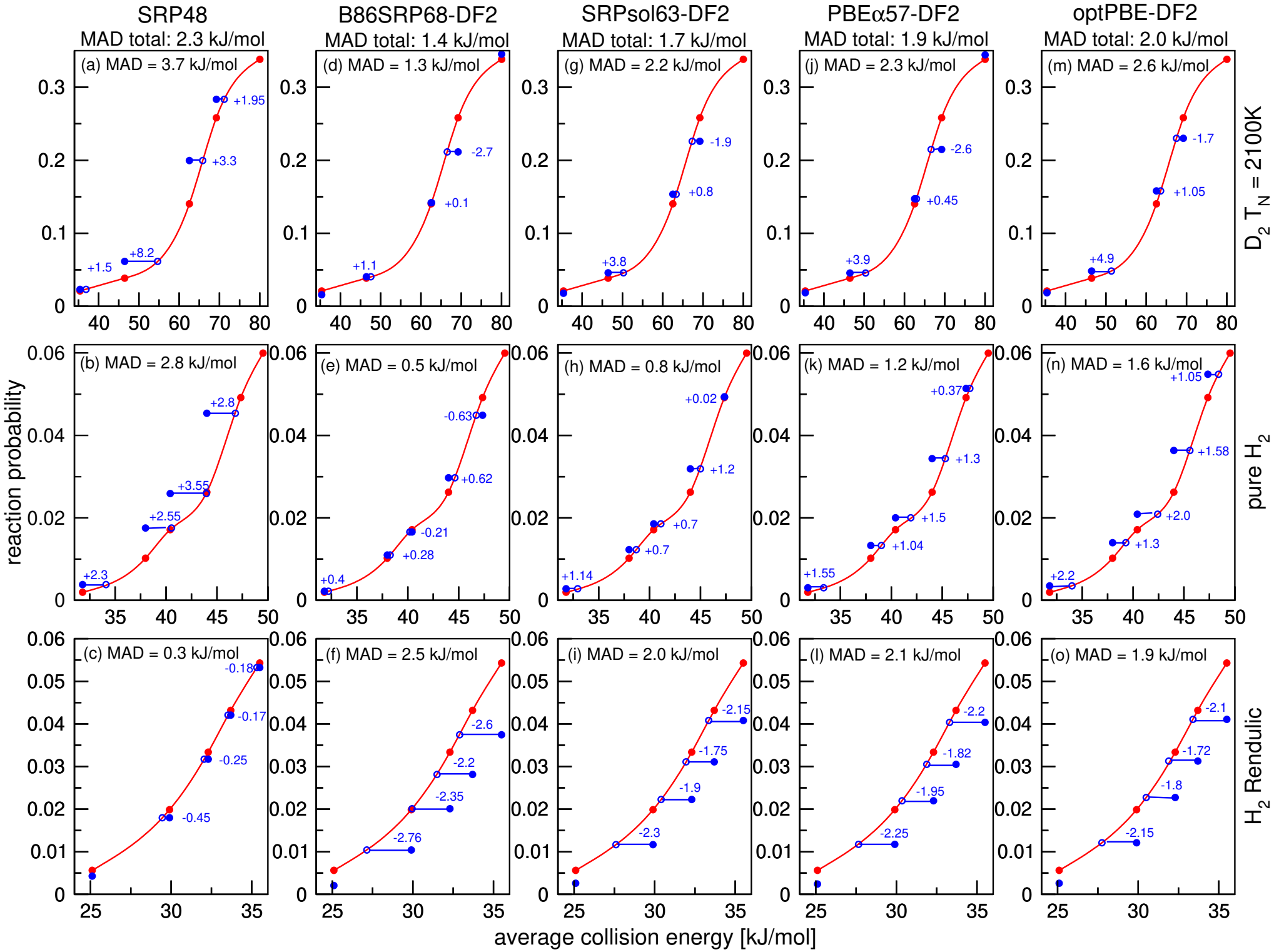
SRP48
MAD total: 2.3 kJ/mol
B86SRP68-DF2
MAD total: 1.4 kJ/mol
SRPsol63-DF2
MAD total: 1.7 kJ/mol
PBEα57-DF2
MAD total: 1.9 kJ/mol
optPBE-DF2
MAD total: 2.0 kJ/mol
(a) MAD = 3.7 kJ/mol
(b) MAD = 2.8 kJ/mol
(c) MAD = 0.3 kJ/mol
(d) MAD = 1.3 kJ/mol
(e) MAD = 0.5 kJ/mol
(f) MAD = 2.5 kJ/mol
(g) MAD = 2.2 kJ/mol
(h) MAD = 0.8 kJ/mol
(i) MAD = 2.0 kJ/mol
(j) MAD = 2.3 kJ/mol
(k) MAD = 1.2 kJ/mol
(l) MAD = 2.1 kJ/mol
(m) MAD = 2.6 kJ/mol
(n) MAD = 1.6 kJ/mol
(o) MAD = 1.9 kJ/mol
reaction probability
average collision energy [kJ/mol]
D2 TN = 2100K
pure H2
H2 Rendulic