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SUPPORTING INFORMATION

for

Straightforward computational determination of energy-transfer kinetics through the application of the Marcus theory

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1 Additional details about the application of the Marcus theory.

Classical vs. Semi-classical Marcus theory.

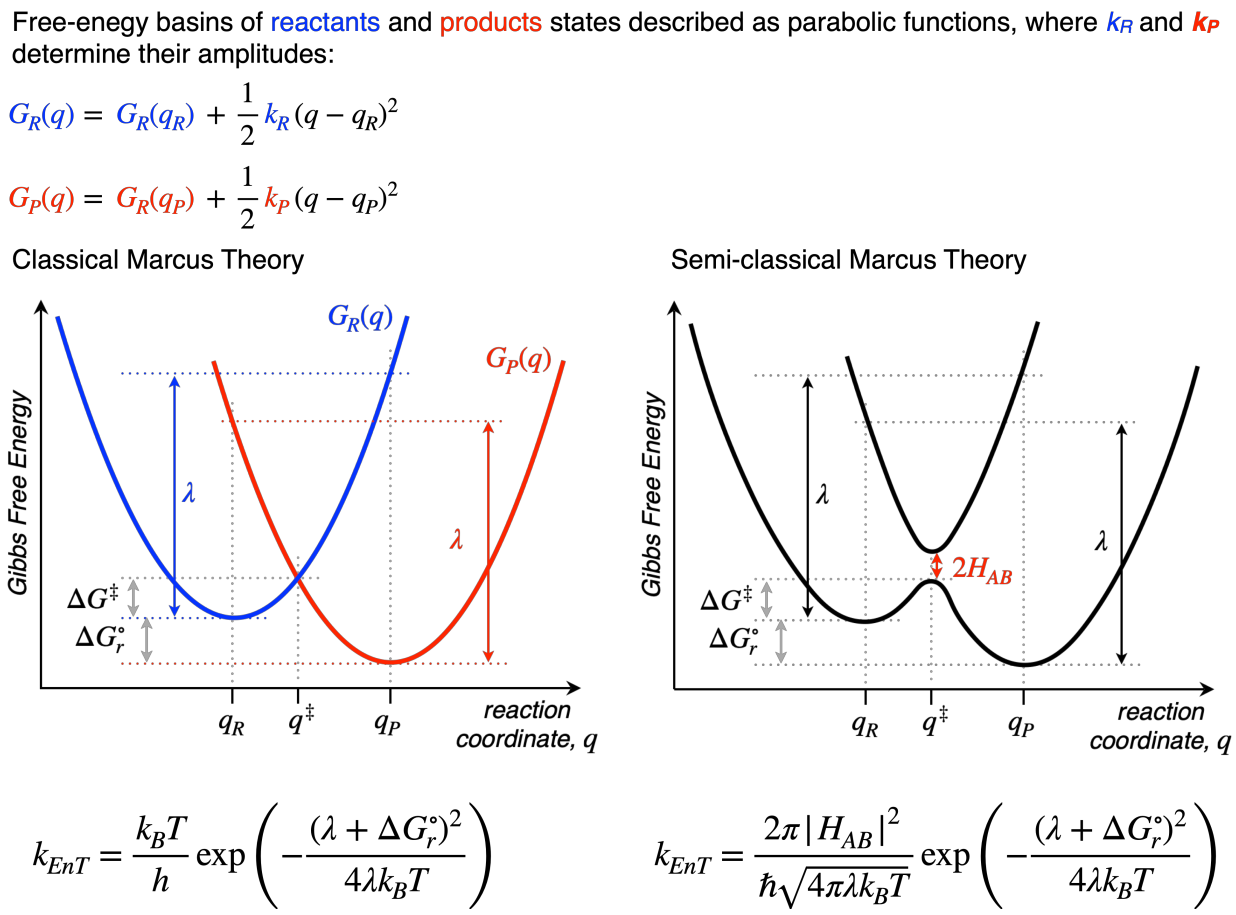


Figure S 1: Comparison of the classical (left) and semi-classical (right) versions of the Marcus Theory and their impact on EnT rate constants. H_{AB} stands for the electronic coupling between initial and final states.

Symmetric vs. Asymmetric Marcus approach.

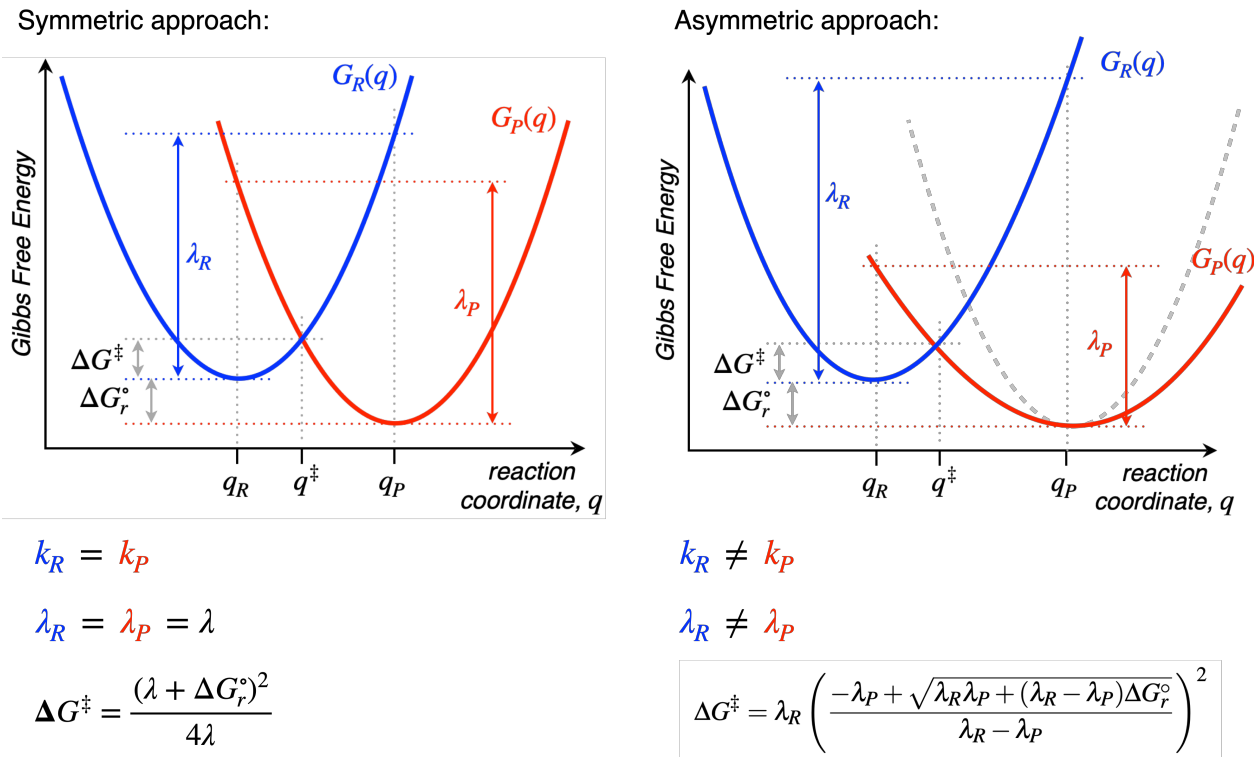


Figure S 2: Graphical representation of the impact of the relative amplitude of parabolas describing reactants and products states on the height of the free-energy barrier. In the asymmetric scenario, the gray dashed parabola represents what would be assumed if the symmetric approach were applied to a system where the free-energy curves of reactants and products have distinct amplitudes.

2 Discussion about the existence of two minima on the triplet surface of 4.

As mentioned in the main text and shown in Figure 5, we characterized two minima for substrate **4** on the triplet-state energy surface. The first one, labeled as ^{3}**4**, corresponds to the twisted configuration analogous to that obtained for **1**-**3** (see Figure S3 for a representation of the spin density on the optimized geometry of ^{3}**4**), which was obtained when relaxing the *Z* isomer on the triplet-state surface. The second (^{3}**4'**), obtained when steaming from the *E* conformer, is 6.8 kcal mol^{-1} less stable and corresponds to a structure whereby the planarity of the system is preserved (Figure S3 and Figure 5, main text). The existence of this second minimum for **4** was ascribed to a higher delocalization of the spin density in the flat configuration compared to the other substrates, granted by the hihgly-conjugated naphtalene substituent, thus stabilizing a local minimum with $\Phi = 180°$ by reducing the repulsion between electrons of the same spin. Note that a flat triplet minimum with a *Z*-like configuration could not be located, most likely due to steric repulsion between the oxygen atom of the ester group and the naphtalene substituent, which destabilizes the flat configuration, preventing an efficient conjugation of the π system. As a matter of fact, deviation from planarity of the naphtalene group with respect to the double bond was found to be larger in the *Z* isomer (54.1°) compared to the *E* one (20.6°).

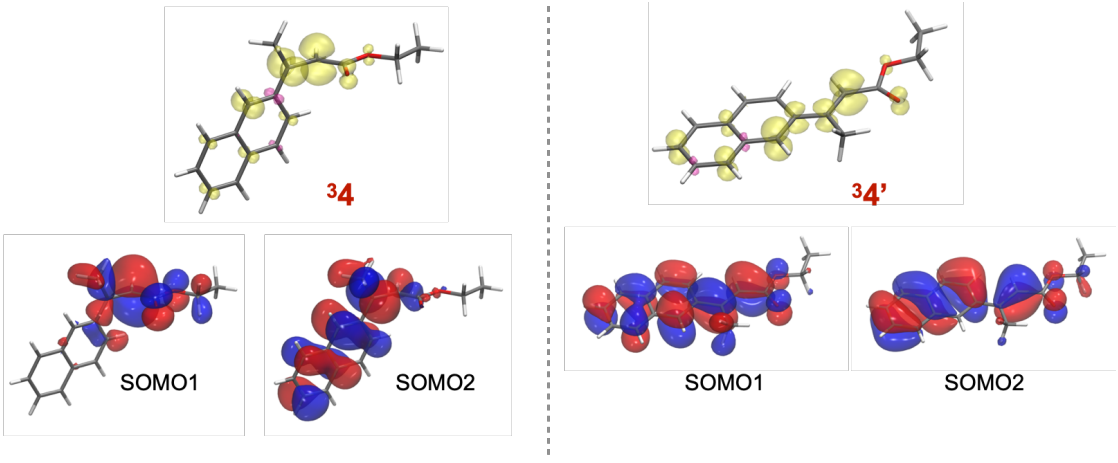


Figure S 3: Spin density distribution and singly occupied molecular orbitals (SOMOs) represented on the optimized structures of ^{3}**4**, $\Phi \approx 90°$ (left) and ^{3}**4'**, $\Phi \approx 180°$ (right)

3 Summary of the calculated parameters used in the Marcus theory.

Table S 1: Calculated reorganization energies (kcal mol^{-1}) for all the studied species on the reactants (λ_R) and products (λ_P) surfaces of the ^{3}PC + substrate $\rightarrow$ PC + ^{3}substrate reaction

pair	λ_R	λ_P
^{3}TX*/TX	4.8	4.1
$1_E/^3 1$	71.9	32.7
$1_Z/^3 1$	71.0	26.1
$2_E/^3 2$	61.3	21.7
$2_Z/^3 2$	59.8	33.0
$3_E/^3 3$	63.0	23.3
$3_Z/^3 3$	62.9	33.8
$4_E/^3 4$'	10.5	9.2
$4_Z/^3 4$	59.2	22.3
^{3}Ir-A/Ir-A	13.1	8.3
^{3}Ir-B/Ir-B	7.3	5.1
^{3}Ir-C/Ir-C	6.6	3.3
^{3}Ir-D/Ir-D	7.9	5.9
^{3}Ir-E/Ir-E	11.1	11.8
^{3}Ru/Ru	8.2	3.5

Table S 2: Kinetic and thermodynamic parameters (kcal mol^{-1}) for the sensitization of $\mathbf{3}_E$ and $\mathbf{3}_Z$ by Ir(III)- and Ru(II)-based photocatalysts (PCs).

