cross\_1 cross.angle\_1 para\_1 para.angle\_1

basic 1657.145 88.87598 1680.272 0.8135640

m\_Br 1641.563 86.52798 1669.350 5.3064891

m\_Cl 1647.623 87.99223 1672.190 0.5571530

m\_F 1667.799 89.43099 1687.475 1.2303741

m\_I 1635.908 86.10668 1665.188 5.0361022

m\_nitro 1652.893 89.52036 1670.161 15.3229206

o\_Br 1640.950 86.10140 1667.603 4.2814122

o\_Cl 1644.388 83.39964 1669.814 8.4329035

o\_F 1661.212 82.36304 1690.324 7.0039394

o\_I 1636.017 86.95176 1662.298 4.5800455

o\_nitro 1648.916 77.71427 1697.301 6.5969508

p\_amine 1650.795 85.49212 1695.094 1.7959744

p\_azide 1646.569 81.15264 1686.111 9.0181962

p\_boc 1655.074 88.66046 1690.612 0.1978967

p\_Br 1643.592 85.79180 1667.277 4.0653936

p\_Cl 1644.973 87.69119 1673.792 1.7897188

p\_F 1668.675 88.39884 1686.741 1.2790767

p\_I 1637.713 84.99666 1663.926 4.0806195

p\_Me 1647.258 88.63994 1691.186 0.4467172

p\_nitro 1651.780 88.73170 1675.980 0.2146471 - Switch

p\_OEt 1650.561 78.02302 1691.921 10.5863019 - Switch

p\_OH 1664.378 77.38406 1692.697 12.1684053 - Switch

p\_OMe 1651.727 79.27003 1692.978 10.2378371 - Switch

p\_Ph 1657.143 89.28811 1687.744 1.3011375 – Wrong ring

p\_tfm 1656.701 87.30995 1693.811 3.0571887 - Switch

penta\_F 1705.867 84.38950 1721.704 4.2085974 - Switch

Bend Vibration –CH2 example: threshold 1300 :

problematic 3 existing vibrations mixed : basic 1460-bending 3084-twist 3133-rocking

0 1 2 3 4 5 Frequency Cross\_mag

7 -0.13 0.70 -0.03 -0.04 0.10 -0.66 1460.0055 0.466972

18 0.03 -0.05 -0.53 -0.20 0.79 0.20 3084.1379 0.420979

21 -0.04 0.06 0.84 -0.13 0.50 0.11 3135.4327 0.426651

Strech –

Finds C=O at 1800, needs to adjust threshold from 3000 default for C-H

Finds C-H at 3080~ even when lowering threshold