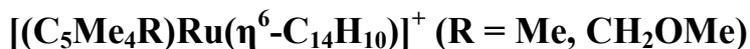


Photodimerization of the anthracene ruthenium complexes



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Table S1 Energy decomposition analysis (at BP86/TZ2P) for the interaction between two $[RuCp]^+$ cations in the $[Ru_2Cp_2]^{2+}$ moiety with the geometry it has in complexes **2c** and **3c**.

| | 2c (<i>anti</i> -) | 3c (<i>syn</i> -) |
|----------------------------|----------------------------|---------------------------|
| ΔE_{int} | 37.16 | 40.10 |
| ΔE_{Pauli} | 0.02 | 0.02 |
| ΔE_{elstat} | 37.69 | 40.92 |
| ΔE_{orb} | -0.55 | -0.83 |

Cartesian coordinates and energies for structures optimized at PBE/L1(Ru), L2 (C,H,O)

$[2c]^{2+}$ $E = -10527.60564514$ a.u.

| | | | |
|----|------------|-------------|------------|
| 44 | 5.66652409 | 2.10799444 | 8.00868557 |
| 44 | 3.81983322 | 7.99465715 | 3.41629393 |
| 6 | 3.62728802 | 2.98474510 | 8.05193091 |
| 1 | 3.12772123 | 3.44715165 | 8.90329879 |
| 6 | 3.52243519 | 1.57997971 | 7.85173589 |
| 1 | 2.94790131 | 0.97162544 | 8.54869368 |
| 6 | 4.22346751 | 0.96406570 | 6.77994389 |
| 1 | 4.18714188 | -0.11706234 | 6.65432535 |
| 6 | 5.02709180 | 1.75500265 | 5.91219858 |
| 1 | 5.60224033 | 1.27349018 | 5.12126934 |
| 6 | 8.04757159 | 5.33507637 | 5.85958288 |
| 1 | 8.59256014 | 4.85394800 | 5.04461264 |
| 6 | 8.70955602 | 6.22951069 | 6.70750390 |
| 1 | 9.76597006 | 6.44704225 | 6.54958536 |
| 6 | 8.01988374 | 6.83542775 | 7.75935123 |
| 1 | 8.53641283 | 7.52731483 | 8.42475582 |
| 6 | 6.66638361 | 6.54830786 | 7.96638638 |
| 1 | 6.13255617 | 7.01466165 | 8.79716907 |
| 6 | 4.54239585 | 5.28863728 | 7.29931463 |
| 1 | 4.20674247 | 5.59785835 | 8.29763132 |
| 6 | 5.92319561 | 4.07655226 | 5.19149698 |
| 1 | 6.62672081 | 3.47326765 | 4.60326928 |
| 6 | 6.69526780 | 5.05153818 | 6.05830308 |