PC	substrate	$\Delta G^{\ddagger}_{exp.}$	$\Delta G^{\circ}{}_r$	λ_R	λ_P	$\Delta G^{\ddagger}_{symm.}$	$\Delta\Delta G^{\ddagger}_{symm.}$	$\Delta G^{\ddagger}_{asymm.}$	$\Delta\Delta G^{\ddagger}_{asymm.}$
Ir-A	3_E	8.2	-3.1	76.1	31.6	12.0	-3.8	9.9	-1.7
	3_Z	9.7	-3.2	76.0	42.0	13.2	-3.5	12.0	-2.3
Ir-B	3_E	6.5	-8.2	70.3	28.4	8.6	-2.1	6.0	+0.5
	3_Z	8.1	-8.4	70.2	38.1	9.8	-1.7	8.3	-0.3
Ir-C	3_E	5.4	-15.4	69.6	26.6	5.6	-0.2	2.3	+3.0
	3_Z	6.7	-15.6	69.5	37.0	6.7	0.0	4.7	+2.0
Ir-D	3_E	5.1	-12.8	70.9	29.2	6.9	-1.8	4.1	+1.1
	3_Z	6.4	-13.0	70.9	39.6	8.1	-1.7	6.4	0.0
Ir-E	3_E	4.6	-15.3	74.1	35.0	7.1	-2.5	4.6	+0.1
	3_Z	5.0	-15.5	74.0	45.5	8.2	-3.2	6.7	-1.7
Ru	3_E	-	-0.6	71.2	26.8	11.9	-	9.9	-
	3_Z	-	-0.8	71.2	37.3	13.2	-	12.1	-
						MAE =	2.0	MAE =	1.3

4 Analysis of the theoretical rate constants derived from the application of the asymmetric Marcus approach.

Owing to the good agreement between calculated barriers and those derived from experimental rate constants (see main text), the theoretical rate constants are also in line with the experimental ones, as shown in Table S3. Note however, that rate constants are strongly sensitive to computational error due to their exponential dependence on free-energy barriers. In fact, a difference of only 1 kcal mol^{-1} in the height of the barrier, which falls within the range of computational uncertainty, entails variations of one order of magnitude on the derived rate constant. On these grounds, we consider that the agreement between experimental and theoretical rate constants is more than acceptable. Additionally, the theoretical barriers can also reproduce the experimental selectivity trends.[1] Specifically, they lead to a k_Z/k_E ratio >1 for substrate **1**, indicating minor *E*-isomer sensitization and thus, major *E*-isomer formation; and k_Z/k_E ratios <1 for substrates **2** and **3**, for which a preference for the *Z*-isomer formation was also experimentally reported.[1] In fact, as shown in Figure S4, the construction of microkinetic models based on theoretical rate constants can correctly reproduce the experimental selectivity trend. Unfortunately, a quantitative theoretical determination of reaction outcomes in terms of amounts of *E* and *Z* isomer would require extremely accurate barriers with errors significantly smaller than 1 kcal mol^{-1}, which is out of reach for DFT, and most likely, even for more sophisticated and demanding computational methods. As a matter of fact, decreasing the $\Delta\Delta G^{\ddagger}$ between *E*- and *Z*-isomer sensitization by only 1.5 kcal mol^{-1} for substrates **2** and **3** leads to *E*:*Z* product ratios that are in good quantitative agreement with experimental ones (see Figure S4)

Obviously, the above analysis cannot apply to substrate **4**, whose sensitization is diffusion controlled. In these cases, a *E*:*Z* ratio close to 50:50 (as experimentally found by Kerzig, Gilmour and co-workers)[1] may be always expected, as diffusion barriers cannot discern between *E* and *Z* isomers of the same molecule and hence, the sensitization process cannot be selective at all.

Table S 3: Comparison of experimental and theoretical rate constants and constants and barrier ratios for the sensitization of Z and E isomers of substrates **1-3**

Substrate	k_{EnT} exp. / 10^9 M^{-1} s^{-1}	k_{EnT} calc. 10^9 M^{-1} s^{-1}	k_Z/k_E exp.	k_Z/k_E calc.	$\Delta G_Z^\ddagger/\Delta G_E^\ddagger$ exp.	$\Delta G_Z^\ddagger/\Delta G_E^\ddagger$ calc.
1_Z	0.583	0.142	30.7	39.3	0.73	0.74
1_E	0.019	0.004				
2_Z	2.60	0.54	0.38	0.03	1.14	1.62
2_E	6.76	18.9				
3_Z	3.25	0.14	0.46	0.02	1.05	1.51
3_E	7.02	8.38				

Equations used in microkinetic models to produce the results shown in Figure S4:

$$TX \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} TX* \tag{4.1}$$

$$TX^* + subs_E \xrightarrow{k_2} TX + subs^* \tag{4.2}$$

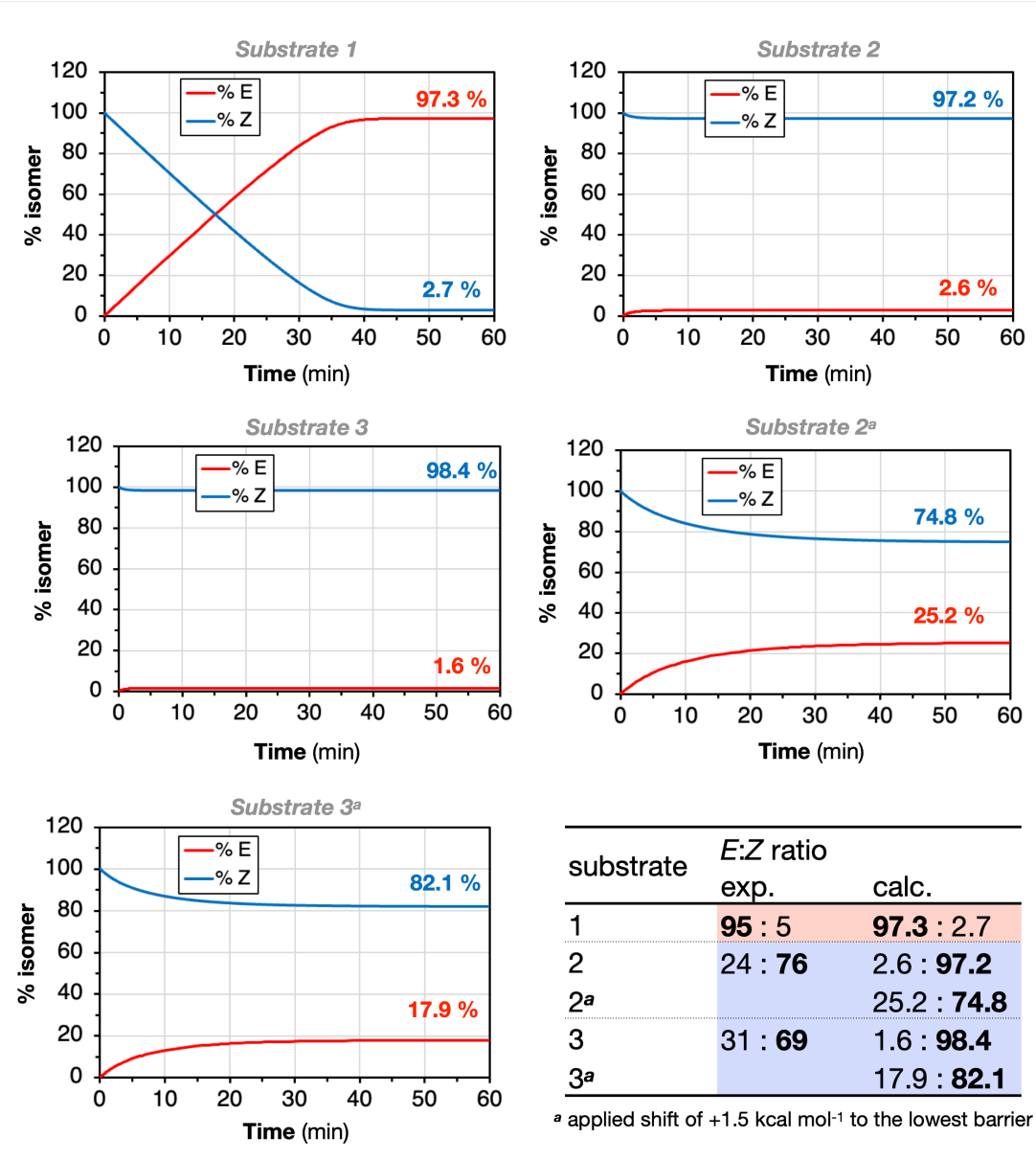
$$TX^* + subs_Z \xrightarrow{k_3} TX + subs^* \tag{4.3}$$

$$subs^* \xrightarrow{k_4} subs_E \tag{4.4}$$

$$subs* \xrightarrow{k_5} subs_Z \tag{4.5}$$

k_1 was fitted to 10^{-1} s^{-1}, so that the reaction is completed within 1h, as in the experimental reference.[1] k_{-1} was estimated from the experimental lifetime of TX* (77 μs), assuming first-order kinetics.k_2 and k_3 (EnT events) were derived from theoretical free-energy barriers. Finally, k_4 and k_5 were both set to 10^{11} s^{-1} for the sake of being faster than EnT processes and equal for subs* to yield either E or Z products. Initial concentrations:[1]

[subs$_Z$] = 6×10^{-2} M; [TX] = 6×10^{-4} M; [subs$_E$] = [subs*] = [TX*] = 0.



substrate	*E*:*Z* ratio exp.	calc.
1	**95** : 5	**97.3** : 2.7
2	24 : **76**	2.6 : **97.2**
2[a]		25.2 : **74.8**
3	31 : **69**	1.6 : **98.4**
3[a]		17.9 : **82.1**

[a] applied shift of +1.5 kcal mol^{-1} to the lowest barrier

Figure S 4: Evolution of E:Z product ratios as function of reaction time as derived from the microkinetic model presented above. Asterisk marks denote that in those models, the free-energy barrier for the fastest EnT event has been shifted by +1.5 kcal mol^{-1} and the table compares E:Z ratios at the end of the simulation with experimental ones.[1] Within the table, red and blue coloring represents experimental selectivity towards E or Z isomers, respectively, which is qualitatively, if not quantitatively reproduced by our microkinetic models in all cases.

5 Analysis of the factors governing the EnT free-energy barriers from excited photocatalysts to $\mathbf{3}_E$ and $\mathbf{3}_Z$.

As shown in Figure S5, neither the computationally-determined barriers nor the experimental ones are solely determined by the triplet energy of the analyzed PCs, which are implicit in the reaction free energies (Figure S5a,d), although they roughly correlate. Conversely, our results also evidence that their intrinsic reorganization energies have an important weight on the height of the barriers (Figure S5b,c,e,f), correlating even better with the barriers than the reaction energies themselves.

Consequently, this causes that PCs that entail distinct reaction energies display similar barriers, due to the compensating effect of the reorganization energies. For instance, even though the EnT from **Ir-A** to $\mathbf{3}_E$ is thermodynamically less favorable than that of **Ir-B** to $\mathbf{3}_Z$ (ΔG_r° of -3.1 vs -8.4 kcal mol^{-1}, respectively, entries 1 and 4 in Table S2), they both exhibit very similar barriers, which is explained by the fact that the λ_P of the latter is significantly higher.

Similarly, although **Ir-A** and **Ru** exhibit rather different triplet energies (see Table S5) they were predicted to show similar barriers, owing to the much smaller reorganization energies determined for **Ru** compared to **Ir-A** (Table S1).

