

Appendix 3

Ordering of octane isomers based on vertex degree weighted path indices $P_N(a, b, \dots)$

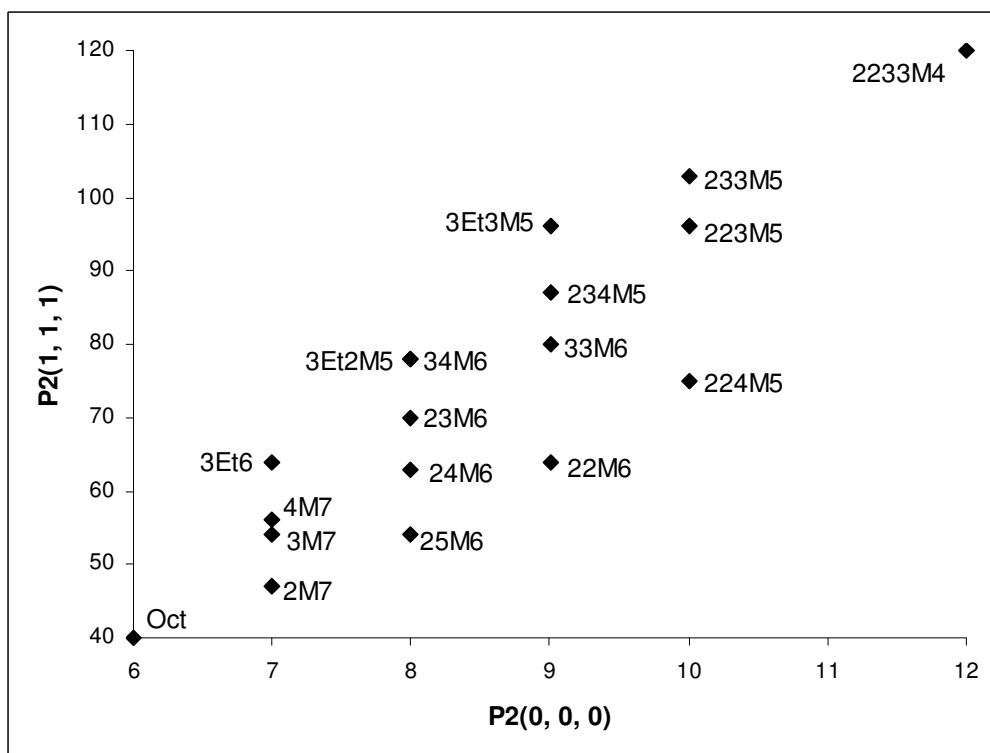


Figure A3a. Ordering of octane isomers based on vertex degree weighted path indices $P_2(0, 0, 0)$ and $P_2(1, 1, 1)$.