| | | | |
|---|-------------|-------------|-------------|
| 6 | 6.00050547 | 5.66171015 | 7.11835288 |
| 6 | 4.40921126 | 3.78247454 | 7.17120001 |
| 6 | 5.11433676 | 3.16313232 | 6.09382209 |
| 6 | 7.56482660 | 2.88085519 | 8.83191495 |
| 6 | 6.66004748 | 2.61638488 | 9.90993255 |
| 6 | 6.35229153 | 1.21674380 | 9.89866713 |
| 6 | 7.06800047 | 0.61584435 | 8.81202995 |
| 6 | 7.81696246 | 1.64518196 | 8.15363016 |
| 1 | 7.98224370 | 3.84905040 | 8.57128115 |
| 1 | 6.28138204 | 3.34529065 | 10.62039423 |
| 1 | 5.70061076 | 0.69943925 | 10.59699496 |
| 1 | 7.05364528 | -0.43647297 | 8.54301645 |
| 1 | 8.47056812 | 1.50778708 | 7.29728636 |
| 6 | 5.85905341 | 7.11788428 | 3.37337659 |
| 1 | 6.35865730 | 6.65549596 | 2.52202038 |
| 6 | 5.96388971 | 8.52264659 | 3.57360431 |
| 1 | 6.53855130 | 9.13103028 | 2.87677833 |
| 6 | 5.26269886 | 9.13853853 | 4.64530694 |
| 1 | 5.29909293 | 10.21965663 | 4.77099624 |
| 6 | 4.45892222 | 8.34760498 | 5.51290775 |
| 1 | 3.88364976 | 8.82914397 | 6.30373033 |
| 6 | 1.43855914 | 4.76749658 | 5.56554181 |
| 1 | 0.89357360 | 5.24859351 | 6.38053095 |
| 6 | 0.77654548 | 3.87318693 | 4.71750636 |
| 1 | -0.27987323 | 3.65566127 | 4.87540197 |
| 6 | 1.46620351 | 3.26737972 | 3.66558804 |
| 1 | 0.94965072 | 2.57560039 | 3.00008993 |
| 6 | 2.81971822 | 3.55445605 | 3.45860681 |
| 1 | 3.35353751 | 3.08813767 | 2.62779878 |
| 6 | 4.94375328 | 4.81400525 | 4.12580043 |
| 1 | 5.27957363 | 4.50482017 | 3.12754229 |
| 6 | 3.56291822 | 6.02606150 | 6.23363340 |
| 1 | 2.85940040 | 6.62932233 | 6.82189378 |
| 6 | 2.79085765 | 5.05104732 | 5.36683518 |
| 6 | 3.48561759 | 4.44097379 | 4.30670577 |
| 6 | 5.07695206 | 6.32016599 | 4.25395621 |
| 6 | 4.37170131 | 6.93947584 | 5.33126236 |
| 6 | 1.91965191 | 7.22346086 | 2.59584546 |
| 6 | 2.82449212 | 7.48338365 | 1.51678012 |
| 6 | 3.13503106 | 8.88243744 | 1.52433327 |
| 6 | 2.42096600 | 9.48753627 | 2.60971785 |
| 6 | 1.67025135 | 8.46137439 | 3.27106777 |
| 1 | 1.50041339 | 6.25675558 | 2.85907266 |
| 1 | 3.20138130 | 6.75191098 | 0.80801702 |
| 1 | 3.78751408 | 9.39664362 | 0.82446917 |
| 1 | 2.43745322 | 10.54051768 | 2.87599740 |
| 1 | 1.01734244 | 8.60227918 | 4.12737562 |

$[3c]^{2+}$ $E = -10527.60039613$ a.u.

| | | | |
|----|------------|-------------|------------|
| 44 | 8.09960197 | 4.90077258 | 7.76579107 |
| 44 | 3.79137789 | 7.98907089 | 3.36301628 |
| 6 | 4.01364001 | 2.96827472 | 8.02617604 |
| 1 | 3.47977061 | 3.41660625 | 8.86648764 |
| 6 | 4.02907085 | 1.57805463 | 7.87205880 |
| 1 | 3.50680148 | 0.94647846 | 8.59063337 |
| 6 | 4.71144590 | 1.00106415 | 6.79967431 |
| 1 | 4.72332486 | -0.08211938 | 6.67894626 |
| 6 | 5.38093214 | 1.81212601 | 5.87735568 |
| 1 | 5.91456626 | 1.35784150 | 5.04009761 |
| 6 | 8.19909447 | 5.53092843 | 5.64261554 |
| 1 | 8.75222803 | 5.04181485 | 4.84040373 |
| 6 | 8.84515844 | 6.51182180 | 6.44793611 |

