

# A NEW POLARITY SCALE FOR GC PHASES

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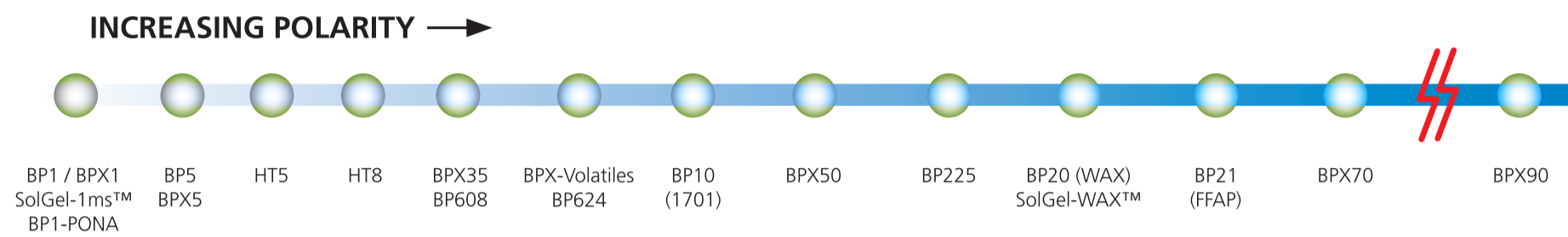


Figure 1: The linear or two dimensional polarity scale does not recognize differences in polar phase chemistries or the relationship between polar and non-polar.

## Introduction

Traditionally, the polarity of GC phases has been represented on a qualitative polarity scale in one dimension (Figure 1). While different presentations have been adopted by various manufacturers, the information content has remained essentially the same in each case.

We present here a three-dimensional GC polarity scale (Figure 2) that considers the selectivity of the GC phase towards any analyte as being dependent on at least three types of interactions: van der Waals forces, hydrogen bonding (or proton donor and acceptor type bonding) and bonding between  $\pi$ - and n-type orbitals. Because the scale is in three dimensional space, it can easily show that a phase may exhibit elements of all bonding types or a dominance of one.

Importantly, it also illustrates what the phase is not. The one dimensional polarity scale does not show different types of interactions and also does not show that if one bonding type becomes dominant then such dominance must logically be at the expense of at least one of the other bonding types. This information is readily conveyed in a three dimensional format.

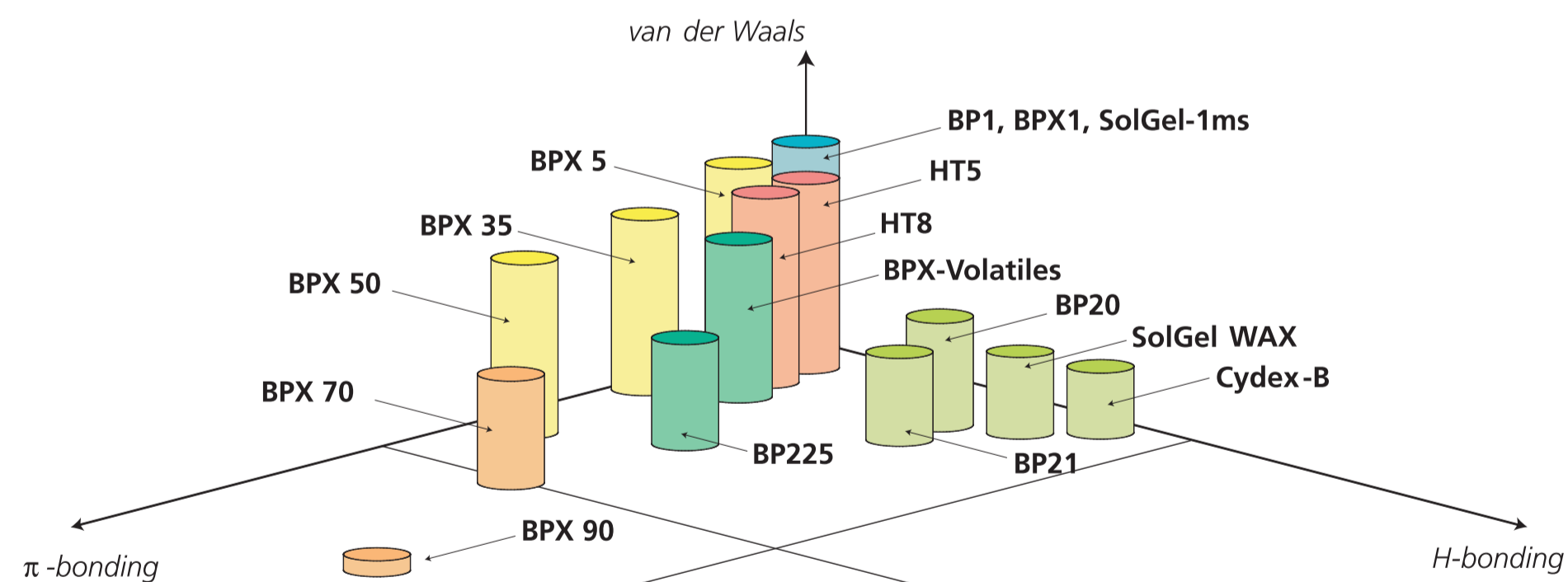


Figure 2: A three-dimensional GC polarity scale.