It is also interesting to note that Gilmour and Kerzig observed that thioxanthone-based photocatalysts sensitize substrates faster than Ir-based photocatalysts with similar triplet energies.[1] This can be easily rationalized using the Marcus theory and the above-reported parameters as follows:

According to the Marcus theory, barriers are a function of reaction free energies (ΔG_r°) and reorganization energies (λ parameters). The more exergonic the reaction, the lower the barrier; and the smaller the reorganization energy, the lower the barrier too (see eq. 3 and 4 in the main text). When comparing the **Ir-D** and **TX** catalysts, although they exhibit similar triplet energies, which translate into almost equal reaction free energies (see Table 1 in the main text and Table S2), they sensitize alkene substrates at a different rate. Hence, the discrepancies in the rate constants (and thus the barriers) arise from their distinct reorganization energies. As shown in Table S1, the reorganization energies calculated for **TX** (4.1-4.8 kcal mol^{-1}) are smaller than those measured for **Ir-D** (5.9-7.9 kcal mol^{-1}). Consequently, the EnT barriers are lower for **TX**, explaining the experimental outcomes by

Gilmour and Kerzig and co-workers.[1]

To further support these conclusions, we have carried out additional calculations on the sensitization of 3_E and 3_Z by 2,7-Dimethoxy-9*H*-thioxanthen-9-one (**MeOTX**), which was also found to sensitize substrates faster than Ir-based PCs with similar triplet energies. Specifically, the reorganization energy of **MeOTX** (4.2 kcal mol^{-1}, both on reactants and products surfaces) was computed to be very similar to that of **TX** (4.4 kcal mol^{-1}, on average) and hence, also smaller than that of Ir-based PCs, which are typically larger than 6 kcal mol^{-1} when averaged over reactants and products surfaces. Also in qualitative agreement with experimental findings,[1] free-energy barriers obtained for **MeOTX** were found to be *ca.* 5 kcal mol^{-1} higher than those involving **TX**. This can be explained by the lower triplet energy of **MeOTX**,[1] which leads to less favorable EnT thermodynamics. Specifically, the sensitization free energies by **MeOTX** (-2.5 and -2.7 kcal mol $^{-1}$ for 3_E and 3_Z, respectively) are significantly less exergonic than those involving **TX** (-11.9 and -12.1 kcal mol^{-1}). Thus, although both PCs display similar reorganization energies, their distinct reaction kinetics are due to different thermodynamic driving forces.

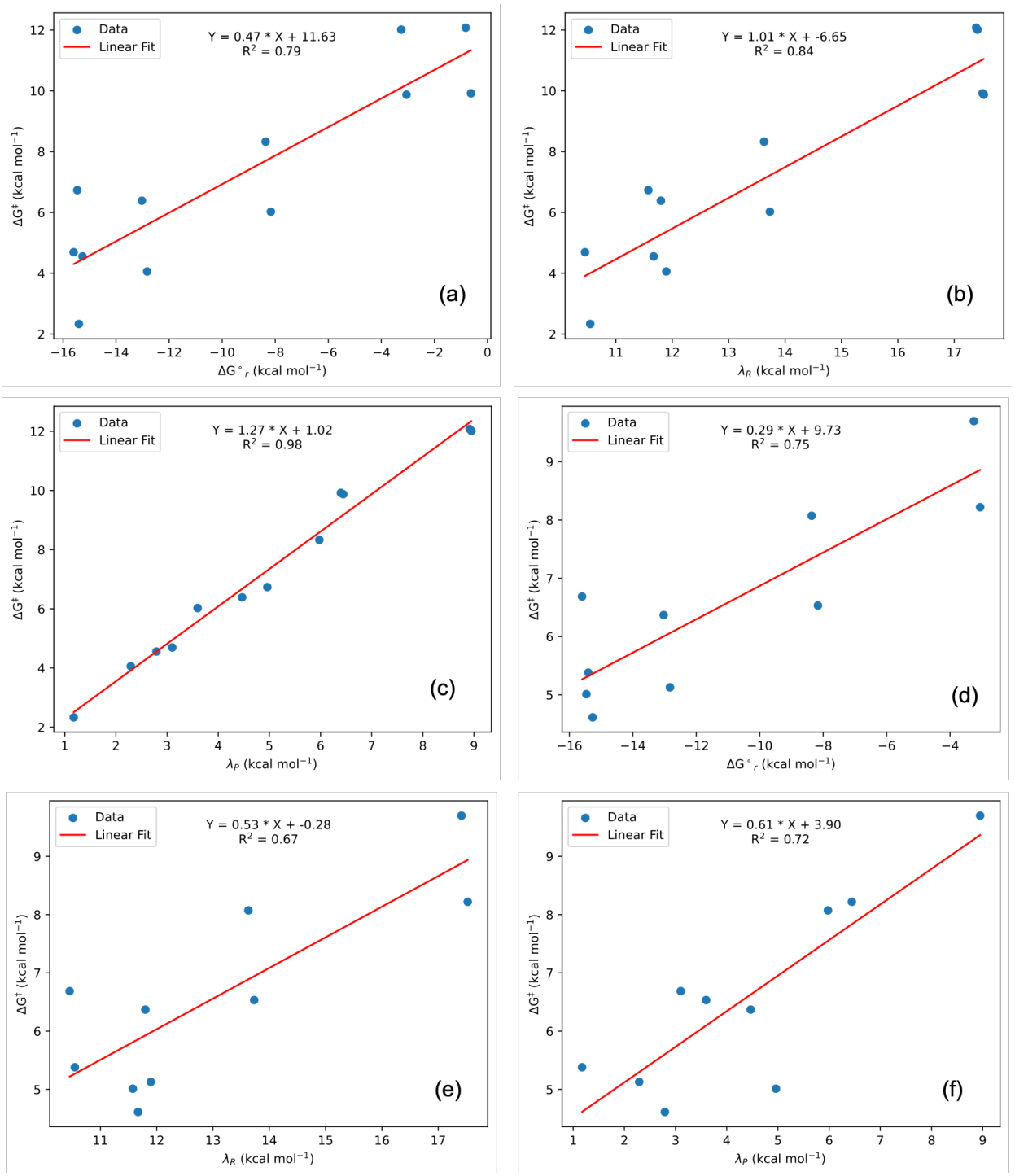


Figure S 5: Linear fitting of the ΔG_r° for EnT processes from Ir- and Ru-based photocatalysts to $\mathbf{3}_E$ and $\mathbf{3}_Z$ and contributions to λ_R and λ_P of the PCs with the free-energy barriers obtained either computationally through the asymmetric Marcus equation (a-c) or from experimental rate constants[1] (d-f).

6 Methodology benchmark and calculated triplet energies for the studied photocatalysts.

Table S 4: Comparison of the performance of several density functionals in predicting the triplet energy of **TX**. The experimental value of 63.4 kcal mol^{-1} was determined from the phosphorescense emission wavelength in 2-Methyltetrahydrofuran ($\epsilon = 6.97$).[1]

E[ρ]	$\Delta E_{triplet-singlet}$	
	IEF-PCM (MeCN, $\epsilon = 35.69$)	IEF-PCM (THF, $\epsilon = 7.43$)
B3LYP-D3BJ	60.3	61.0
ωB97X-D	67.0	67.9
PBE0-D3BJ	61.2	61.9
TPSSh-D3BJ	58.6	59.2
PBE-D3BJ	55.5	56.1

Table S 5: Comparison of the DFT (B3LYP-D3BJ)-derived triplet energies (kcal mol^{-1}) for Ir- and Ru-based photocatalysts with the experimental ones.[1]

PC	$\Delta E_{triplet-singlet}$	
	exp.	calc.
Ir-A	55.6	51.3
Ir-B	59.3	57.0
Ir-C	62.5	61.9
Ir-D	63.4	62.6
Ir-E	67.1	64.2
Ru	50.5	49.5

