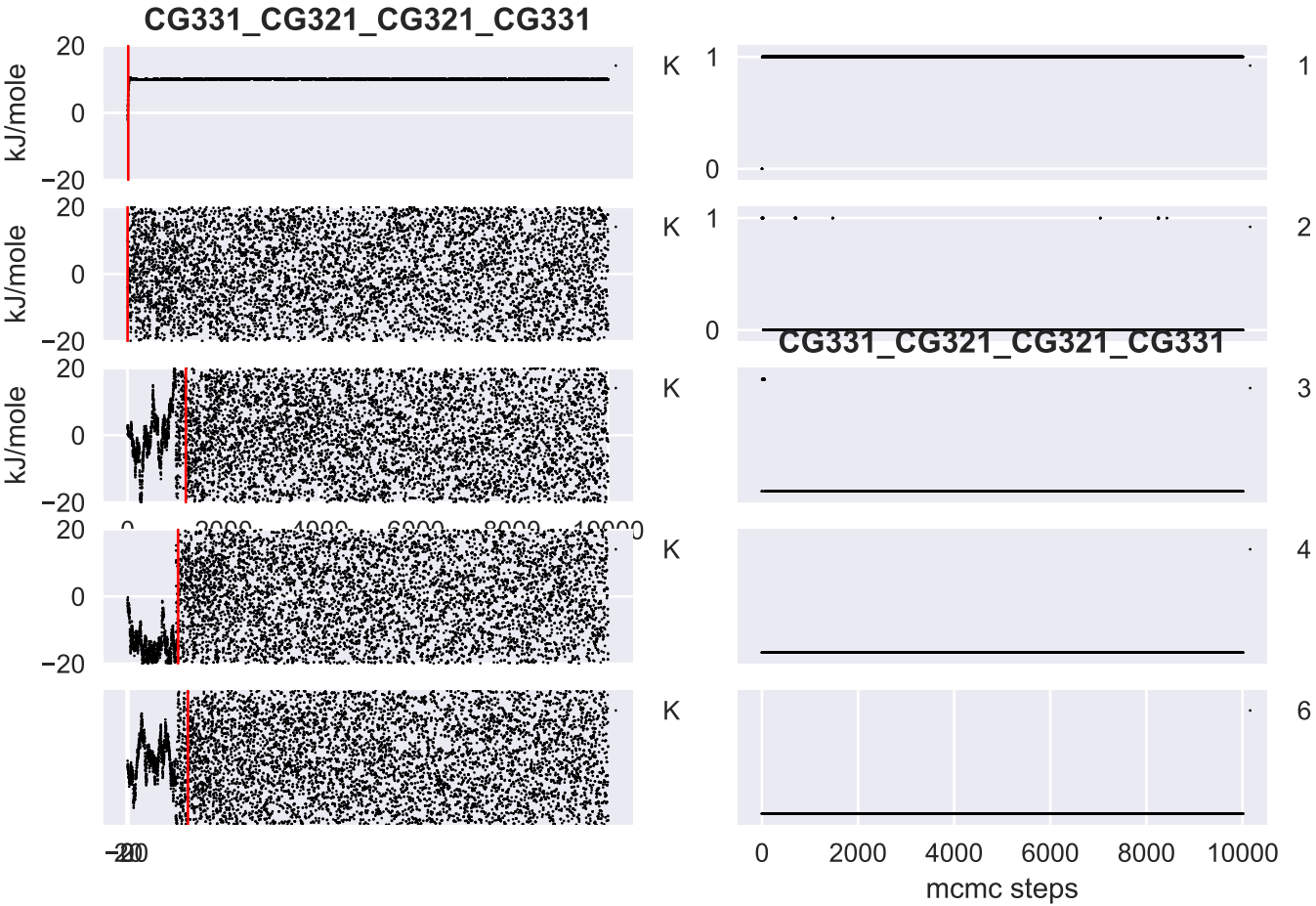
CG331_CG321_CG321_CG331
kJ/mole
20
0
−20
K
1
0
1
2
3
4
6
CG331_CG321_CG321_CG331
0
2000
4000
6000
8000
10000
mcmc steps