

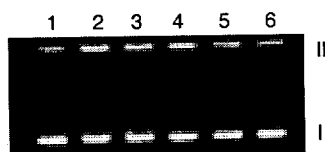
# Supporting Information

## The Relative Efficiencies of $\text{CpM}(\text{CO})_n\text{CH}_3$ and $\text{CpM}(\text{CO})_n\text{Ph}$ Complexes in Photoinduced DNA Cleavage

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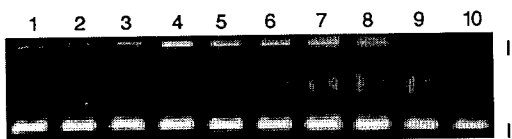
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### Plasmid relaxation by $[\text{CpW}(\text{CO})_3]_2$ .

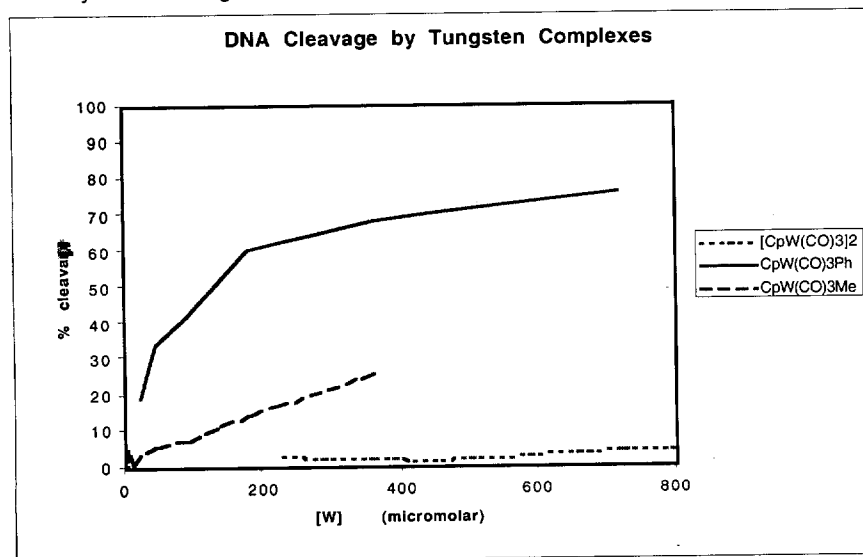


**Figure S1.** Relaxation of pBR322 DNA (30  $\mu\text{M}$ /bp in 10% DMSO/20 mM Tris buffer, pH 8) by  $[\text{CpW}(\text{CO})_3]_2$ . Lane 1, DNA alone; lanes 2—6, DNA + complex (3600, 1800, 900, 450, and 225  $\mu\text{M}$ ). Reactions in lane 2—6 were irradiated with Pyrex-filtered light from a 450 W medium pressure mercury arc lamp for 20 minutes.

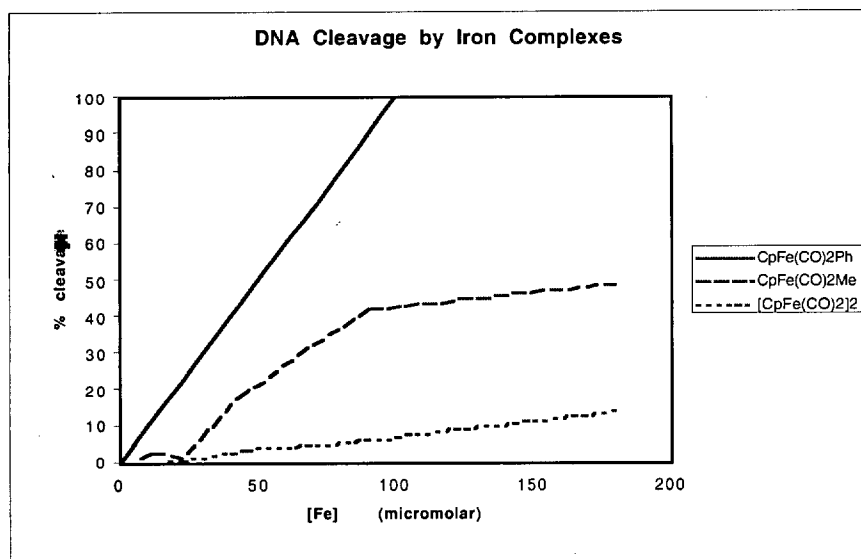
### Plasmid relaxation by $[\text{CpFe}(\text{CO})_2]_2$ .