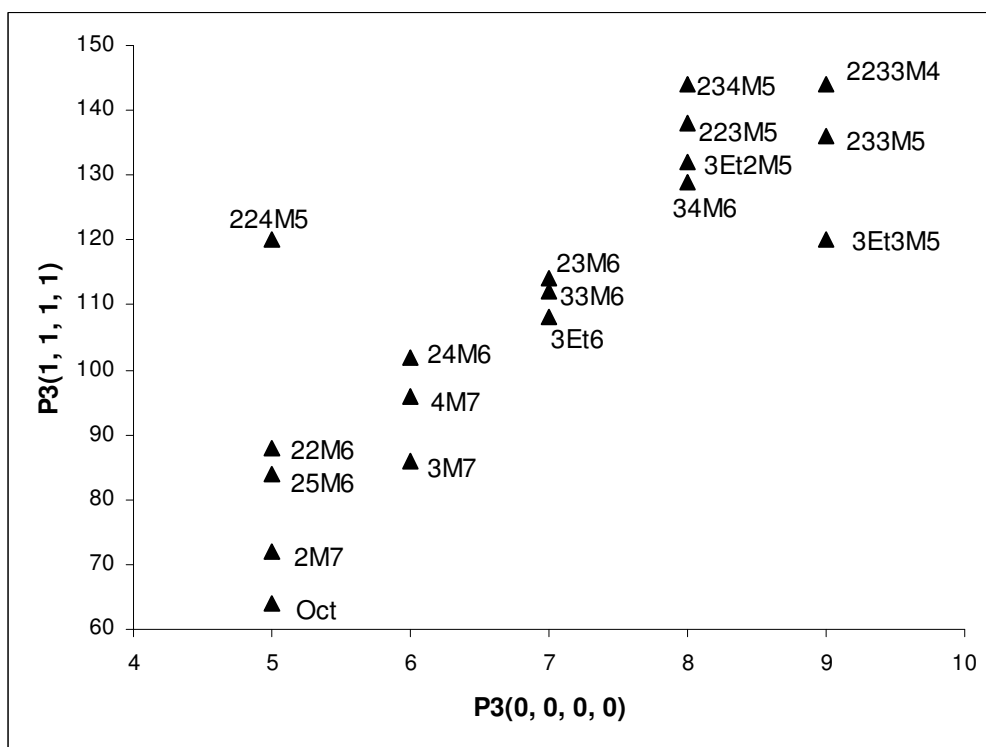


Figure A3b. Ordering of octane isomers based on vertex degree weighted path indices $P_3(0, 0, 0, 0)$ and $P_3(1, 1, 1, 1)$.

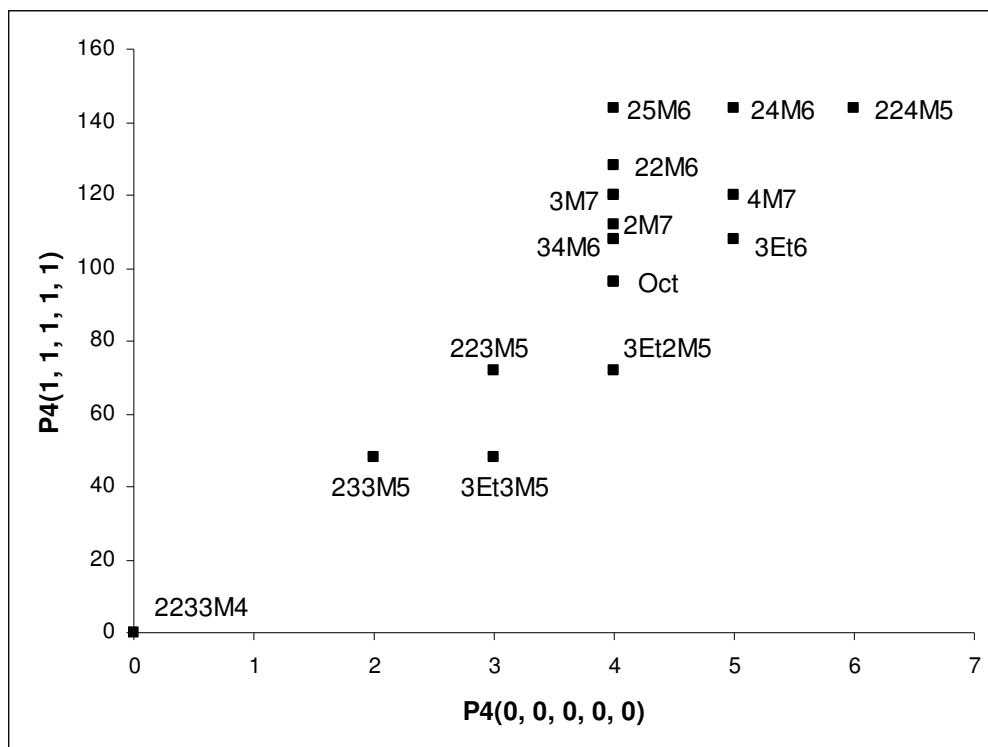


Figure A3c. Ordering of octane isomers based on vertex degree weighted path indices $P_4(0, 0, 0, 0, 0)$ and $P_4(1, 1, 1, 1, 1)$.

