148	0.012	0.074	None	m
COOH	0.480	0.015	0.015	0.077	Possible	m
CCl ₃	0.634	0.029	0.029	0.091	None	m
NO ₂	0.671	-0.129	0.033	0.095	Possible	m
SO ₃ H	0.736	-0.039	0.038	0.101	Possible	m
NH ₃ ⁺	0.805	-0.120	0.043	0.105	None	m
CF ₃	0.975	0.060	0.060	0.123	None	m

* All charge values were calculated by the methods described in references 1 and 2.

the ring, as well as the partial charges on carbon and hydrogen atoms, is given. Also indicated are the possibility of substituent conjugation with the ring and the usual orientation effect. It is extremely important in studying the charge data to keep in mind that they represent solely the partial charges that would be expected from bond polarities resulting from initial electronegativity differences. The mobility of certain electrons in these multiple-bonded systems also has an important influence on the over-all charge distribution in the molecule, but the quantitative effect of this influence cannot easily be reckoned.

If the general reactivity of a benzene ring may be taken as a reflection of the availability of pi electrons, the data of Table 1 are of especial interest. Electron availability will be determined chiefly by two factors: the charge on the carbon atom, and the capacity of the rest of the molecule to supply electrons without the result of excessive positive charge on any one atom. The first factor is evaluated in Table 1; the lower the positive charge or the higher the negative charge on carbon, the greater the electron availability. The second factor depends essentially on the number and kinds of atoms of the substituent group: if the electron release to the ring is equal for two different substituents, the substituent that is the better electron reservoir will contribute more to the availability of pi electrons.

The problem of orientation effects of substituents on the benzene ring seems

too complex to be susceptible to complete solution by any one simple rule or formula. In part, the complexity may arise from differences in polarizing effects exerted by attacking molecules. These differences require a different interpretation of each substitution. The following observations from Table 1 are of interest, however. Groups that are predominantly meta directors are generally either highly electronegative groups with strong electron-withdrawing power and with a positively charged atom attached directly to ring carbon, or groups of lesser withdrawing power that have a multiple bond capable of conjugation with the ring. Groups that are predominantly ortho, para directors are usually either electron-releasing groups, or electron-withdrawing groups in which the atom attached directly to ring carbon has an appreciable negative charge. The latter type may be regarded as an example of the electrostatic influence on pi electrons that is exerted by high charge on the substituent atom directly attached to ring carbon (4). This charge, if it is negative, may tend to compensate for the electron withdrawal by the group by repulsion of the pi electrons. Similarly, the weakness of the ortho, para directing powers of the (CH₃)₃Si-group (5), despite the group's strong electron-releasing action, may be associated with the electrostatic attraction of the positively charged silicon for the pi electrons.

R. T. SANDERSON

Department of Chemistry,
State University of Iowa, Iowa City

References and Notes

1. R. T. Sanderson, *J. Chem. Educ.* 31, 2, 238 (1954); 32, 140 (1955).
2. —, *Science* 121, 207 (1955).
3. See, for example, L. B. Ferguson, *Electronic Structures of Organic Molecules* (Prentice-Hall, New York, 1952); A. E. Remick, *Electronic Interpretations of Organic Chemistry* (Wiley, New York, ed. 2, 1949); and similar works.
4. A similar effect, in the addition to olefinic double bonds, has been noted elsewhere: R. T. Sanderson, *Science* 122, 244 (1955).
5. J. L. Speier, *J. Am. Chem. Soc.* 75, 2930 (1953).

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Polygonization of a Plastically Bent Sapphire Crystal

If one thinks of edge-type dislocations as arising formally from the insertion of an extra partial plane of atoms, then a plastically bent crystal must have more of these wedges going in from the convex surface than from the concave one (1). From the extensive work on polygonization of plastically bent metal crystals it has been shown that thermal activation can induce these excess dislocations of like sign to segregate and form plane walls perpendicular to the slip planes (2). In fact, these walls are simply small-angle grain boundaries, which then separate blocks or polygons of unbent structure. Each recovered block thus differs slightly in orientation from its neighbors.

In recent years it has been demonstrated that many ionic crystals that are hard and brittle at room temperature can be deformed plastically at elevated temperatures (3). Of particular interest, from the point of polygonization, is the case of plane bending of crystals that deform on only one slip system. Figure 1 illustrates the geometry of a bent sapphire (Al₂O₃) (4). It shows in particular that the slip planes curve into in-

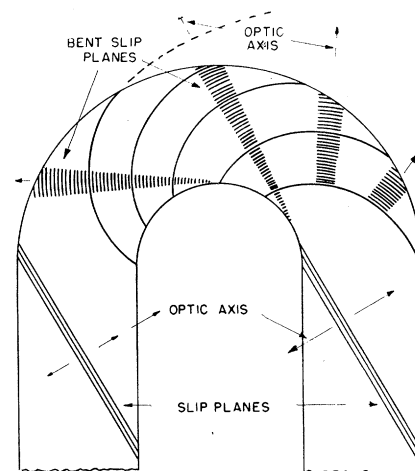


Fig. 1 Plane bending by slip on a single set of planes. The bent slip planes have the shape of an involute of a cylinder. Normals to the curved planes define the positions of the optic axis.

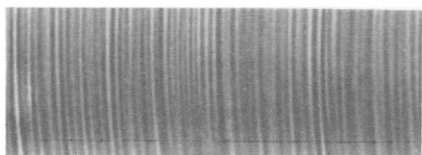


Fig. 2. Slip lines on the convex surface of a plane bent sapphire crystal. ($\times 125$)

volutes, yet the normals to these planes are preserved as straight lines. Accordingly, if polygonization can be induced in such a sample, then the positions of the dislocation walls should be defined by planes normal to the plane of the figure and parallel to the optic axis.

