

This file contains the errata to "Generalized Transition State Theory," D. G. Truhlar, A. D. Isaacson, and B. C. Garrett, in *Theory of Chemical Reaction Dynamics*, edited by M. Baer (CRC Press, Boca Raton, FL, 1985), Vol. 4, pp. 65-137.

Errata for "Generalized Transition State Theory"

This section contains all known errata to the GTST book chapter (Ref. 5 in Sect. 21) by D. G. Truhlar, A. D. Isaacson, and B. C. Garrett.

1. p. 71, line 1: $V[x_{i\gamma}]$ should be $V([x_{i\gamma}])$.
2. p. 71, third line after eq. (6): "coordinate(s)" should be "coordinate (s)".
3. p. 77, Fig. caption line 3: "1 molecule and per centimeter, anharmonicity" should be "1 molecule per centimeter, and anharmonicity".
4. p. 78, second line after eq. (15): $\nabla V(R)_j'$ should be $\nabla V(R'_j)$.
5. p. 81, eq. (31): $x_{i'\gamma'}$ should be $x_{i'\beta'}$.
6. p. 82, eq. (35), line 1: $(m_A + m_B)^{-1}$ should be M^{-1} where M is the total mass.
7. same equation, line 2: insert " μ_j " in numerator.
8. p. 83, line 2: $Q^{\text{GT},0}(T,s)$ should be $Q^{\text{GT}}(T,s)$.
9. p. 83, line 8: $\Phi_V^{\text{R}}(T)$ should be $\Phi_C^{\text{R}}(T)$.
10. p. 83, second line from the bottom: Δ should be ΔG .
11. p. 84, first line after eq. (42): ΔG_C^{GT} should be $\Delta G_C^{\text{GT},0}$
12. p. 88, line 16: "accurage" should be "accurate".
13. p. 94, eq.(85c): add " β " before " V " in first exponential.
14. p. 95, line after eq. (91): "MED" should be "MEP".
15. p. 97, eq. (98) should read

$$B_{mF} = - \sum_{i=1}^N \sum_{\gamma} \frac{d\{[\text{sign}(s)]v_{i\gamma}(s)\}}{ds} L_{i\gamma,m}^{\text{GT}}(s)$$

or

$$B_{mF} = -\sum_{i=1}^N \sum_{\gamma} \frac{dv_{i\gamma}(s)}{d|s|} L_{i\gamma,m}^{GT}(s)$$

16. p. 97, second line after eq. (98): $B_{mF}(s)$ should be $-B_{mF}(s)$.
17. p. 97, third line after eq. (98): $[1 - \kappa(s) \bullet \mathbf{Q}(s)]^2$ should be $[1 - \kappa(s) \bullet \mathbf{Q}(s)]^2$.
18. p. 97, second and third lines after eq. (100): " μ " should not be a subscript.
19. p. 97, third line after eq. (101): $[\hbar/\mu\omega_m(s)]/2$ should be $[\hbar/\mu\omega_m(s)]^{1/2}$.
20. p. 101, in the last sentence, the gradient in the product channel (or reactant channel) should be multiplied by -1.
21. p. 102, line 7: "is $\mathbf{x}(s)$ " should be "is $\dot{\mathbf{x}}(s)$."
22. p. 102, fourth and fifth lines after eq. (126): " \mathbf{x} " should be " $\dot{\mathbf{x}}$ " in three places.
23. p. 102, line after eq. (127b): "B" should be β in two places, and "B/2" should be $\pi/2$. Thus below eq. (127), the inequality should be $0 < \beta < \pi/2$.
24. p. 102, line after eq. (128): "XB" should be "A + XB".
25. p. 102, second line after eq. (128): x^R should be \dot{x}^R .
26. p. 103: eq. (130) should be the special case of eq. (157) with $\tilde{\alpha}_0 = 1$, i.e., insert $\sin(\chi(\tilde{\alpha}_0 = 1, s_0))$ before $d\tilde{s}_0$.
27. p. 104, fifth line after eq. (131): "mass-weighted coordinates \mathbf{x} the" should be "mass-scaled coordinates \mathbf{x} ; the".
28. p. 104, second line after eq. (133): \tilde{s}_1 should be \tilde{s}_0 .
29. p. 104, second line after eq. (134): "zt" should be "at" and "normal" should be "generalized normal coordinates".
30. p. 104, third line after eq. (134): "coordinate(s)" should be "coordinate (s)".
31. p. 104, eq. (135) and following: notice that $q_{\perp,m}$ depends on \tilde{s}_1 as well as \tilde{s}_0 .
32. p. 106, eq. (144): insert a minus sign before the left-hand side because every term in the sum is negative.
33. p. 106, eq. (146): the condition $Q_m < t_m$ should be replaced by eq. (143).
34. p. 106: eq. (147) should be the special case of eq. (159) with $\tilde{\alpha}_0 = \tilde{\alpha}_1 = 1$.

35. p. 110, line 6: 147 should be 148a.
36. p. 117, line 3: "reactant" should be "reactants".
37. p. 117, second line from bottom: $p_2 : p_1$ should be p_2/p_1 .
38. p. 118, second line from bottom: ":" should be "/" in two places.
39. p. 121, line below eq. (209): " $N_m - 1/2$ " should be " $(N_m + 1/2)/h$ ".
40. p. 121, eq. (210): $1/4\pi h$ should be π .
41. p. 123, second line above eq. (217): "sätte" should be "state".
42. Ref. 58, line 1: "B.D." should be "B.C."
43. Ref. 71, line 2: "Vol. 2" should be "Vol. 4 of Modern Theoretical Chemistry".
44. Ref. 192, line 2: "*Phyus*" should be "*Phys*".
45. Ref. 231, line 2: "52" should be "62".