7 Cartesian coordinates (Å) of the optimized structures at the B3LYP-D3BJ/cc-pVDZ,LANL2DZ(f) level

$\mathbf{1}_E$

Atom X Y Z

1 C -1.0181 0.3787 0.0131

2 C -0.2812 1.5059 0.0290

3 H 0.8102 1.5017 -0.0371

4 C -0.3870 -0.9805 -0.1032

5 H 0.7103 -0.9328 -0.1658

6 H -0.6680 -1.6079 0.7607

7 H -0.7725 -1.5039 -0.9956

8 C -0.9509 2.8134 0.1356

9 O -2.1638 2.9683 0.2101

10 O -0.0769 3.8339 0.1409

11 C -0.6436 5.1643 0.2419

12 H -1.3281 5.3196 -0.6065

13 H -1.2370 5.2239 1.1674

14 B -2.5889 0.4205 0.1171

15 O -3.4001 0.3219 -0.9841

16 O -3.2569 0.3195 1.3103

17 C -4.7825 0.4248 -0.5085

18 C -4.6527 0.0013 1.0039

19 C -5.2065 1.8818 -0.7006

20 C -5.6494 -0.4968 -1.3557

21 C -4.8097 -1.5031 1.2307

22 C -5.5439 0.7804 1.9616

23 H -4.5656 2.5604 -0.1233

24 H -5.1036 2.1410 -1.7652

25 H -6.2565 2.0331 -0.4102

26 H -5.2668 -1.5255 -1.3612

27 H -6.6832 -0.5078 -0.9772

28 H -5.6711 -0.1324 -2.3936

29 H -4.5107 -1.7400 2.2625

30 H -5.8514 -1.8260 1.0892

31 H -4.1678 -2.0792 0.5481

32 H -5.3800 0.4270 2.9907

33 H -5.3278 1.8558 1.9284

34 H -6.6052 0.6261 1.7128

35 C 0.5069 6.1467 0.2356

36 H 1.0894 6.0634 -0.6950

37 H 0.1179 7.1737 0.3105

38 H 1.1808 5.9679 1.0878

1$_Z$

Atom X Y Z

1 C -0.9859 0.2637 0.1096

2 C -0.3940 1.4766 0.0128

3 H 0.6803 1.5389 -0.1725

4 C -2.4587 0.0573 0.3605

5 H -3.0602 0.4821 -0.4591

6 H -2.6933 -1.0112 0.4546

7 H -2.7858 0.5818 1.2712

8 C -1.0901 2.7723 0.1403

9 O -2.2840 2.9424 0.3297

10 O -0.2122 3.7937 0.0167

11 C -0.7660 5.1260 0.1218

12 H -1.5382 5.2504 -0.6536

13 H -1.2587 5.2281 1.1017

14 B -0.0649 -0.9918 -0.0502

15 O 1.2911 -0.9213 -0.2467

16 O -0.5460 -2.2739 -0.0040

17 C 1.7506 -2.2720 -0.5787

18 C 0.6122 -3.1719 0.0297

19 C 1.8277 -2.3428 -2.1045

20 C 3.1280 -2.4796 0.0345

21 C 0.8409 -3.5272 1.4994

22 C 0.2812 -4.4197 -0.7763

23 H 0.8378 -2.2016 -2.5628

24 H 2.4904 -1.5427 -2.4652

25 H 2.2348 -3.3077 -2.4398

26 H 3.1281 -2.2727 1.1123

27 H 3.4677 -3.5143 -0.1257

28 H 3.8525 -1.8052 -0.4458

29 H -0.0807 -3.9677 1.9072

30 H 1.6539 -4.2591 1.6118

31 H 1.0875 -2.6351 2.0936

32 H -0.5263 -4.9781 -0.2797

33 H -0.0479 -4.1709 -1.7932

34 H 1.1606 -5.0785 -0.8422

35 C 0.3752 6.1055 -0.0474

36 H 0.8555 5.9828 -1.0306

37 H -0.0049 7.1360 0.0267

38 H 1.1369 5.9598 0.7342

^{3}1

Atom X Y Z

1 C -1.2831 0.5983 0.6766

2 C -0.6177 1.6122 -0.1333

3 H -0.1142 1.3585 -1.0727

4 C -0.4892 -0.0917 1.7477

5 H -0.1349 0.6453 2.4940

6 H -1.0877 -0.8544 2.2647

7 H 0.4188 -0.5664 1.3325

8 C -0.6305 3.0063 0.2748

9 O -1.1824 3.4315 1.2859

10 O 0.0387 3.7984 -0.5976

11 C 0.0688 5.2073 -0.2762

12 H -0.9664 5.5768 -0.2015

13 H 0.5398 5.3367 0.7114

14 B -2.7899 0.3510 0.4980

15 O -3.5552 0.9927 -0.4507

16 O -3.5097 -0.5231 1.2817

17 C -4.9537 0.6994 -0.1394

18 C -4.8415 -0.6351 0.6856

19 C -5.4712 1.8781 0.6878

20 C -5.7289 0.5830 -1.4441

21 C -4.8231 -1.8873 -0.1929

22 C -5.8620 -0.7836 1.8053

23 H -4.9228 1.9714 1.6367

24 H -5.3241 2.8057 0.1154

25 H -6.5432 1.7734 0.9099

26 H -5.2722 -0.1482 -2.1234

27 H -6.7690 0.2801 -1.2482

28 H -5.7484 1.5589 -1.9518

29 H -4.5314 -2.7505 0.4232

30 H -5.8140 -2.0890 -0.6252

31 H -4.0964 -1.7892 -1.0128

32 H -5.7045 -1.7399 2.3262

33 H -5.7766 0.0263 2.5411

34 H -6.8843 -0.7823 1.3970

35 C 0.8447 5.9051 -1.3724

36 H 0.3593 5.7601 -2.3501

37 H 0.8921 6.9854 -1.1655

38 H 1.8738 5.5180 -1.4324

2$_E$

Atom X Y Z

1 C -0.9746 0.2685 -0.0741

2 C -0.4207 1.5030 0.0271

3 H 0.6621 1.6008 0.1047

4 C -2.4594 0.0243 -0.1241

5 H -3.0089 0.9545 -0.2889

6 H -2.7018 -0.7076 -0.9099

7 H -2.8035 -0.4092 0.8306

8 C -1.1302 2.7940 0.0585

9 O -2.3335 3.0040 0.0179

10 O -0.2255 3.7996 0.1446

11 C -0.7641 5.1406 0.1852

12 H -1.3605 5.3115 -0.7249

13 H -1.4432 5.2247 1.0484

14 C 0.4065 6.0948 0.2862

15 H 1.0743 5.9907 -0.5831

16 H 0.0393 7.1322 0.3190

17 H 0.9905 5.9047 1.2001

18 C -0.0933 -0.9280 -0.1196

19 C -0.5577 -2.1754 0.3411

20 C 1.2187 -0.8587 -0.6303

21 C 0.2672 -3.3018 0.3211

22 H -1.5684 -2.2675 0.7385

23 C 2.0390 -1.9858 -0.6594

24 H 1.5923 0.0821 -1.0361

25 C 1.5694 -3.2131 -0.1784

26 H -0.1122 -4.2542 0.6966

27 H 3.0481 -1.9080 -1.0692

28 H 2.2118 -4.0955 -0.2017

2$_Z$

Atom X Y Z

1 C -1.1610 0.4306 -0.0602

2 C -0.5047 1.6113 -0.0649

3 H 0.5625 1.6204 -0.2948

4 C -0.4323 -0.8409 -0.4052

5 H 0.6194 -0.6553 -0.6630

6 H -0.4790 -1.5468 0.4411

7 H -0.9213 -1.3453 -1.2553

8 C -1.0969 2.9451 0.1587

9 O -2.2707 3.2258 0.3256

10 O -0.1176 3.8824 0.1301

11 C -0.5430 5.2513 0.3170

12 H -1.2649 5.5100 -0.4737

13 H -1.0656 5.3321 1.2833

14 C 0.6947 6.1210 0.2644

15 H 1.2032 6.0221 -0.7073

16 H 0.4147 7.1766 0.4032

17 H 1.4040 5.8430 1.0595

18 C -2.5951 0.2606 0.3032

19 C -3.0583 0.6153 1.5805

20 C -3.4912 -0.3291 -0.6026

21 C -4.3872 0.3912 1.9410

22 H -2.3659 1.0653 2.2931

23 C -4.8277 -0.5347 -0.2487

24 H -3.1471 -0.6116 -1.5996

25 C -5.2788 -0.1796 1.0255

26 H -4.7303 0.6663 2.9406

27 H -5.5161 -0.9791 -0.9706

28 H -6.3203 -0.3494 1.3063

^{3}2

Atom X Y Z

1 C -1.4305 0.4930 -0.0738

2 C -0.6984 1.6479 0.4576

3 H -0.0136 1.5509 1.3075

4 C -0.7818 -0.2707 -1.1972

5 H 0.2664 0.0311 -1.3303

6 H -0.8050 -1.3591 -1.0206

7 H -1.3049 -0.0841 -2.1537

8 C -0.8043 2.9526 -0.1787

9 O -1.4943 3.1960 -1.1622

10 O -0.0419 3.8801 0.4482

11 C -0.0828 5.2130 -0.1106

12 H 0.2488 5.1675 -1.1603

13 H -1.1259 5.5674 -0.1066

14 C 0.8192 6.0864 0.7343

15 H 1.8546 5.7122 0.7192

16 H 0.8162 7.1146 0.3409

17 H 0.4725 6.1137 1.7790

18 C -2.7241 0.1574 0.4262

19 C -3.3226 0.9110 1.4790

20 C -3.4746 -0.9318 -0.1055

21 C -4.5826 0.5906 1.9677

22 H -2.7740 1.7528 1.9068

23 C -4.7356 -1.2421 0.3912

24 H -3.0588 -1.5296 -0.9168

25 C -5.3020 -0.4883 1.4301

26 H -5.0149 1.1849 2.7757

27 H -5.2893 -2.0814 -0.0355

28 H -6.2923 -0.7376 1.8155

3$_E$

Atom X Y Z

1 C -1.1078 0.7335 -0.0523

2 C -0.3849 1.8793 -0.1441

3 B -2.6371 0.5617 0.0860

4 O -3.1922 -0.6945 0.2110

5 O -3.5889 1.5605 0.1001

6 C -4.6412 -0.5548 0.0971

7 C -4.8638 0.9535 0.4791

8 C -4.9995 -0.8683 -1.3572

9 C -5.3015 -1.5579 1.0335

10 C -5.0260 1.1791 1.9835

11 C -5.9788 1.6528 -0.2861

12 H -4.5363 -0.1478 -2.0472

13 H -4.6255 -1.8720 -1.6077

14 H -6.0879 -0.8550 -1.5147

15 H -4.9328 -1.4561 2.0622

16 H -6.3940 -1.4226 1.0360

17 H -5.0862 -2.5812 0.6911

18 H -4.9644 2.2575 2.1911

19 H -5.9993 0.8126 2.3414

20 H -4.2308 0.6743 2.5516

21 H -6.0534 2.7003 0.0425

22 H -5.7950 1.6450 -1.3681

23 H -6.9459 1.1651 -0.0896

24 H -0.5462 -0.2074 -0.0634

25 C -1.0219 3.2456 -0.0736

26 H -0.7373 3.7581 0.8613

27 H -0.6705 3.8847 -0.8999

28 H -2.1138 3.1792 -0.1019

29 C 1.0959 1.8447 -0.3028

30 C 1.8950 2.9243 0.1218

31 C 1.7455 0.7421 -0.8946

32 C 3.2854 2.8899 -0.0091

33 H 1.4309 3.7989 0.5777

34 C 3.1326 0.7103 -1.0342

35 H 1.1529 -0.0914 -1.2740

36 C 3.9124 1.7829 -0.5868

37 H 3.8807 3.7359 0.3410

38 H 3.6078 -0.1533 -1.5044

39 H 4.9984 1.7587 -0.6967

3$_Z$

Atom X Y Z

1 C -1.1235 0.6643 0.7557

2 C -0.3910 1.7004 0.2843

3 B -2.6593 0.4809 0.7046

4 O -3.5131 1.0907 -0.1857

5 O -3.3107 -0.3869 1.5556

6 C -4.8765 0.8081 0.2512

7 C -4.6920 -0.5068 1.0919

8 C -5.3257 2.0057 1.0917

9 C -5.7607 0.6650 -0.9799

10 C -4.7613 -1.7789 0.2450

11 C -5.6041 -0.6259 2.3051

12 H -4.7055 2.1174 1.9931

13 H -5.2199 2.9207 0.4911

14 H -6.3771 1.9087 1.3995

15 H -5.3626 -0.0801 -1.6806

16 H -6.7802 0.3671 -0.6904

17 H -5.8234 1.6304 -1.5041

18 H -4.4179 -2.6304 0.8510

19 H -5.7891 -1.9837 -0.0888

20 H -4.1132 -1.7041 -0.6405

21 H -5.4010 -1.5706 2.8316

22 H -5.4496 0.2001 3.0111

23 H -6.6601 -0.6298 1.9938

24 H -0.5555 -0.1620 1.2022

25 C 1.1169 1.6884 0.3132

26 H 1.5307 1.7937 -0.7041

27 H 1.5017 2.5447 0.8930

28 H 1.5051 0.7571 0.7489

29 C -1.0128 2.9417 -0.2571

30 C -0.6332 3.4562 -1.5090

31 C -1.9718 3.6451 0.4912

32 C -1.2192 4.6210 -2.0111

33 H 0.1112 2.9285 -2.1085

34 C -2.5487 4.8161 -0.0024

35 H -2.2575 3.2697 1.4747

36 C -2.1788 5.3063 -1.2593

37 H -0.9234 4.9951 -2.9936

38 H -3.2900 5.3484 0.5975

39 H -2.6315 6.2207 -1.6483

^{3}**3**

Atom X Y Z

1 C -0.9863 0.3824 1.4503

2 C -0.1331 1.5713 1.3265

3 B -2.4102 0.3215 0.8796

4 O -3.2382 -0.7741 0.9955

5 O -2.9803 1.3620 0.1789

6 C -4.3803 -0.5426 0.1107

7 C -4.3873 1.0241 -0.0271

8 C -4.0661 -1.2613 -1.2030

9 C -5.6244 -1.1351 0.7578

10 C -5.1726 1.7245 1.0836

11 C -4.8159 1.5453 -1.3919

12 H -3.1732 -0.8375 -1.6860

13 H -3.8706 -2.3227 -0.9909

14 H -4.9089 -1.1978 -1.9068

15 H -5.7770 -0.7477 1.7733

16 H -6.5174 -0.9065 0.1559

17 H -5.5255 -2.2293 0.8181

18 H -4.9566 2.8023 1.0465

19 H -6.2563 1.5835 0.9595

20 H -4.8816 1.3502 2.0761

21 H -4.7851 2.6451 -1.3947

22 H -4.1557 1.1819 -2.1898

23 H -5.8470 1.2327 -1.6177

24 H -0.5856 -0.4858 1.9947

25 C -0.1966 2.5877 2.4374

26 H 0.8011 2.7832 2.8698

27 H -0.5827 3.5579 2.0740

28 H -0.8554 2.2484 3.2487

29 C 0.6875 1.7771 0.1768

30 C 1.5051 2.9369 0.0310

31 C 0.7141 0.8259 -0.8870

32 C 2.2907 3.1237 -1.1012

33 H 1.5160 3.6926 0.8169

34 C 1.5040 1.0230 -2.0123

35 H 0.0982 -0.0723 -0.8061

36 C 2.3005 2.1730 -2.1332

37 H 2.9062 4.0225 -1.1851

38 H 1.5020 0.2760 -2.8097

39 H 2.9191 2.3262 -3.0195

4$_E$

Atom X Y Z

1 C -0.9448 0.2529 0.2369

2 C -0.4205 1.4948 0.0741

3 H 0.6265 1.6075 -0.2047

4 C -2.3937 0.0096 0.5674

5 H -2.9117 -0.4326 -0.3004

6 H -2.4839 -0.7129 1.3930

7 H -2.9009 0.9416 0.8274

8 C -1.1208 2.7836 0.2159

9 O -2.2894 2.9919 0.5071

10 O -0.2500 3.7925 -0.0322

11 C -0.7818 5.1331 0.0654

12 H -1.6204 5.2350 -0.6416

13 H -1.1827 5.2831 1.0803

14 C 0.3472 6.0911 -0.2484

15 H 0.7354 5.9212 -1.2647

16 H -0.0162 7.1283 -0.1850

17 H 1.1756 5.9696 0.4668

18 C -0.0792 -0.9420 0.0654

19 C 1.3462 -0.8539 0.1627

20 C -0.6387 -2.1871 -0.1924

21 C 2.1448 -1.9585 -0.0098

22 H 1.8116 0.1008 0.4067

23 C 0.1593 -3.3453 -0.3866

24 H -1.7198 -2.3018 -0.2711

25 C 1.5847 -3.2356 -0.2960

26 C -0.4171 -4.6160 -0.6669

27 C 2.3811 -4.3965 -0.4850

28 C 0.3815 -5.7261 -0.8477

29 H -1.5043 -4.6969 -0.7361

30 C 1.7930 -5.6156 -0.7559

31 H -0.0705 -6.6964 -1.0624

32 H 3.2296 -1.8681 0.0814

33 H 3.4675 -4.3077 -0.4132

34 H 2.4135 -6.5022 -0.9012

4$_Z$

Atom X Y Z

1 C -1.2388 0.5652 -0.1798

2 C -0.4930 1.6906 -0.1156

3 H 0.5704 1.6328 -0.3549

4 C -0.6096 -0.7316 -0.6150

5 H 0.4531 -0.6087 -0.8650

6 H -0.7101 -1.4894 0.1799

7 H -1.1348 -1.1362 -1.4963

8 C -0.9833 3.0476 0.1923

9 O -2.1339 3.3997 0.3867

10 O 0.0598 3.9128 0.2103

11 C -0.2660 5.2953 0.4802

12 H -0.9783 5.6478 -0.2825

13 H -0.7689 5.3571 1.4583

14 C 1.0290 6.0784 0.4552

15 H 1.5164 5.9999 -0.5291

16 H 0.8257 7.1413 0.6575

17 H 1.7274 5.7071 1.2213

18 C -2.6786 0.4829 0.1900

19 C -3.1081 0.8519 1.4988

20 C -3.6068 -0.0222 -0.7037

21 C -4.4235 0.7153 1.8747

22 H -2.3725 1.2362 2.2056

23 C -4.9789 -0.1502 -0.3553

24 H -3.2997 -0.3144 -1.7103

25 C -5.3995 0.2207 0.9638

26 C -5.9470 -0.6444 -1.2734

27 C -6.7697 0.0803 1.3153

28 C -7.2704 -0.7672 -0.9039

29 H -5.6230 -0.9258 -2.2782

30 C -7.6857 -0.4018 0.4027

31 H -8.0047 -1.1472 -1.6169

32 H -4.7378 0.9916 2.8839

33 H -7.0857 0.3628 2.3224

34 H -8.7361 -0.5038 0.6830

^{3}4'