It is pertinent to realize a significant difference between the structures of an edge-type dislocation in a simple metal such as zinc and a structurally similar crystal such as sapphire. In the former, a single extra partial plane is required as an insert, whereas for the latter a double one is needed. Thus, for sapphire, it will be composed of contiguous planes of oxygen ions and aluminum ions, respectively. Since polygonization requires both glide and climb of dislocations, it is therefore implicit that the process necessitates self-diffusion of both types of ions.

In order to evaluate these various simple concepts, the following experiment was performed. A long, single crystal rod of Linde synthetic sapphire was plane bent in an oxygen-gas flame at a temperature of the order of 1800°C . Microscopic examination of the deformed sample showed well-developed slip lines (Fig. 2) when viewed normal to the axis of bending but none could be detected when viewed parallel to the axis, in accordance with the requirements for plane bending. Significantly, no evidence was obtained for polygonization at this stage.

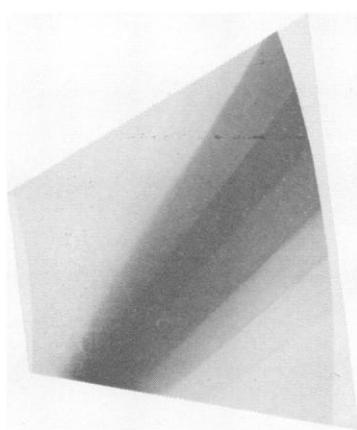


Fig. 3. Portion of a plane bent and polygonized sapphire crystal, viewed parallel to the axis of bending. For photographing, the sample was immersed in ethylene iodide and illuminated by transmitted polarized light. ($\times 18$)

The sample was then annealed in the flame for 10 minutes at a temperature of the order of 2000°C . After this treatment, striking evidence for the expected polygonization was obtained, as is shown in Fig. 3.

With this discovery of polygonization in plane bent sapphire, it was clear that polygonization of a plane bent crystal of zinc should produce an identical macrostructure. This prediction has been fully verified by my colleague, J. J. Gilman (5).

M. L. KRONBERG

Research Laboratory, General Electric Company, Schenectady, New York

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4. C. D. West, *ONR Tech. Rept. No. N7ONR-39102* (1952); J. F. Nye, *Acta Metals* 1, 153 (1953).
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On Responsibility of Scientists

In his informative article, "The work of many people" [*Science* 121, 267 (1955)], Edward Teller discusses the role of scientists in the development of the atom and hydrogen bombs. I feel that, in view of the fundamental assistance that the scientist might give in helping to understand and ameliorate the present world tension, I should present to the readers of *Science* a humanistic point of view, which I am sharing with others and which is at least complementary to the one set forth by Teller.

I fully realize that the purpose of Teller's article was not the discussion of the wider cultural background against which the development of the atom bomb must be seen. Yet in the last two paragraphs the awful gravity of the human situation springs into focus. Teller states: "... I also believe that we would be unfaithful to the tradition of Western civilization if we were to shy away from exploring the limits of human achievement. It is our specific duty as scientists to explore and to explain. Beyond that our responsibilities cannot be any greater than those of any other citizen of our democratic society. ... To be in possession of this instrument [thermonuclear weapon] is an even greater challenge to the free community in which we live. I am confident that, whatever the scientists are able to discover or invent, the people will be good enough ... to control it for the ultimate benefit of everyone."

Teller's faith in the organizing ability

of the human community is a healthy sign, but we must also admit that there are many who have long observed the dangerous course that Western civilization has been taking, and they are alarmed that atom and hydrogen bombs have, at this point, become, so to speak, the symbol of man's ability or inability to practice ordinary human virtues on a world-wide scale. The mere creation of fear and of weapons has in the past never produced a turn of heart among potential trouble makers. The delicate equilibrium of international and interhuman relationships is now taxed to the utmost by conflicting ideologies and self-propelling material interests. So, many of us would rather not wait until the control of those disorganizing forces becomes even more urgent as a result of more dreadful external catastrophes. One of the chief dangers is that we continue to apply too simple and too static a formula to the present situation. We scientists are readily tempted to succumb to this tendency, since, in the traditional thinking of science, the idea of automatic scientific and social progress has been prominent. I believe that our hope lies in an ever-growing understanding of the psychological and historical factors that control man's destiny and that everyone should try to acquire and help to disseminate such understanding. Let me be more specific.

The majority of scientists, in speaking of the principles of their profession, readily identify themselves with an ideal that has its main origin in the 17th-century individualistic and cultural renaissance. But history shows that the purity of an original ideal, whether religious or scientific, whether envisioned by an inspired individual or a small brotherhood, changes when it is forced to operate within the more material medium of human society. Science has been no exception to this process, which was pointed out especially by Lewis Mumford and Arnold Toynbee. "Why is this secular cult of science," wrote Toynbee (*New York Times Magazine*, 26 Dec. 1954), "not enough? Because science operates in a medium from which it can never detach itself. Our Western science is the child of moral virtues; and it must now become the father of further moral virtues if its extraordinary material triumphs in our times are not to bring human history to an abrupt, unpleasant and discreditable end. ... The virtues of prudence, self-control, tolerance, wisdom, and—far above all these—love have become necessities of life in the literal sense."

There are, I am confident, many among us who share this growing general awareness that such laws of human behavior are now more important than material interests, theories of supply and demand, systems of attack and counterat-