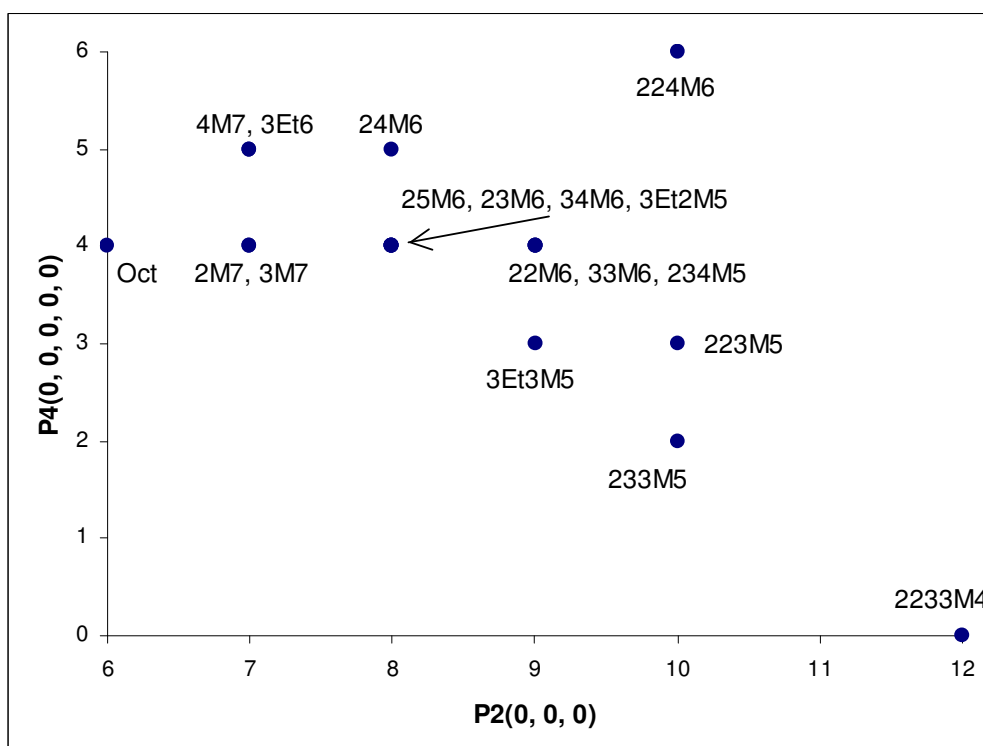


Figure A3d. Ordering of octane isomers based on vertex degree weighted path indices $P_2(0, 0, 0)$ and $P_4(0, 0, 0, 0, 0)$.