Atom X Y Z

1 C -0.9519 0.2117 0.0096

2 C -0.3982 1.5464 0.0028

3 H 0.6741 1.6713 -0.1277

4 C -2.4395 0.0029 0.1686

5 H -2.8596 -0.5354 -0.6979

6 H -2.6623 -0.6088 1.0592

7 H -2.9580 0.9596 0.2677

8 C -1.0990 2.8030 0.1537

9 O -2.3037 3.0003 0.3211

10 O -0.2077 3.8379 0.0862

11 C -0.7641 5.1597 0.2220

12 H -1.5172 5.3166 -0.5675

13 H -1.2842 5.2341 1.1911

14 C 0.3798 6.1462 0.1169

15 H 0.8867 6.0569 -0.8567

16 H -0.0023 7.1740 0.2159

17 H 1.1212 5.9736 0.9127

18 C -0.1086 -0.8974 -0.1332

19 C 1.3325 -0.8055 -0.2910

20 C -0.6569 -2.2568 -0.1301

21 C 2.1155 -1.9086 -0.4275

22 H 1.8118 0.1713 -0.3016

23 C 0.1457 -3.3953 -0.2704

24 H -1.7302 -2.3972 -0.0150

25 C 1.5704 -3.2505 -0.4248

26 C -0.4045 -4.7141 -0.2656

27 C 2.3684 -4.3853 -0.5645

28 C 0.4132 -5.8273 -0.4064

29 H -1.4840 -4.8318 -0.1487

30 C 1.8019 -5.6722 -0.5567

31 H -0.0243 -6.8274 -0.4005

32 H 3.1959 -1.7953 -0.5441

33 H 3.4481 -4.2667 -0.6812

34 H 2.4424 -6.5487 -0.6672

^{3}**4**

Atom X Y Z

1 C -1.5684 0.8157 -0.3571

2 C -0.7032 1.7853 0.3250

3 H -0.0545 1.4879 1.1565

4 C -0.9943 0.1284 -1.5672

5 H 0.0946 0.2658 -1.6237

6 H -1.2040 -0.9537 -1.5626

7 H -1.4289 0.5434 -2.4958

8 C -0.6187 3.1621 -0.1394

9 O -1.2476 3.6188 -1.0872

10 O 0.2461 3.8906 0.6059

11 C 0.3975 5.2767 0.2228

12 H 0.7473 5.3195 -0.8211

13 H -0.5889 5.7657 0.2635

14 C 1.3856 5.9061 1.1807

15 H 2.3617 5.3993 1.1271

16 H 1.5306 6.9663 0.9221

17 H 1.0184 5.8489 2.2172

18 C -2.9020 0.5921 0.0805

19 C -3.4205 1.2870 1.2361

20 C -3.7710 -0.2966 -0.5870

21 C -4.7008 1.0905 1.6750

22 H -2.7658 1.9812 1.7669

23 C -5.0991 -0.5130 -0.1493

24 H -3.4279 -0.8373 -1.4698

25 C -5.5869 0.1884 1.0052

26 C -5.9771 -1.4111 -0.8227

27 C -6.9161 -0.0323 1.4386

28 C -7.2690 -1.6056 -0.3764

29 H -5.6082 -1.9454 -1.7015

30 C -7.7453 -0.9119 0.7636

31 H -7.9301 -2.2973 -0.9026

32 H -5.0680 1.6276 2.5529

33 H -7.2792 0.5051 2.3180

34 H -8.7687 -1.0735 1.1077

TX

Atom X Y Z

1 C -9.1456 -0.3853 0.0081

2 C -7.7590 -0.4653 0.0198

3 C -6.9823 0.7096 0.0147

4 C -7.6078 1.9733 -0.0023

5 C -9.0183 2.0233 -0.0139

6 C -9.7835 0.8671 -0.0089

7 C -6.8786 3.2651 -0.0089

8 C -5.3952 3.2740 0.0032

9 C -4.5954 2.1128 0.0206

10 C -3.1911 2.2199 0.0308

11 H -2.5813 1.3143 0.0441

12 C -2.5864 3.4703 0.0239

13 C -3.3703 4.6369 0.0067

14 C -4.7527 4.5307 -0.0034

15 H -9.7364 -1.3034 0.0123

16 H -7.2646 -1.4387 0.0330

17 H -9.4816 3.0098 -0.0271

18 H -10.8730 0.9285 -0.0180

19 H -1.4969 3.5397 0.0319

20 H -2.8940 5.6187 0.0014

21 H -5.3890 5.4156 -0.0168

22 S -5.2359 0.4706 0.0310

23 O -7.5043 4.3295 -0.0246

^{3}TX

Atom X Y Z

1 C -9.1421 -0.4126 0.0085

2 C -7.7501 -0.4704 0.0200

3 C -6.9987 0.7167 0.0145

4 C -7.6118 2.0132 -0.0029

5 C -9.0257 2.0266 -0.0142

6 C -9.7680 0.8485 -0.0086

7 C -6.8795 3.2666 -0.0092

8 C -5.4282 3.2970 0.0026

9 C -4.5936 2.1306 0.0203

10 C -3.1909 2.2096 0.0307

11 H -2.6015 1.2906 0.0440

12 C -2.5643 3.4539 0.0242

13 C -3.3616 4.6142 0.0071

14 C -4.7520 4.5388 -0.0034

15 H -9.7313 -1.3294 0.0127

16 H -7.2340 -1.4324 0.0334

17 H -9.5138 2.9999 -0.0274

18 H -10.8587 0.9068 -0.0177

19 H -1.4766 3.5227 0.0322

20 H -2.8821 5.5957 0.0019

21 H -5.3645 5.4390 -0.0165

22 S -5.2609 0.5132 0.0304

23 O -7.5333 4.3783 -0.0251

Ir-A

Atom X Y Z

1 N -1.8879 -1.0683 0.2227

2 H 0.7437 -3.7588 3.6816

3 H -0.6975 3.7488 3.5577

4 H 4.0151 -1.0898 2.8483

5 H -4.0120 1.0518 3.0473

6 H 3.0908 -3.0194 4.0970

7 H -3.0145 3.0339 4.1487

8 H 0.6115 2.4978 1.8778

9 H -0.6683 -2.5842 2.0307

10 H 4.6501 0.6128 1.7193

11 H -4.7132 -0.7022 2.0398

12 H -5.3469 -2.7265 0.7365

13 H 3.4487 3.4467 -1.3109

14 H -3.6929 -3.6753 -0.9226

15 H 1.2308 2.3023 -1.3819

16 H -1.4857 -2.5371 -1.1822

17 C 0.3556 -2.2426 2.1936

18 C -0.4002 2.1660 2.1188

19 C 2.1884 -0.7395 1.7214

20 C -2.2573 0.6468 1.8285

21 C 1.1531 -2.9094 3.1290

22 C -1.1393 2.8760 3.0702

23 C 2.9883 -1.4105 2.6623

24 C -2.9987 1.3616 2.7848

25 C 2.4716 -2.4965 3.3660

26 C -2.4407 2.4772 3.4058

27 C 2.6498 0.4076 0.9378

28 C -2.7646 -0.5346 1.1284

29 C 3.9132 1.0084 1.0220

30 C -4.0193 -1.1299 1.3178

31 C -4.3715 -2.2605 0.5893

32 C 3.2539 2.5914 -0.6649

33 C -3.4609 -2.7906 -0.3306

34 C 2.0184 1.9608 -0.7128

35 C -2.2321 -2.1638 -0.4835

36 Ir -0.0885 -0.0856 0.0439

37 C 4.2194 2.1031 0.2216

38 H 5.2016 2.5734 0.2871

39 C -0.9379 1.0406 1.4708

40 C 1.4649 -2.2732 -1.6360

41 C 0.2417 -0.7279 -2.8689

42 C -0.6183 0.4229 -2.8660

43 C -1.0909 0.9535 -4.0902

44 C -0.6893 0.3316 -5.3215

45 C 0.1385 -0.7545 -5.3248

46 C 0.6291 -1.3161 -4.0967

47 C 1.4869 -2.4387 -4.0392

48 C 1.9053 -2.9117 -2.8087

49 H 2.5682 -3.7729 -2.7289

50 H 1.8096 -2.9186 -4.9645

51 H -1.0604 0.7502 -6.2582

52 H 0.4417 -1.2190 -6.2641

53 C -1.7501 2.0300 -1.6250

54 C -1.9405 2.0820 -4.0260

55 H -2.3265 2.5194 -4.9480

56 C -2.2705 2.6148 -2.7930

57 H -2.9245 3.4822 -2.7081

58 N -0.9427 0.9695 -1.6576

59 N 0.6524 -1.2163 -1.6619

60 H 1.7675 -2.6211 -0.6479

61 H -1.9826 2.4255 -0.6358

62 C 0.8503 -1.1480 1.4636

63 N 1.7184 0.9006 0.0641

^{3}Ir-A

Atom X Y Z

1 N -1.8819 -1.0789 0.2736

2 H 0.8629 -3.9040 3.5626

3 H -0.8208 3.8888 3.4348

4 H 4.1027 -1.1845 2.7387

5 H -4.1052 1.1435 2.9390

6 H 3.2119 -3.1597 3.9283

7 H -3.1431 3.1692 3.9784

8 H 0.5472 2.5840 1.8352

9 H -0.6048 -2.6754 1.9919

10 H 4.7307 0.5305 1.5831

11 H -4.8049 -0.6209 1.9027

12 H -5.3805 -2.6778 0.6197

13 H 3.3992 3.4538 -1.3049

14 H -3.6479 -3.6848 -0.9138

15 H 1.1538 2.3363 -1.2761

16 H -1.4049 -2.5736 -1.0737

17 C 0.4201 -2.3372 2.1478

18 C -0.4661 2.2566 2.0700

19 C 2.2511 -0.7952 1.6745

20 C -2.3229 0.6998 1.7823

21 C 1.2445 -3.0310 3.0298

22 C -1.2346 2.9931 2.9677

23 C 3.0721 -1.4956 2.5641

24 C -3.0875 1.4433 2.6871

25 C 2.5689 -2.6111 3.2383

26 C -2.5437 2.5874 3.2765

27 C 2.6858 0.3785 0.9128

28 C -2.8035 -0.5070 1.1047

29 C 3.9594 0.9552 0.9430

30 C -4.0731 -1.0779 1.2388

31 C -4.3928 -2.2265 0.5195

32 C 3.2265 2.5880 -0.6668

33 C -3.4375 -2.7893 -0.3305

34 C 1.9772 1.9785 -0.6608

35 C -2.1903 -2.1835 -0.4290

36 Ir -0.0855 -0.0857 0.1473

37 C 4.2323 2.0675 0.1512

38 H 5.2229 2.5232 0.1704

39 C -0.9828 1.0915 1.4639

40 C 1.4931 -2.2739 -1.5441

41 C 0.2343 -0.7115 -2.7817

