**Enantioseparation and identification for the rationalization of the environmental impact of four polychlorinated biphenyls**

Fangjie Guo,[a] Qiaozhi Tang,[a] Jingqian Xie,[a] Lu Zhao,[a] Kai Liu,[b] and Weiping Liu\*[a]

**Supporting Information**

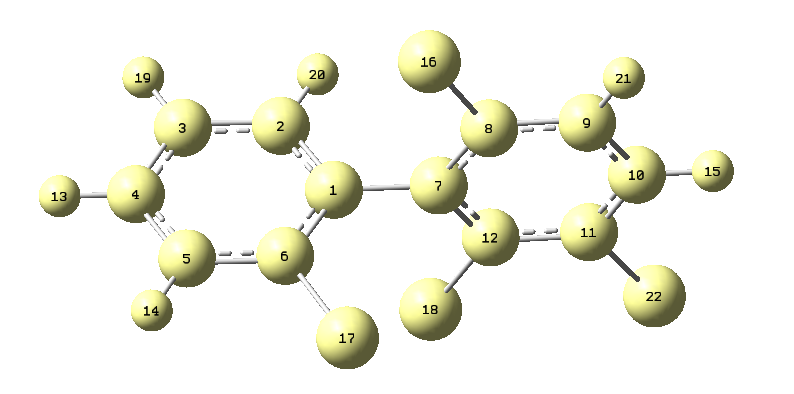


Figure S1. The atom serial number in Gaussian view of PCB45 (*S*).

Table S1. Effects of column temperature on the retention and separation factor of four PCBs on OD-H and OJ-H.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Factor | 10 °C | 15 °C | 20 °C | 25 °C | 30 °C |
| OJ-45 | *t*0 | 6.527 | 6.163 | 6.437 | 6.397 | 6.330 |
| *t*1 | 12.587 | 11.460 | 11.580 | 11.271 | 11.030 |
| *t*2 | 15.060 | 13.403 | 13.377 | 12.916 | 12.527 |
| *k*1 | 0.928 | 0.859 | 0.799 | 0.762 | 0.742 |
| *k*2 | 1.307 | 1.175 | 1.078 | 1.019 | 0.979 |
| *a* | 1.408 | 1.367 | 1.349 | 1.338 | 1.319 |
| OD-95 | *t*0 | 6.270 | 6.250 | 6.210 | 6.193 | 6.170 |
| *t*1 | 15.903 | 15.597 | 14.480 | 14.363 | 13.917 |
| *t*2 | 17.827 | 17.497 | 15.933 | 15.973 | 15.427 |
| *k*1 | 1.536 | 1.496 | 1.332 | 1.319 | 1.256 |
| *k*2 | 1.843 | 1.800 | 1.566 | 1.579 | 1.500 |
| *a* | 1.200 | 1.203 | 1.176 | 1.197 | 1.195 |
| OD-136 | *t*0 | 6.277 | 6.250 | 6.220 | 6.200 | 6.170 |
| *t*1 | 18.380 | 17.620 | 16.563 | 16.130 | 15.510 |
| *t*2 | 22.377 | 21.167 | 19.470 | 19.010 | 18.147 |
| *k*1 | 1.928 | 1.819 | 1.663 | 1.602 | 1.514 |
| *k*2 | 2.565 | 2.387 | 2.130 | 2.066 | 1.941 |
| *a* | 1.330 | 1.312 | 1.281 | 1.290 | 1.282 |
| OD-149 | *t*0 | 6.278 | 6.250 | 6.223 | 6.197 | 6.170 |
| *t*1 | 13.563 | 13.143 | 12.650 | 14.010 | 11.943 |
| *t*2 | 15.757 | 15.197 | 14.397 | 15.643 | 13.520 |
| *k*1 | 1.160 | 1.103 | 1.033 | 1.261 | 0.936 |
| *k*2 | 1.510 | 1.432 | 1.314 | 1.524 | 1.191 |
| *a* | 1.301 | 1.298 | 1.272 | 1.209 | 1.273 |

Table S2. Van ’t Hoff equations and thermodynamic parameters of the four PCBs.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| PCB | ln*k* =-*ΔH°/RT*+*ΔS°/R* | *R*2 | Δ*H°*(KJ mol-1) | Δ*S*(J mol-1) | Results |
| 45P1 | ln*k* = 3.3869*/T* - 0.4004 | 0.973 | -0.407 | -0.048 | enthalpy-driven |
| 45P2 | ln*k* = 4.3143*/T* - 0.1498 | 0.980 | -0.519 | -0.018 | enthalpy-driven |
| 95P1 | ln*k* = 3.0437*/T* + 0.1481 | 0.871 | -0.366 | 0.018 | dual-driven |
| 95P2 | ln*k* = 3.159*/T* + 0.3188 | 0.845 | -0.380 | 0.038 | dual-driven |
| 136P1 | ln*k* = 3.5225*/T* + 0.3255 | 0.927 | -0.424 | 0.039 | dual-driven |
| 136P2 | ln*k* = 4.1005*/T* + 0.5536 | 0.939 | -0.493 | 0.067 | dual-driven |
| 149P1 | ln*k* = 1.5194*/T* + 0.0007 | 0.127 | -0.183 | 0.000 | none enthalpy/entropy-driven |
| 149P2 | ln*k* = 2.2318*/T* + 0.1986 | 0.327 | -0.268 | 0.024 | none enthalpy/entropy-driven |
| PCB | ln*α*=-ΔΔ*H*°/RT+ΔΔ*S*°/R | *R*2 | ΔΔ*H°*(KJ mol-1) | Δ*S°*(J mol-1) | Results |
| 45 | ln*k* = 0.9274*/T* + 0.2505 | 0.983 | -0.112 | 0.030 | - |
| 95 | ln*k* = 0.1152*/T* + 0.1707 | 0.115 | -0.014 | 0.021 | - |
| 136 | ln*k* = 0.578*/T* + 0.2281 | 0.884 | -0.070 | 0.027 | - |
| 149 | ln*k* = 0.7124*/T* + 0.1978 | 0.412 | -0.086 | 0.024 | - |