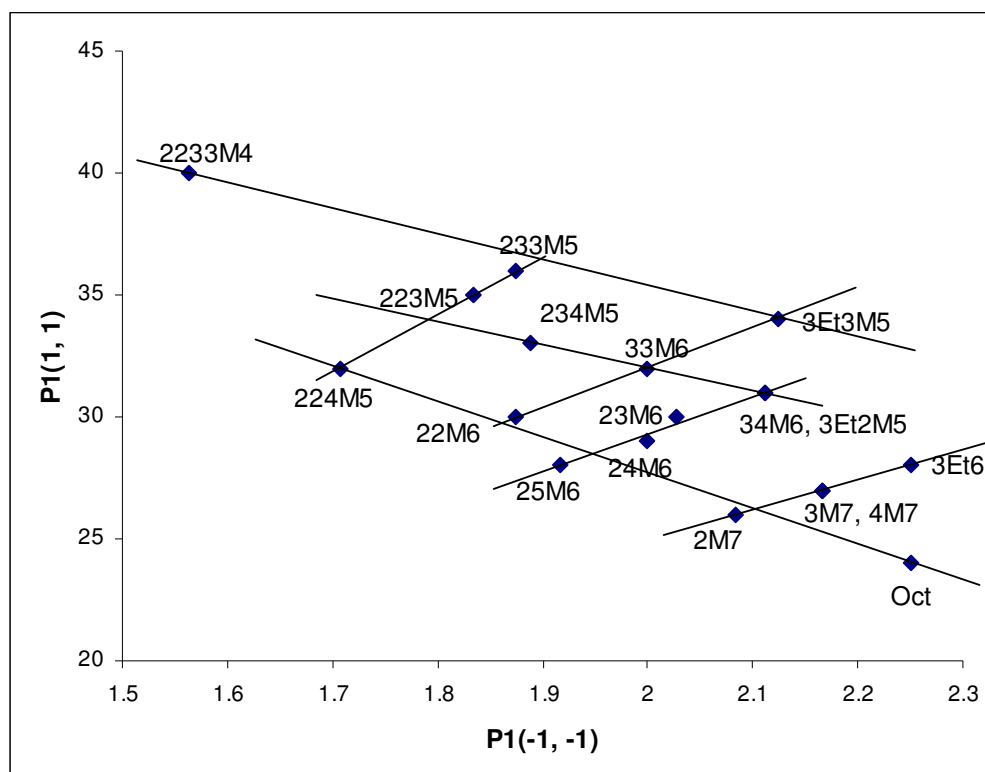


Figure A3e. Ordering of octane isomers based on vertex degree weighted path indices $P_1(-1, -1)$ and $P_1(1, 1)$.

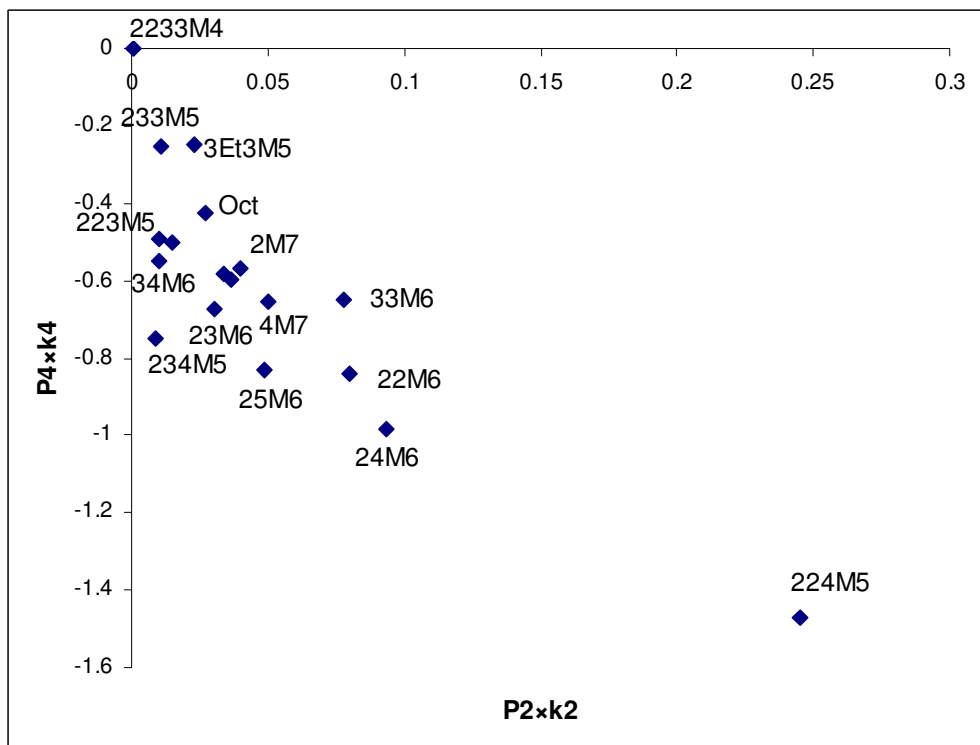


Figure A3f. Ordering of octane isomers based on vertex degree weighted path indices $P_2(3.5, -6.1, 3.0)$ and $P_4(0.65, 1.06, 0.063, 0.97, -0.154)$, which contribute together 54.9% of information about Tc of octanes.