42 C -0.6039 0.4110 -2.7783

43 C -1.0951 0.9680 -4.0037

44 C -0.6820 0.3368 -5.2334

45 C 0.1436 -0.7486 -5.2371

46 C 0.6420 -1.3235 -4.0114

47 C 1.4932 -2.4261 -3.9578

48 C 1.9287 -2.9037 -2.7000

49 H 2.5975 -3.7603 -2.6210

50 H 1.8175 -2.9078 -4.8819

51 H -1.0494 0.7543 -6.1734

52 H 0.4460 -1.2090 -6.1802

53 C -1.7747 2.0316 -1.5295

54 C -1.9402 2.0748 -3.9418

55 H -2.3268 2.5155 -4.8625

56 C -2.2879 2.6105 -2.6802

57 H -2.9493 3.4722 -2.5945

58 N -0.9411 0.9672 -1.5477

59 N 0.6563 -1.2118 -1.5533

60 H 1.8061 -2.6251 -0.5607

61 H -2.0197 2.4278 -0.5439

62 C 0.8951 -1.2014 1.4573

63 N 1.7141 0.9099 0.1125

Ir-B

Atom X Y Z

1 N 0.8061 -1.0838 -1.6597

2 N 1.0369 -1.0842 1.5244

3 N -1.8363 -1.0857 0.1327

4 H 0.6275 -0.8545 -5.0270

5 H -0.6425 0.8107 -4.9966

6 H 2.1149 -2.8385 -4.8519

7 H 2.7650 -3.6807 -2.5589

8 H -2.7323 3.6871 -2.5766

9 H 1.8687 -2.4723 -0.5557

10 H -1.8930 2.5957 -0.5237

11 H 0.8394 -3.6863 3.6642

12 H -0.8674 3.6909 3.6499

13 H 4.0363 -0.8459 3.0638

14 H -4.0094 0.8170 3.0449

15 H 3.1448 -2.8359 4.2574

16 H -3.1329 2.8057 4.2278

17 H 0.4957 2.5941 1.9036

18 H -0.4461 -2.4794 1.8846

19 H 4.6405 0.8262 1.9562

20 H -4.6675 -0.8513 1.9637

21 H -5.2567 -2.8386 0.5918

22 H 3.5899 3.7016 -1.0646

23 H -3.5922 -3.6853 -1.1119

24 H 1.3996 2.5990 -1.3771

25 H -1.4088 -2.4778 -1.3356

26 C 0.4452 -0.6051 -2.8856

27 C -0.4321 0.5711 -2.8449

28 C 0.9152 -1.2366 -4.0486

29 C -0.9120 1.1959 -4.0109

30 C 1.7484 -2.3458 -3.9498

31 C 2.1114 -2.8174 -2.6834

32 C -2.0847 2.8094 -2.6561

33 C 1.6176 -2.1524 -1.5674

34 C -1.6103 2.1902 -1.4972

35 C 0.5532 -2.1560 2.1772

36 C -0.4903 2.1907 2.1426

37 C 2.2760 -0.6010 1.8297

38 C -2.2472 0.5730 1.7931

39 C 1.2722 -2.8202 3.1638

40 C -1.2594 2.8128 3.1289

41 C 3.0474 -1.2314 2.8197

42 C -3.0197 1.2006 2.7879

43 C 2.5473 -2.3440 3.4879

44 C -2.5312 2.3203 3.4568

45 C 2.6775 0.5779 1.0526

46 C -2.7197 -0.6046 1.0548

47 C 3.9233 1.2087 1.2269

48 C -3.9624 -1.2354 1.2279

49 C -4.2918 -2.3464 0.4590

50 C 3.3364 2.8216 -0.4666

51 C -3.3744 -2.8206 -0.4853

52 C 2.0997 2.1963 -0.6425

53 C -2.1607 -2.1560 -0.6146

54 Ir 0.0018 0.0262 -0.0007

55 C 1.7233 1.0615 0.1061

56 C -0.7705 1.0579 -1.5454

57 C 4.2562 2.3304 0.4716

58 C -1.7369 2.3146 -3.9217

59 H 5.2232 2.8183 0.6094

60 H -2.1077 2.7975 -4.8280

61 C -0.9514 1.0583 1.4393

^{3}Ir-B

Atom X Y Z

1 N 0.7818 -1.0846 -1.6258

2 N 1.0091 -1.0610 1.5372

3 N -1.8318 -1.1015 0.1267

4 H 0.6189 -0.8459 -5.0470

5 H -0.5463 0.9564 -5.0150

6 H 2.0900 -2.8298 -4.8665

7 H 2.7534 -3.6660 -2.5458

8 H -2.7285 3.7381 -2.5360

9 H 1.8507 -2.4815 -0.5474

10 H -1.9306 2.5809 -0.4783

11 H 0.7689 -3.5968 3.7471

12 H -0.9286 3.6846 3.6662

13 H 4.0216 -0.8432 3.0497

14 H -4.0259 0.7655 3.0485

15 H 3.0960 -2.7815 4.3001

16 H -3.1776 2.7593 4.2398

17 H 0.4475 2.6226 1.9043

18 H -0.5024 -2.4146 1.9433

19 H 4.6532 0.7807 1.8916

20 H -4.6419 -0.9350 1.9922

21 H -5.1888 -2.9416 0.6349

22 H 3.6409 3.6154 -1.1804

23 H -3.5251 -3.7537 -1.0835

24 H 1.4164 2.5619 -1.4413

25 H -1.3683 -2.4857 -1.3341

26 C 0.4308 -0.5636 -2.8943

27 C -0.3743 0.5951 -2.8580

28 C 0.9115 -1.2268 -4.0679

29 C -0.8396 1.2925 -4.0192

30 C 1.7270 -2.3262 -3.9690

31 C 2.0979 -2.8047 -2.6714

32 C -2.0766 2.8656 -2.6080

33 C 1.5972 -2.1459 -1.5553

34 C -1.6282 2.2113 -1.4598

35 C 0.5042 -2.1020 2.2212

36 C -0.5311 2.2024 2.1453

37 C 2.2568 -0.5937 1.8224

38 C -2.2641 0.5581 1.7887

39 C 1.2159 -2.7537 3.2209

40 C -1.3071 2.8043 3.1396

41 C 3.0232 -1.2135 2.8224

42 C -3.0435 1.1658 2.7905

43 C 2.5035 -2.2969 3.5224

44 C -2.5697 2.2887 3.4646

45 C 2.6742 0.5627 1.0198

46 C -2.7134 -0.6342 1.0571

47 C 3.9368 1.1660 1.1639

48 C -3.9352 -1.2999 1.2487

49 C -4.2398 -2.4233 0.4879

50 C 3.3728 2.7558 -0.5606

51 C -3.3216 -2.8798 -0.4651

52 C 2.1193 2.1587 -0.7103

53 C -2.1277 -2.1856 -0.6115

54 Ir -0.0150 0.0596 -0.0240

55 C 1.7290 1.0531 0.0714

56 C -0.7727 1.0950 -1.5202

57 C 4.2883 2.2614 0.3792

58 C -1.6644 2.3903 -3.8875

59 H 5.2683 2.7275 0.4966

60 H -2.0112 2.9079 -4.7860

61 C -0.9816 1.0729 1.4367

Ir-C

Atom X Y Z

1 N 0.8007 -1.0918 -1.6595

2 N 1.0393 -1.0919 1.5207

3 N -1.8351 -1.0938 0.1377

4 H 0.6281 -0.8532 -5.0267

5 H -0.6292 0.8315 -4.9926

6 H 2.1039 -2.8449 -4.8537

7 H 2.7464 -3.6968 -2.5622

8 H 1.8537 -2.4892 -0.5571

9 H -1.8966 2.6131 -0.5183

10 H 0.8530 -3.7022 3.6509

11 H 4.0388 -0.8477 3.0595

12 H -4.0118 0.8357 3.0350

13 H 3.1552 -2.8444 4.2456

14 H -3.1185 2.8489 4.2059

15 H 0.5001 2.6130 1.9020

16 H -0.4381 -2.4947 1.8759

17 H 4.6331 0.8438 1.9597

18 H -4.6668 -0.8531 1.9675

19 H -5.2523 -2.8479 0.6067

20 H -3.5872 -3.7022 -1.0924

21 H 1.3932 2.6175 -1.3806

22 H -1.4052 -2.4937 -1.3228

23 C 0.4442 -0.6077 -2.8845

24 C -0.4260 0.5723 -2.8421

25 C 0.9122 -1.2388 -4.0486

26 C -0.8973 1.2081 -4.0040

27 C 1.7390 -2.3525 -3.9508

28 C 2.0978 -2.8297 -2.6851

29 C -2.0453 2.7961 -2.6449

30 C 1.6062 -2.1653 -1.5682

31 C -1.5978 2.1903 -1.4783

32 C 0.5597 -2.1682 2.1696

33 C -0.4814 2.1912 2.1217

34 C 2.2766 -0.6046 1.8271

35 C -2.2485 0.5735 1.7877

36 C 1.2818 -2.8326 3.1533

37 C -1.2696 2.7989 3.0900

38 C 3.0511 -1.2355 2.8143

39 C -3.0209 1.2113 2.7743

40 C 2.5553 -2.3521 3.4783

41 C -2.5385 2.3366 3.4381

42 C 2.6725 0.5778 1.0548

43 C -2.7190 -0.6081 1.0570

44 C 3.9113 1.2184 1.2318

45 C -3.9609 -1.2396 1.2338

46 C -4.2882 -2.3551 0.4710

47 C 3.3062 2.8067 -0.4410

48 C -3.3704 -2.8336 -0.4708

49 C 2.0750 2.1962 -0.6410

50 C -2.1577 -2.1687 -0.6039

51 Ir 0.0009 0.0189 -0.0003

52 C 1.7163 1.0583 0.1066

53 C -0.7675 1.0549 -1.5403

54 C 4.2428 2.3455 0.4837

55 C -1.7147 2.3325 -3.9180

56 H 5.1963 2.8599 0.6034

57 H -2.0921 2.8431 -4.8040

58 C -0.9499 1.0554 1.4340

59 F -0.7866 3.8966 3.7310

60 F 3.6174 3.9063 -1.1779

61 F -2.8427 3.8932 -2.5468

^{3}Ir-C

Atom X Y Z

1 N 0.8401 -1.0716 -1.6119

2 N 0.9851 -1.1089 1.4625

3 N -1.8514 -1.0474 0.1576

4 H 0.7194 -0.8797 -4.9820

5 H -0.6091 0.7483 -4.9914

6 H 2.2764 -2.8022 -4.7542

7 H 2.9148 -3.5951 -2.4419

8 H 1.9299 -2.4058 -0.4678

9 H -2.0324 2.5319 -0.5651

10 H 0.8383 -3.8572 3.4195

11 H 4.0435 -0.9817 2.9566

12 H -3.9840 0.9261 3.1050

13 H 3.1836 -3.0556 4.0114

14 H -3.0446 2.9410 4.2092