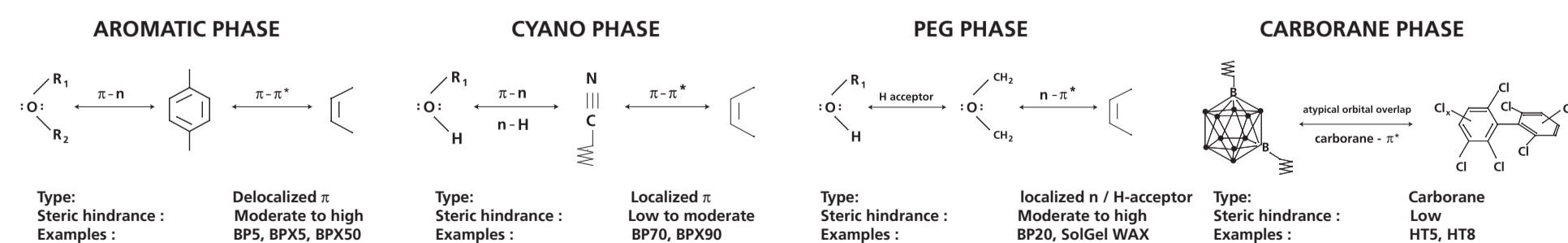


Figure 3: Illustration of the major liquid phase - analyte interactions that operate for polar phases.

## Discussion

A polarity scale for GC-phases is primarily required to show the properties of a GC liquid phase relative to a dimethylpolysiloxane (BP1) phase. Aromatic polarity of a phase may come from aromatic groups that are either embedded in the polysiloxane (polysilylene type e.g. BPX5), from pendant aromatic groups (e.g. BP5) or a combination of both (e.g. BPX50). Such polarity is the result of delocalized  $\pi$ -bonds that may act as  $\pi$ -donors or  $\pi$  and n- receivers. Because the groups are close to the polymer surface, steric hindrance can affect their polarity for some analytes (Figure 3). While polar, the phases are also hydrocarbon based and so retain a relatively high non-polar capacity.

Cyanopropyl and biscyanopropyl polysiloxane phases are isolated  $\pi$ -donors and, because of the free rotational mobility of the functional groups, show little steric hindrance (Figure 3). The acetonitrile like characteristics of the cyano groups mean that the non-polar capacity of these phases are inversely related to the cyano content.

Polyethylene glycol (PEG) or WAX phases are n-donors and hydrogen acceptors (Figure 3). They therefore show high selectivity towards hydrogen bonding analytes that is not typically found for  $\pi$ -donor phases. The n-donor characteristic allows the phases to interact with  $\pi^*$ -orbitals in unsaturated analytes and this interaction is likely to have different selectivity to the  $\pi$ -  $\pi^*$  interaction of aromatic and cyano phases. Because the n-donor atom is embedded, the PEG phases show high steric hindrance and a preference for terminal H-bonding moieties.

Meta-carborane type phases are generally grouped with aromatic phases for convenience. The carborane ring system is unique and is sometimes described as having delocalized  $\sigma$ -bonding. The meta-carborane sits out of the polysiloxane chain and so, while it is imbedded, shows very low steric hindrance (and consequently very high selectivity) towards planar aromatics (Figure 3).

The polarity of all these phase types can be represented in a three dimensional format in such a way that the contribution of each bonding mechanism can be both visualized and rationalized relative to the non-polar (primarily the van der Waals effect) characteristics of the phase. Representing phase chemistries in different colors adds a further dimension to the 3D-polarity scale that assists in phase selection and prediction of analyte solubilities and steric hindrance.

## Conclusion

The 3-D polarity scale for GC phases shows the dominant functionality of a phase and therefore allows simple matching of the analyte and GC-phase chemistry for maximum selectivity.

Because the scale recognizes classically polar phases according to their n- or  $\pi$ -type characteristics, both favorable and unfavorable interactions may be predicted for unsaturated and heteroatomic analytes during interaction with the phase.

Because the scale also shows non-polar properties, the characteristics of a very polar phase may be distinguished from moderately polar and polar phases with the same underlying polar chemistry.

The polarity scale shows that for a polar phase that has a dominant retention mechanism there is also an insignificant non-polar retention.

The 3-D polarity scale better predicts solubility related phenomena (fourth dimensional data) and can also assist in deducing steric factors between phase and analyte (the fifth dimensional variable).