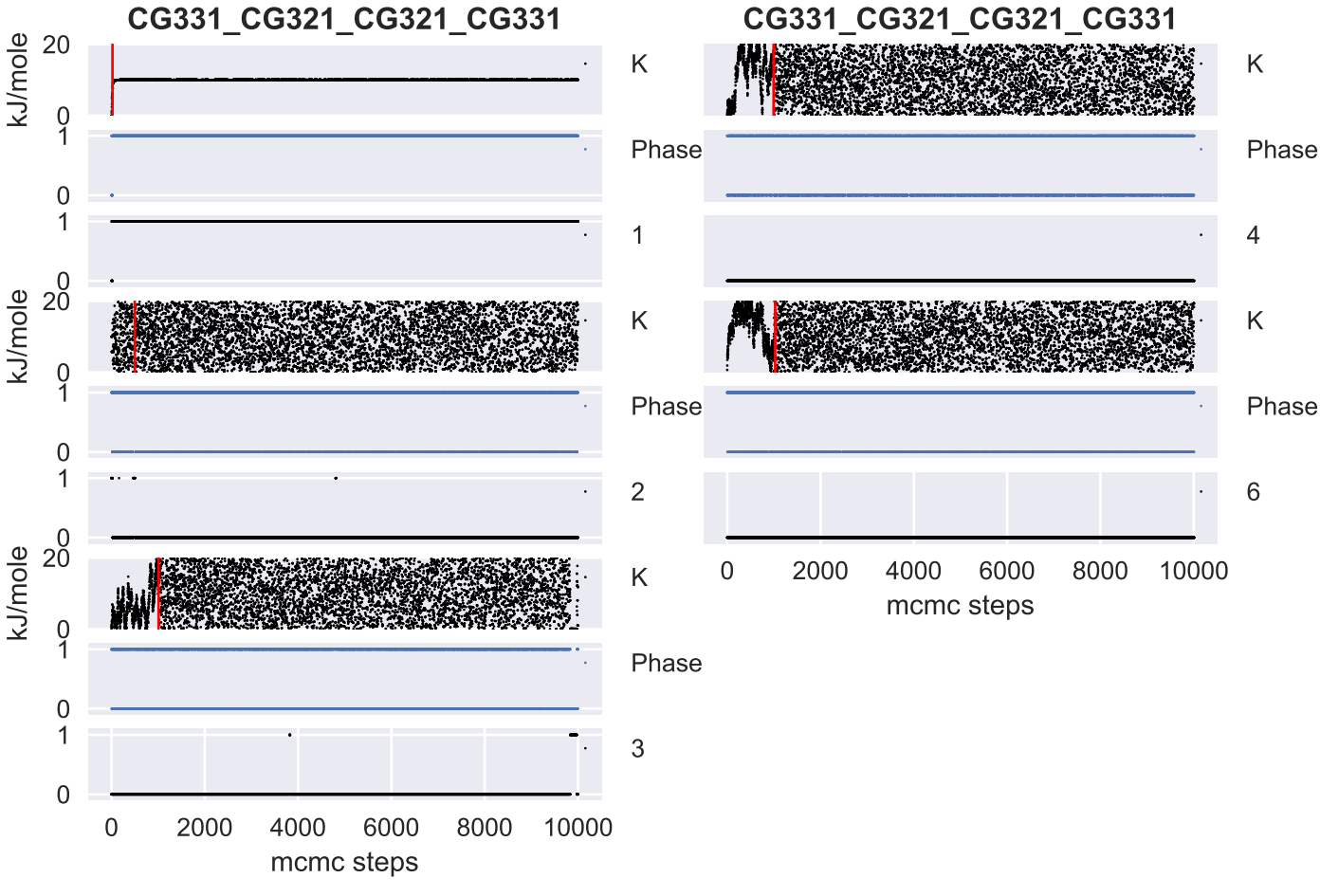
CG331_CG321_CG321_CG331
kJ/mole
20
0
1
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1
0
20
0
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1
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20
0
1
0
1
0
K
Phase
1
K
Phase
2
K
Phase
3
0
2000
4000
6000
8000
10000
mcmc steps
CG331_CG321_CG321_CG331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