15 H 0.5414 2.6518 1.8565

16 H -0.4780 -2.5471 1.7538

17 H 4.5823 0.8874 2.0524

18 H -4.6431 -0.8330 2.0875

19 H -5.2812 -2.7847 0.6943

20 H -3.6793 -3.5837 -1.1087

21 H 1.4000 2.6186 -1.3828

22 H -1.4910 -2.4041 -1.3612

23 C 0.4903 -0.6140 -2.8460

24 C -0.4210 0.5349 -2.8353

25 C 1.0024 -1.2392 -3.9941

26 C -0.9087 1.1271 -4.0134

27 C 1.8744 -2.3142 -3.8649

28 C 2.2315 -2.7589 -2.5871

29 C -2.1602 2.6756 -2.6978

30 C 1.6907 -2.1054 -1.4873

31 C -1.7010 2.1106 -1.5143

32 C 0.5251 -2.2393 2.0512

33 C -0.4404 2.2506 2.1062

34 C 2.2541 -0.6230 1.7939

35 C -2.2570 0.6204 1.8070

36 C 1.2608 -2.9603 2.9673

37 C -1.2061 2.8745 3.0758

38 C 3.0439 -1.3445 2.7162

39 C -2.9969 1.2854 2.8124

40 C 2.5668 -2.5007 3.3031

41 C -2.4813 2.4111 3.4399

42 C 2.6403 0.5851 1.1028

43 C -2.7251 -0.5567 1.1145

44 C 3.8758 1.2468 1.3024

45 C -3.9660 -1.2002 1.3166

46 C -4.3232 -2.2869 0.5380

47 C 3.3012 2.8227 -0.4092

48 C -3.4336 -2.7392 -0.4655

49 C 2.0728 2.2058 -0.6298

50 C -2.2189 -2.0868 -0.6128

51 Ir -0.0246 0.0655 0.0448

52 C 1.7059 1.0893 0.1319

53 C -0.8068 1.0273 -1.5552

54 C 4.2088 2.3684 0.5514

55 C -1.7826 2.2090 -3.9559

56 H 5.1541 2.8933 0.6950

57 H -2.1696 2.6864 -4.8560

58 C -0.9439 1.1165 1.4356

59 F -0.7186 3.9741 3.7072

60 F 3.6301 3.9188 -1.1473

61 F -3.0119 3.7287 -2.6282

Ir-D

Atom X Y Z

1 N 0.8049 -1.0866 -1.6553

2 N 1.0329 -1.0865 1.5226

3 N -1.8338 -1.0889 0.1317

4 H 0.6692 -0.8783 -5.0217

5 H 2.1561 -2.8570 -4.8145

6 H 2.7782 -3.6867 -2.5087

7 H 1.8524 -2.4659 -0.5274

8 H -1.9062 2.5759 -0.4816

9 H 0.7898 -3.6905 3.6540

10 H 4.0139 -0.8729 3.0919

11 H 3.0947 -2.8555 4.2722

12 H -3.0807 2.8462 4.2205

13 H 0.5350 2.5773 1.8899

14 H -0.4641 -2.4707 1.8618

15 H -4.6818 -0.8806 1.9316

16 H -5.2441 -2.8615 0.5430

17 H -3.5576 -3.6916 -1.1479

18 H 1.3655 2.5799 -1.4076

19 H -1.3802 -2.4693 -1.3386

20 C 0.4568 -0.6119 -2.8886

21 C -0.4233 0.5625 -2.8418

22 C 0.9445 -1.2528 -4.0411

23 C -0.9264 1.2353 -3.9663

24 C 1.7782 -2.3604 -3.9193

25 C 2.1257 -2.8251 -2.6482

26 C -2.0751 2.7920 -2.6026

27 C 1.6157 -2.1531 -1.5443

28 C -1.6132 2.1718 -1.4503

29 C 0.5334 -2.1553 2.1671

30 C -0.4503 2.1730 2.1203

31 C 2.2735 -0.6091 1.8398

32 C -2.2493 0.5621 1.7864

33 C 1.2351 -2.8269 3.1605

34 C -1.2183 2.7938 3.0953

35 C 3.0283 -1.2493 2.8384

36 C -2.9725 1.2356 2.7832

37 C 2.5080 -2.3593 3.4973

38 C -2.4891 2.3503 3.4529

39 C 2.6708 0.5673 1.0560

40 C -2.7285 -0.6137 1.0489

41 C 3.8939 1.2439 1.1853

42 C -3.9699 -1.2554 1.2035

43 C -4.2803 -2.3643 0.4220

44 C 3.2849 2.8008 -0.4902

45 C -3.3528 -2.8291 -0.5140

46 C 2.0582 2.1770 -0.6691

47 C -2.1424 -2.1562 -0.6252

48 Ir 0.0004 0.0130 -0.0004

49 C 1.7183 1.0494 0.0994

50 C -0.7748 1.0462 -1.5390

51 C 4.2301 2.3595 0.4324

52 C -1.7496 2.3489 -3.8821

53 H 5.1892 2.8578 0.5620

54 H -2.1196 2.8443 -4.7780

55 C -0.9456 1.0465 1.4394

56 F -0.7215 3.8806 3.7345

57 F 3.5880 3.8886 -1.2394

58 F -2.8784 3.8778 -2.4915

59 F -4.2138 0.8102 3.1432

60 F -0.6174 0.8102 -5.2214

61 F 4.8262 0.8207 2.0815

^{3}Ir-D

Atom X Y Z

1 N 0.8171 -1.0663 -1.6649

2 N 1.0136 -1.0913 1.5253

3 N -1.7761 -1.0958 0.1203

4 H 0.6535 -0.8646 -5.0292

5 H 2.1910 -2.8043 -4.8281

6 H 2.8528 -3.6123 -2.5266

7 H 1.9071 -2.4153 -0.5397

8 H -1.9182 2.5752 -0.4728

9 H 0.7356 -3.6976 3.6459

10 H 3.9828 -0.8999 3.1158

11 H 3.0390 -2.8767 4.2833

12 H -3.0876 2.8921 4.1655

13 H 0.5636 2.5814 1.8781

14 H -0.4966 -2.4637 1.8390

15 H -4.6509 -0.9430 2.0112

16 H -5.2082 -2.9105 0.6180

17 H -3.5355 -3.6750 -1.1589

18 H 1.4167 2.5681 -1.4209

19 H -1.3784 -2.4581 -1.3758

20 C 0.4506 -0.5999 -2.8945

21 C -0.4470 0.5612 -2.8424

22 C 0.9446 -1.2299 -4.0499

23 C -0.9765 1.2190 -3.9637

24 C 1.8073 -2.3155 -3.9311

25 C 2.1772 -2.7682 -2.6621

26 C -2.1256 2.7738 -2.5947

27 C 1.6573 -2.1090 -1.5553

28 C -1.6414 2.1670 -1.4442

29 C 0.4996 -2.1589 2.1593

30 C -0.4267 2.1875 2.1051

31 C 2.2539 -0.6196 1.8505

32 C -2.2708 0.5555 1.7581

33 C 1.1889 -2.8356 3.1572

34 C -1.1975 2.8190 3.0710

35 C 2.9963 -1.2676 2.8532

36 C -3.0003 1.2786 2.7620

37 C 2.4618 -2.3751 3.5047

38 C -2.4973 2.3756 3.4089

39 C 2.6688 0.5551 1.0707

40 C -2.7099 -0.5986 1.0856

41 C 3.9024 1.2122 1.2045

42 C -3.9558 -1.2967 1.2548

43 C -4.2625 -2.3843 0.4825

44 C 3.3344 2.7654 -0.4909

45 C -3.3244 -2.8245 -0.5116

46 C 2.0980 2.1605 -0.6743

47 C -2.1189 -2.1455 -0.6373

48 Ir -0.0077 0.0330 -0.0023

49 C 1.7359 1.0494 0.1040

50 C -0.7930 1.0510 -1.5417

51 C 4.2622 2.3156 0.4445

52 C -1.8119 2.3229 -3.8741

53 H 5.2283 2.7991 0.5787

54 H -2.1990 2.8080 -4.7685

55 C -0.9228 1.0728 1.4186

56 F -0.7157 3.9058 3.7239

57 F 3.6620 3.8401 -1.2462

58 F -2.9376 3.8503 -2.4802

59 F -4.2555 0.8714 3.1013

60 F -0.6810 0.7884 -5.2180

61 F 4.8198 0.7820 2.1108

Ir-E

Atom X Y Z

1 N 0.7767 -1.0277 -1.6510

2 N 1.0113 -1.0823 1.5047

3 N -1.0035 1.0317 1.4424

4 N -1.8293 -1.1047 0.1110

5 H 0.6676 -0.7921 -5.0228

6 H -0.7002 0.9288 -4.9917

7 H 2.1638 -2.7712 -4.8128

8 H 2.7576 -3.6111 -2.5085

9 H -2.7628 3.6578 -2.6436

10 H 1.8206 -2.4198 -0.5237

11 H -1.9711 2.6134 -0.5375

12 H 0.7908 -3.6158 3.7136

13 H -0.7704 3.6430 3.5582

14 H 3.9736 -0.7652 3.1069

15 H -3.9433 0.7591 3.0908

16 H 3.0669 -2.7245 4.3387

17 H -3.0354 2.7639 4.2486

18 H 0.4626 2.4676 1.7417

19 H -0.4646 -2.4917 1.8697

20 H 4.6187 0.8817 1.8808

21 H -4.5931 -0.9121 2.0482

22 H -5.1999 -2.9052 0.6935

23 H 3.6959 3.5731 -1.1360

24 H -3.5884 -3.7226 -1.0673

25 H 1.4665 2.5551 -1.5071

26 H -1.4325 -2.4955 -1.3737

27 C 0.4430 -0.5570 -2.8896

28 C -0.4476 0.6095 -2.8466

29 C 0.9356 -1.1750 -4.0394

30 C -0.9331 1.2428 -3.9760

31 C 1.7734 -2.2815 -3.9204

32 C 2.1053 -2.7502 -2.6482

33 C -2.1058 2.7899 -2.6475

34 C 1.5904 -2.0952 -1.5361

35 C -1.6517 2.1902 -1.4885

36 C 0.5196 -2.1387 2.1746

37 C -0.5127 2.1183 2.0717

38 C 2.2371 -0.5867 1.8285

39 C -2.2264 0.5418 1.8022

40 C 1.2264 -2.7602 3.1989

41 C -1.2106 2.7678 3.0823

42 C 2.9946 -1.1658 2.8487

43 C -2.9698 1.1561 2.8117

44 C 2.4850 -2.2633 3.5402

45 C -2.4607 2.2787 3.4597

46 C 2.6415 0.5702 1.0099

47 C -2.6878 -0.6451 1.0592

48 C 3.8684 1.1946 1.1576

49 C -3.9103 -1.2814 1.2861

50 C -4.2494 -2.3985 0.5251