**Figure S2.** Relaxation of pBR322 DNA (30  $\mu\text{M}$ /bp in 10% DMSO/20 mM Tris buffer, pH 8) by  $[\text{CpFe}(\text{CO})_2]_2$ . Lanes 1 and 3, DNA alone; lanes 2 and 4—10, DNA + complex (90, 90, 45, 23, 11, 5.6, 2.8, and 1.4  $\mu\text{M}$ ). Reactions in lanes 3—10 were irradiated with Pyrex-filtered light from a 450 W medium pressure mercury arc lamp for 20 minutes.



**Figure S3.** Plot of percent relaxation of pBR322 DNA (30  $\mu\text{M}$ /bp in 10% DMSO/20 mM Tris buffer, pH 8) by  $[\text{CpW}(\text{CO})_3]_2$ ,  $\text{CpW}(\text{CO})_3\text{Ph}$ , and  $\text{CpW}(\text{CO})_3\text{Me}$  vs concentration of tungsten species. To obtain value for % cleavage, the highest amount of form II observed in control lanes was subtracted from the sum of % form III and % form II for each concentration.



**Figure S4.** Plot of percent relaxation of pBR322 DNA (30  $\mu\text{M}$ /bp in 10% DMSO/20 mM Tris buffer, pH 8) by  $[\text{CpFe(CO)}_2]_2$ ,  $\text{CpFe(CO)}_2\text{Me}$ , and  $\text{CpFe(CO)}_2\text{Ph}$  vs concentration of iron species. To obtain value for % cleavage, the highest amount of form II observed in control lanes was subtracted from the sum of % form III and % form II for each concentration. Graphs were prepared with Microsoft Excel.

**Plasmid Assay Quantitation Data.** The bands in the scanned gels were quantitated with the NIH ImageJ program to give the following data:

pBR322 cleavage by  $\text{CpW(CO)}_3\text{C}_6\text{H}_5$  (Figure 1a):

| Lane        | $\text{CpW(CO)}_3\text{C}_6\text{H}_5$ ( $\mu\text{M}$ ) | Form I (%) | Form II (%) | Form III (%) |
|-------------|----------------------------------------------------------|------------|-------------|--------------|
| 1 (control) |                                                          | 93.5       | 6.5         | 0.0          |
| 2 (control) | 360                                                      | 82.1       | 17.9        | 0.0          |
| 3 (control) |                                                          | 84.7       | 15.3        | 0.0          |
| 4           | 360                                                      | 56.7       | 63.3        | 0.0          |
| 5           | 180                                                      | 67.9       | 32.1        | 0.0          |
| 6           | 90                                                       | 75.0       | 25.0        | 0.0          |
| 7           | 45                                                       | 76.5       | 23.5        | 0.0          |
| 8           | 22.5                                                     | 78.7       | 21.3        | 0.0          |
| 9           | 11.3                                                     | 81.8       | 18.2        | 0.0          |
| 10          | 5.6                                                      | 77.1       | 22.9        | 0.0          |
| 11          | 2.8                                                      | 81.7       | 18.3        | 0.0          |
| 12          | 1.4                                                      | 82.0       | 18.0        | 0.0          |

pBR322 cleavage by  $\text{CpFe}(\text{CO})_2\text{CH}_3$  (Figure 1b):

| Lane        | $\text{CpFe}(\text{CO})_2\text{CH}_3$ ( $\mu\text{M}$ ) | Form I (%) | Form II (%) | Form III (%) |
|-------------|---------------------------------------------------------|------------|-------------|--------------|
| 1 (control) |                                                         | 91.9       | 8.1         | 0.0          |
| 2 (control) | 360                                                     | 83.7       | 16.3        | 0.0          |
| 3 (control) |                                                         | 91.2       | 8.8         | 0.0          |
| 4           | 360                                                     | 15.8       | 73.6        | 10.6         |
| 5           | 180                                                     | 35.0       | 57.2        | 7.8          |
| 6           | 90                                                      | 41.5       | 55.2        | 3.3          |
| 7           | 45                                                      | 64.1       | 34.5        | 1.4          |
| 8           | 22.5                                                    | 82.6       | 17.4        | 0.0          |
| 9           | 11.3                                                    | 81.1       | 18.9        | 0.0          |
| 10          | 5.6                                                     | 87.2       | 12.8        | 0.0          |
| 11          | 2.8                                                     | 87.3       | 12.7        | 0.0          |
| 12          | 1.4                                                     | 91.3       | 8.7         | 0.0          |

