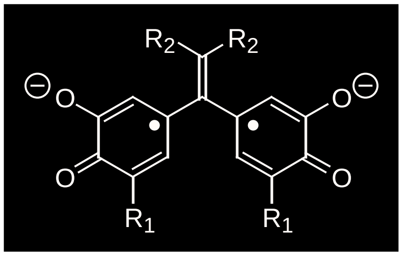
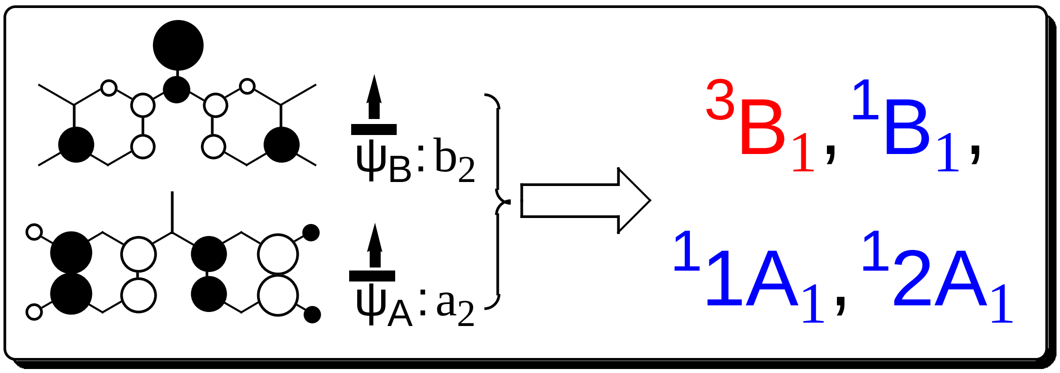
Our TMM- and *meta*-Phenylene-type bis(semiquinone)s have approximate C_{2v} symmetry. As such, the two singly-occupied MOs transform as a_2 and b_2. The four electronic states formed are: two open-shell states, ${}^3B_1$, ${}^1B_1$, and two zwitterionic ${}^1A_1$ states.



C_{2v}	E	C_2	σ_v	σ_v'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1



Open-shell singlet: 0.707<AB+BA>

Repulsion Energy = $0.5\langle(AB+BA)|e^2/r|(AB+BA)\rangle = J_{AB} + K_{AB}$

E(AB+BA) = +(AB+BA)

$C_2(AB+BA) = (C_2A)(C_2B)+(C_2B)(C_2A) = (A)(-B)+(-B)(A) =$ -(AB+BA)

$\sigma_v(AB+BA) = (\sigma_vA)(\sigma_vB)+(\sigma_vB)(\sigma_vA) = (-A)(-B)+(-B)(-A) =$ +(AB+BA)

$\sigma_v'(AB+BA) = (\sigma_v'A)(\sigma_v'B)+(\sigma_v'B)(\sigma_v'A) = (-A)(B)+(B)(-A) =$ -(AB+BA)

Therefore, (AB+BA) transforms as b_1 (+1, -1, +1, -1)

Open-shell triplet: 0.707<AB-BA>

Repulsion Energy = $0.5\langle(AB-BA)|e^2/r|(AB-BA)\rangle = J_{AB} - K_{AB}$

E(AB-BA) = +(AB-BA)

$C_2(AB-BA) = (C_2A)(C_2B)-(C_2B)(C_2A) = (A)(-B)-(-B)(A) =$ -(AB-BA)

$\sigma_v(AB-BA) = (\sigma_vA)(\sigma_vB)-(\sigma_vB)(\sigma_vA) = (-A)(-B)-(-B)(-A) =$ +(AB-BA)

$\sigma_v'(AB-BA) = (\sigma_v'A)(\sigma_v'B)-(\sigma_v'B)(\sigma_v'A) = (-A)(B)-(B)(-A) =$ -(AB-BA)

Therefore, (AB-BA) transforms as b_1 (+1, -1, +1, -1)

Closed-shell singlet 1: 0.707<AA-BB>

Repulsion Energy = $0.5\langle(AA-BB)|e^2/r|(AA-BB)\rangle = 1/2(J_{AA} + J_{BB}) - K_{AB}$

E(AA-BB) = +(AA-BB)

$C_2(AA-BB) = (C_2A)(C_2A)-(C_2B)(C_2B) = (A)(A)-(-B)(-B) =$ +(AA-BB)

$\sigma_v(AA-BB) = (\sigma_vA)(\sigma_vA)-(\sigma_vB)(\sigma_vB) = (-A)(-B)-(-B)(-A) =$ +(AA-BB)

$\sigma_v'(AA-BB) = (\sigma_v'A)(\sigma_v'A)-(\sigma_v'B)(\sigma_v'B) = (-A)(-A)-(B)(B) =$ +(AA-BB)

Therefore, (AB+BA) transforms as a_1 (+1, +1, +1, +1)

Closed-shell singlet 2: 0.707<AA+BB>

Repulsion Energy = $0.5\langle(AA+BB)|e^2/r|(AA+BB)\rangle = 1/2(J_{AA} + J_{BB}) + K_{AB}$

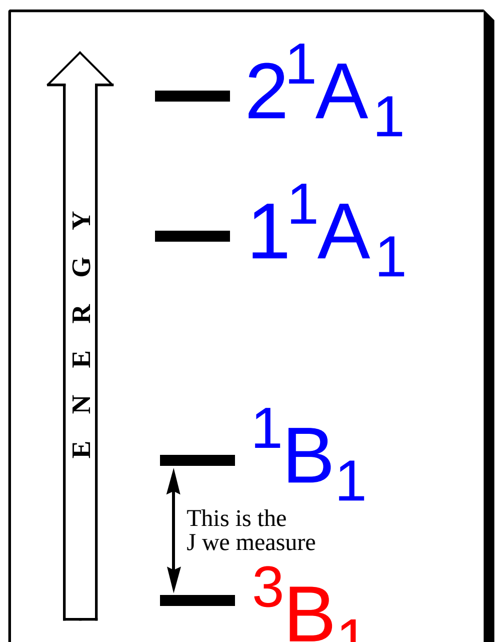
E(AA+BB) = +(AA+BB)

$C_2(AA+BB) = (C_2A)(C_2A)+(C_2B)(C_2B) = (A)(A)+(-B)(-B) =$ +(AA+BB)

$\sigma_v(AA+BB) = (\sigma_vA)(\sigma_vA)+(\sigma_vB)(\sigma_vB) = (-A)(-B)+(-B)(-A) =$ +(AA+BB)

$\sigma_v'(AA+BB) = (\sigma_v'A)(\sigma_v'A)+(\sigma_v'B)(\sigma_v'B) = (-A)(-A)+(B)(B) =$ +(AA+BB)

Therefore, (AB+BA) transforms as a_1 (+1, +1, +1, +1)



The ${}^1A_1$ states can mix into ${}^1B_1$ via b_1 normal modes