51 C 3.3524 2.7213 -0.5521

52 C -3.3614 -2.8548 -0.4492

53 C 2.1153 2.1345 -0.7410

54 C -2.1592 -2.1777 -0.6275

55 Ir -0.0148 0.0167 -0.0522

56 C 1.7054 1.0370 0.0374

57 C -0.8016 1.0704 -1.5432

58 N 4.2083 2.2531 0.3872

59 N -1.7483 2.3174 -3.8673

60 C -2.2316 2.9724 -5.0989

61 H -1.3750 3.3837 -5.6477

62 H -2.7544 2.2328 -5.7177

63 H -2.9184 3.7782 -4.8243

64 C 5.5261 2.8881 0.5898

65 H 5.5880 3.2644 1.6183

66 H 6.3136 2.1449 0.4139

67 H 5.6323 3.7170 -0.1160

^{3}Ir-E

Atom X Y Z

1 N 0.7904 -1.0280 -1.6604

2 N 1.0248 -1.0815 1.5045

3 N -0.9631 1.0380 1.4213

4 N -1.7876 -1.1143 0.0945

5 H 0.6578 -0.7954 -5.0316

6 H -0.7272 0.9122 -4.9921

7 H 2.1734 -2.7602 -4.8294

8 H 2.7915 -3.5918 -2.5286

9 H -2.7730 3.6454 -2.6341

10 H 1.8550 -2.4082 -0.5382

11 H -1.9551 2.6108 -0.5310

12 H 0.7932 -3.6071 3.7205

13 H -0.7707 3.5985 3.6015

14 H 3.9828 -0.7639 3.1140

15 H -4.0148 0.8054 3.0371

16 H 3.0691 -2.7183 4.3478

17 H -3.0923 2.7692 4.2279

18 H 0.4869 2.4499 1.7986

19 H -0.4553 -2.4853 1.8670

20 H 4.6347 0.8778 1.8837

21 H -4.6205 -0.9005 2.0576

22 H -5.2320 -2.8748 0.6980

23 H 3.7207 3.5716 -1.1336

24 H -3.6087 -3.6961 -1.0742

25 H 1.4885 2.5578 -1.5069

26 H -1.4372 -2.5111 -1.3739

27 C 0.4444 -0.5611 -2.8967

28 C -0.4517 0.6013 -2.8486

29 C 0.9350 -1.1751 -4.0495

30 C -0.9509 1.2294 -3.9754

31 C 1.7843 -2.2735 -3.9348

32 C 2.1297 -2.7375 -2.6645

33 C -2.1137 2.7794 -2.6411

34 C 1.6156 -2.0866 -1.5495

35 C -1.6463 2.1855 -1.4843

36 C 0.5286 -2.1348 2.1755

37 C -0.4998 2.0905 2.0870

38 C 2.2500 -0.5855 1.8301

39 C -2.2518 0.5195 1.7619

40 C 1.2314 -2.7541 3.2037

41 C -1.2193 2.7404 3.1041

42 C 3.0039 -1.1634 2.8537

43 C -3.0247 1.1849 2.7951

44 C 2.4901 -2.2582 3.5465

45 C -2.5154 2.2689 3.4506

46 C 2.6570 0.5710 1.0115

47 C -2.6757 -0.6040 1.0731

48 C 3.8855 1.1925 1.1601

49 C -3.9450 -1.2738 1.2914

50 C -4.2808 -2.3672 0.5389

51 C 3.3746 2.7205 -0.5502

52 C -3.3786 -2.8343 -0.4502

53 C 2.1361 2.1364 -0.7401

54 C -2.1492 -2.1652 -0.6236

55 Ir -0.0003 0.0193 -0.0550

56 C 1.7238 1.0404 0.0381

57 C -0.7954 1.0673 -1.5447

58 N 4.2282 2.2502 0.3899

59 N -1.7674 2.3022 -3.8623

60 C -2.2643 2.9518 -5.0916

61 H -1.4138 3.3624 -5.6502

62 H -2.7917 2.2088 -5.7024

63 H -2.9497 3.7574 -4.8130

64 C 5.5473 2.8822 0.5939

65 H 5.6093 3.2572 1.6229

66 H 6.3332 2.1375 0.4176

67 H 5.6557 3.7117 -0.1109

Ru

Atom X Y Z

1 Ru -0.0332 -0.0934 -0.0163

2 C 1.4591 -2.3037 -1.6003

3 C 0.2689 -0.7438 -2.8440

4 C -0.5632 0.4207 -2.8387

5 C -1.0299 0.9658 -4.0571

6 C -0.6515 0.3289 -5.2888

7 C 0.1469 -0.7798 -5.2941

8 C 0.6338 -1.3505 -4.0681

9 C 1.4627 -2.4940 -4.0053

10 C 1.8733 -2.9641 -2.7705

11 H 2.5133 -3.8417 -2.6841

12 H 1.7694 -2.9920 -4.9263

13 H -1.0177 0.7533 -6.2248

14 H 0.4296 -1.2552 -6.2344

15 C -1.6434 2.0477 -1.5806

16 C -1.8476 2.1167 -3.9834

17 H -2.2289 2.5698 -4.8996

18 C -2.1517 2.6515 -2.7442

19 H -2.7798 3.5369 -2.6494

20 N -0.8659 0.9628 -1.6191

21 N 0.6742 -1.2239 -1.6283

22 H 1.7635 -2.6582 -0.6162

23 H -1.8650 2.4523 -0.5937

24 N 0.9902 -1.1586 1.4645

25 C 2.2516 -0.6825 1.6983

26 C 0.5571 -2.1952 2.1863

27 C 2.6811 0.4339 0.9123

28 C 3.1181 -1.2484 2.6619

29 C 1.3525 -2.8147 3.1664

30 H -0.4525 -2.5461 1.9756

31 C 3.9756 0.9735 1.0931

32 N 1.7873 0.9369 0.0063

33 C 4.4289 -0.6830 2.8289

34 C 2.6324 -2.3474 3.4070

35 H 0.9448 -3.6582 3.7228

36 C 4.8401 0.3808 2.0766

37 C 4.3389 2.0754 0.2853

38 C 2.1595 1.9764 -0.7446

39 H 5.0924 -1.1252 3.5735

40 H 3.2681 -2.8134 4.1612

41 H 5.8372 0.8026 2.2103

42 C 3.4286 2.5711 -0.6311

43 H 5.3287 2.5217 0.3917

44 H 1.4240 2.3514 -1.4554

45 H 3.6748 3.4184 -1.2705

46 N -1.8477 -1.1154 0.1933

47 C -2.6661 -0.5711 1.1456

48 C -2.2809 -2.1822 -0.4830

49 C -2.1753 0.5761 1.8466

50 C -3.9425 -1.0974 1.4512

51 C -3.5374 -2.7663 -0.2442

52 H -1.6056 -2.5881 -1.2355

53 C -2.9612 1.1846 2.8523

54 N -0.9372 1.0383 1.4919

55 C -4.7254 -0.4606 2.4747

56 C -4.3705 -2.2303 0.7218

57 H -3.8349 -3.6373 -0.8274

58 C -4.2549 0.6318 3.1469

59 C -2.4166 2.3114 3.5101

60 C -0.4469 2.1019 2.1332

61 H -5.7091 -0.8724 2.7043

62 H -5.3488 -2.6678 0.9263

63 H -4.8564 1.1071 3.9231

64 C -1.1601 2.7637 3.1482

65 H -2.9891 2.8102 4.2934

66 H 0.5420 2.4403 1.8263

67 H -0.7085 3.6278 3.6347

^{3}Ru

Atom X Y Z

1 Ru -0.0057 -0.1080 0.0394

2 C 1.6111 -2.2087 -1.6311

3 C 0.2764 -0.7257 -2.8285

4 C -0.6243 0.3839 -2.7885

5 C -1.1678 0.9017 -3.9859

6 C -0.7873 0.2992 -5.2337

7 C 0.0822 -0.7541 -5.2730

8 C 0.6422 -1.2991 -4.0673

9 C 1.5455 -2.3866 -4.0348

10 C 2.0280 -2.8355 -2.8181

11 H 2.7261 -3.6696 -2.7589

12 H 1.8543 -2.8600 -4.9679

13 H -1.2100 0.7041 -6.1540

14 H 0.3665 -1.2037 -6.2251

15 C -1.7757 1.9281 -1.4783

16 C -2.0612 1.9919 -3.8727

17 H -2.5046 2.4222 -4.7717

18 C -2.3625 2.4984 -2.6211

19 H -3.0477 3.3365 -2.4999

20 N -0.9252 0.9032 -1.5614

21 N 0.7532 -1.1871 -1.6348

22 H 1.9718 -2.5456 -0.6598

23 H -1.9859 2.3058 -0.4790

24 N 1.0117 -1.1507 1.5208

25 C 2.2840 -0.6937 1.7346

26 C 0.5468 -2.1618 2.2601

27 C 2.7262 0.4052 0.9366

28 C 3.1416 -1.2635 2.7013

29 C 1.3361 -2.7815 3.2423

30 H -0.4742 -2.4830 2.0577

31 C 4.0319 0.9201 1.0982

32 N 1.8363 0.9160 0.0339

33 C 4.4646 -0.7230 2.8524

34 C 2.6297 -2.3392 3.4635

35 H 0.9148 -3.6050 3.8175

36 C 4.8917 0.3224 2.0824

37 C 4.4044 2.0037 0.2691

38 C 2.2137 1.9334 -0.7404

39 H 5.1238 -1.1677 3.5988

40 H 3.2574 -2.8097 4.2215

41 H 5.8979 0.7254 2.2036

42 C 3.4960 2.5036 -0.6472

43 H 5.4028 2.4340 0.3582

44 H 1.4764 2.3093 -1.4494

45 H 3.7532 3.3363 -1.3007

46 N -1.8076 -1.1370 0.1956

47 C -2.6679 -0.5256 1.1004

48 C -2.2441 -2.1969 -0.4975

49 C -2.1853 0.5958 1.7763

50 C -3.9901 -1.0262 1.3312

51 C -3.5242 -2.7309 -0.3253

52 H -1.5404 -2.6397 -1.2032

53 C -2.9752 1.2550 2.7599

54 N -0.8878 1.0285 1.4581

55 C -4.7908 -0.3390 2.3055

56 C -4.4015 -2.1434 0.5993

57 H -3.8183 -3.6019 -0.9092

58 C -4.3054 0.7428 2.9881

59 C -2.4124 2.3371 3.4458

60 C -0.3511 2.0626 2.1889

61 H -5.8014 -0.7045 2.4969

62 H -5.4021 -2.5518 0.7518

63 H -4.9252 1.2444 3.7338

64 C -1.0685 2.7245 3.1540

65 H -2.9905 2.8648 4.2050

66 H 0.6690 2.3469 1.9351

67 H -0.6023 3.5525 3.6875

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