pBR322 cleavage by  $\text{CpFe}(\text{CO})_2\text{C}_6\text{H}_5$  (Figure 1c):

| Lane        | $\text{CpFe}(\text{CO})_2\text{C}_6\text{H}_5$ ( $\mu\text{M}$ ) | Form I (%) | Form II (%) | Form III (%) |
|-------------|------------------------------------------------------------------|------------|-------------|--------------|
| 1 (control) |                                                                  | 73.2       | 26.8        | 0.0          |
| 2 (control) | 360                                                              | 71.3       | 28.7        | 0.0          |
| 3 (control) |                                                                  | 71.4       | 28.6        | 0.0          |
| 4           | 360                                                              | 0.0        | 0.0         | 0.0          |
| 5           | 180                                                              | 0.0        | 0.0         | 0.0          |
| 6           | 90                                                               | 0.0        | 0.0         | 0.0          |
| 7           | 45                                                               | 0.0        | 0.0         | 0.0          |
| 8           | 22.5                                                             | 0.0        | 60.4        | 39.6         |
| 9           | 11.3                                                             | 8.9        | 80.5        | 10.6         |
| 10          | 5.6                                                              | 66.3       | 33.7        | 0.0          |
| 11          | 2.8                                                              | 65.9       | 34.1        | 0.0          |
| 12          | 1.4                                                              | 79.8       | 20.2        | 0.0          |

pBR322 cleavage by  $\text{CpW}(\text{CO})_3\text{CH}_3$  (data from Figure 1 of reference #2):

| Lane        | $\text{CpW}(\text{CO})_3\text{CH}_3$ ( $\mu\text{M}$ ) | Form I (%) | Form II (%) | Form III (%) |
|-------------|--------------------------------------------------------|------------|-------------|--------------|
| 1 (control) |                                                        | 99.1       | 0.9         | 0.0          |
| 2 (control) |                                                        | 96.3       | 3.7         | 0.0          |
| 3 (control) | 720                                                    | 96.0       | 4.0         | 0.0          |
| 4           | 720                                                    | 20.6       | 79.4        | 0.0          |
| 5           | 360                                                    | 28.5       | 71.5        | 0.0          |
| 6           | 180                                                    | 36.6       | 63.4        | 0.0          |
| 7           | 90                                                     | 55.0       | 45.0        | 0.0          |
| 8           | 45                                                     | 62.4       | 37.6        | 0.0          |
| 9           | 22.5                                                   | 77.5       | 22.5        | 0.0          |

pBR322 cleavage by  $[\text{CpW}(\text{CO})_3]_2$  (Figure S1):

| Lane        | $[\text{CpW}(\text{CO})_3]_2$ ( $\mu\text{M}$ ) | Form I (%) | Form II (%) | Form III (%) |
|-------------|-------------------------------------------------|------------|-------------|--------------|
| 1 (control) |                                                 | 83.5       | 16.5        | 0.0          |
| 2           | 3600                                            | 68.2       | 31.8        | 0.0          |
| 3           | 1800                                            | 71.2       | 28.8        | 0.0          |
| 4           | 900                                             | 77.9       | 22.1        | 0.0          |
| 5           | 450                                             | 82.2       | 17.8        | 0.0          |
| 6           | 225                                             | 80.6       | 19.4        | 0.0          |

pBR322 cleavage by  $[\text{CpFe}(\text{CO})_2]_2$  (Figure S2):

| Lane        | $[\text{CpFe}(\text{CO})_2]_2$ ( $\mu\text{M}$ ) | Form I (%) | Form II (%) | Form III (%) |
|-------------|--------------------------------------------------|------------|-------------|--------------|
| 1 (control) |                                                  | 88.2       | 11.8        | 0.0          |
| 2 (control) |                                                  | 94.3       | 5.7         | 0.0          |
| 3 (control) | 90                                               | 90.2       | 9.8         | 0.0          |
| 4           | 90                                               | 74.5       | 25.5        | 0.0          |
| 5           | 45                                               | 82.2       | 17.8        | 0.0          |
| 6           | 22.5                                             | 85.2       | 14.8        | 0.0          |
| 7           | 11.25                                            | 87.6       | 12.4        | 0.0          |
| 8           | 5.63                                             | 90.2       | 9.8         | 0.0          |
| 9           | 2.81                                             | 92.3       | 7.7         | 0.0          |
| 10          | 1.41                                             | 91.8       | 8.2         | 0.0          |