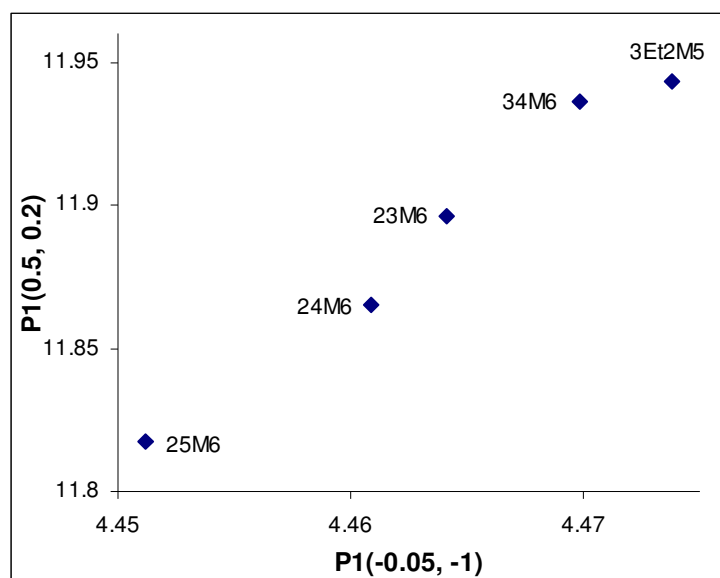
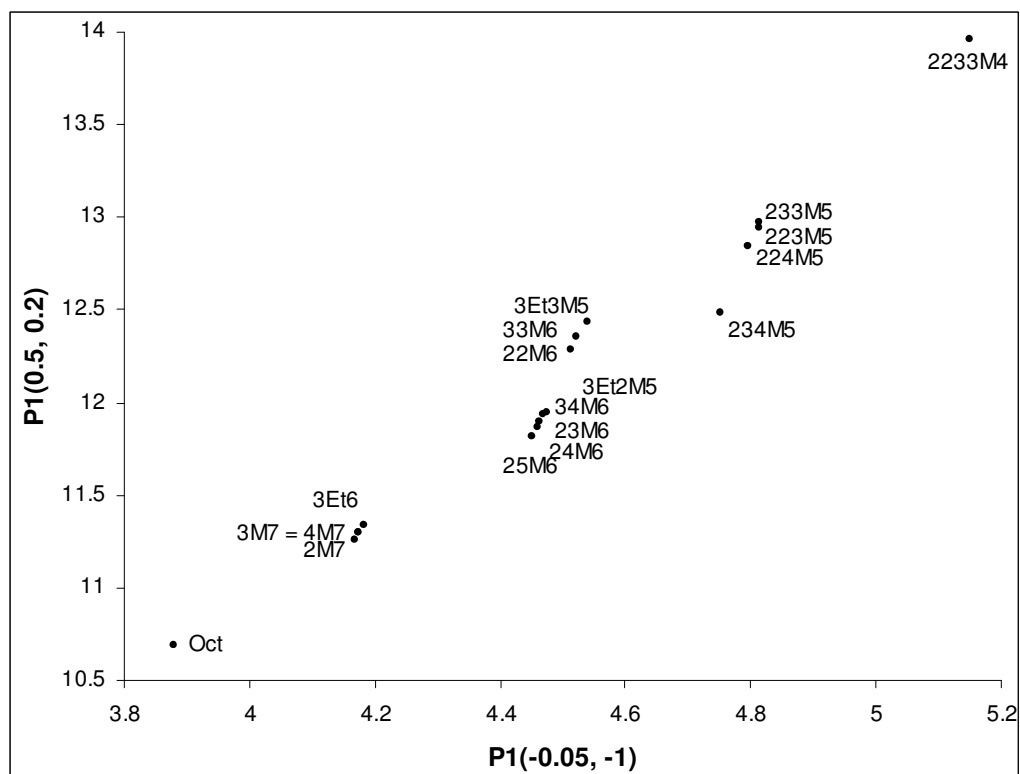


Figure A3g. Ordering of octane isomers based on vertex degree weighted path index $P_1(-0.05, -1)$ and $P_1(0.5, 0.2)$, presenting the "regular" sequence of octane isomers based on this index.