| | | | |
|---|-------------|-------------|-------------|
| 1 | 9.88691048 | 6.76968593 | 6.26226528 |
| 6 | 8.15019617 | 7.09941840 | 7.54042744 |
| 1 | 8.65869645 | 7.80838441 | 8.19235025 |
| 6 | 6.81154164 | 6.70429897 | 7.82327579 |
| 1 | 6.30033878 | 7.11497478 | 8.69433996 |
| 6 | 4.72110391 | 5.28932073 | 7.22554709 |
| 1 | 4.40073651 | 5.58796500 | 8.23214087 |
| 6 | 6.08683181 | 4.13443892 | 5.07900520 |
| 1 | 6.79621821 | 3.56226111 | 4.46708969 |
| 6 | 6.85116979 | 5.15317563 | 5.90433243 |
| 6 | 6.15170300 | 5.74466430 | 7.00364744 |
| 6 | 4.67677261 | 3.78007617 | 7.10569638 |
| 6 | 5.36381251 | 3.19910100 | 6.02586618 |
| 6 | 7.79235636 | 2.89686282 | 8.64770060 |
| 6 | 9.02635637 | 2.90534144 | 7.92182786 |
| 6 | 9.89127702 | 3.87575728 | 8.52546652 |
| 6 | 9.18989493 | 4.46778691 | 9.62632222 |
| 6 | 7.89314208 | 3.86187860 | 9.70045339 |
| 1 | 6.92816250 | 2.27523753 | 8.43141355 |
| 1 | 9.26958926 | 2.27866891 | 7.06880469 |
| 1 | 10.90421111 | 4.11264046 | 8.21264605 |
| 1 | 9.57829403 | 5.23186081 | 10.29366285 |
| 1 | 7.12530821 | 4.08865906 | 10.43430038 |
| 6 | 5.86256799 | 7.20590695 | 3.25487069 |
| 1 | 6.35009409 | 6.76381565 | 2.38561364 |
| 6 | 5.90969288 | 8.61605832 | 3.44815323 |
| 1 | 6.43021903 | 9.24776908 | 2.72967826 |
| 6 | 5.21460798 | 9.20379125 | 4.54049300 |
| 1 | 5.20198648 | 10.28629105 | 4.65984949 |
| 6 | 4.47498628 | 8.37919671 | 5.43554508 |
| 1 | 3.89794901 | 8.83724549 | 6.23925707 |
| 6 | 1.60871292 | 4.69237471 | 5.56843606 |
| 1 | 1.07209509 | 5.14270800 | 6.40592313 |
| 6 | 0.95606887 | 3.78110472 | 4.73157437 |
| 1 | -0.08598597 | 3.52221307 | 4.91892269 |
| 6 | 1.63840715 | 3.20411870 | 3.65916225 |
| 1 | 1.13042459 | 2.49360386 | 3.00714619 |
| 6 | 2.97594428 | 3.53623453 | 3.41960684 |
| 1 | 3.50674827 | 3.08392719 | 2.57948263 |
| 6 | 5.06933268 | 4.86388749 | 4.03919023 |
| 1 | 5.39236061 | 4.56874523 | 3.03241229 |
| 6 | 3.70357775 | 6.01877207 | 6.18571671 |
| 1 | 2.99687011 | 6.59438977 | 6.79750346 |
| 6 | 2.94381541 | 5.02242269 | 5.33472257 |
| 6 | 3.63087143 | 4.44145121 | 4.25489438 |
| 6 | 5.14770203 | 6.37439021 | 4.16351268 |
| 6 | 4.44821299 | 6.96585695 | 5.26281327 |
| 6 | 1.89629840 | 7.12348758 | 2.62307260 |
| 6 | 2.75048886 | 7.40330268 | 1.50873272 |
| 6 | 3.00144031 | 8.81417800 | 1.48341712 |
| 6 | 2.30085472 | 9.40678421 | 2.58447049 |
| 6 | 1.61857019 | 8.36076363 | 3.28768712 |
| 1 | 1.53172326 | 6.14374619 | 2.91840761 |
| 1 | 3.13360704 | 6.67554085 | 0.79942870 |
| 1 | 3.60545573 | 9.34367186 | 0.75211171 |
| 1 | 2.28105410 | 10.46394041 | 2.83353718 |
| 1 | 0.99178340 | 8.48724273 | 4.16556540 |