***Definitions***

interaction energy: $E_{int} = E(AB,r_c)^{AB} - E(A,r_e) - E(B,r_e)$

BSSE correction: $E_{BSSE} = \Delta E^{counterpoise} = [E(A, r_c)^{AB} + E(B, r_c)^{AB}] - [E(A, r_c) + E(B, r_c)]$

deformation energy: $E_{deformation,total} = E_{deformation}(A) + E_{deformation}(B) = [E(A, r_c) - E(A, r_e)] + [E(B, r_c) - E(B, r_e)]$

**BSSE corrected interaction energy:**

$E_{int,corr} = E_{int} - E_{BSSE}$

$E_{int,corr} = E(AB,r_c)^{AB} - E(A,r_e) - E(B, r_e) - E_{BSSE}$

$E_{int,corr} = E(AB, r_c)^{AB} - E(A, r_e) - E(B, r_e) - [E(A, r_c)^{AB} + E(B, r_c)^{AB}] + [E(A, r_c) + E(B, r_c)]$

$E_{int,corr} = E(AB, r_c)^{AB} - E(A, r_e) - E(B, r_e) + [E(A, r_c) - E(A, r_c)^{AB}] + [E(B, r_c) - E(B, r_c)^{AB}]$

$E_{int,corr} = E(AB, r_c)^{AB} - E(A, r_c)^{AB} - E(B, r_c)^{AB} + [E(A, r_c) - E(A,r_e)] + [E(B, r_c) - E(B, r_e)]$

$E_{int,corr} = E(AB, r_c)^{AB} - E(A, r_c)^{AB} - E(B, r_c)^{AB} + E_{deformation,total}$