

Table 1: Molecular orbital energy and fractional orbital mixing (%) of ETRP.

Mol. Orbital	Energy / eV	Ru ^{II}	Cl ⁻	Cl-Phen	Pyridyl	Porphyrin
469	-4.70	0.06	0.00	5.68	2.87	91.38
468	-4.85	0.54	0.01	99.40	0.05	0.00
467	-4.93	0.55	0.01	99.23	0.18	0.04
466	-4.93	0.56	0.01	99.16	0.22	0.05
465	-4.97	1.13	0.03	98.74	0.09	0.01
464	-5.03	0.56	0.01	99.16	0.22	0.05
463	-5.08	1.15	0.03	98.60	0.22	0.01
462	-5.10	1.19	0.03	98.52	0.26	0.01
461	-5.18	1.17	0.03	98.52	0.27	0.01
460	-5.30	1.38	0.03	97.25	1.30	0.05
459	-5.38	1.11	0.03	98.78	0.07	0.00
458	-5.38	1.06	0.02	98.87	0.04	0.00
457	-5.48	1.08	0.03	98.85	0.04	0.00
456	-5.60	0.26	0.09	1.86	94.09	3.71
455	-5.62	0.19	0.11	2.46	90.43	6.82
454	-5.64	0.04	0.10	0.66	98.20	1.00
453	-5.68	0.55	0.08	7.36	76.55	15.46
452	-5.72	0.47	0.05	5.71	78.66	15.11
451	-5.92	3.35	0.07	9.79	79.01	7.77
450	-5.98	3.45	0.07	11.11	77.62	7.75
449	-6.05	3.24	0.06	9.50	79.28	7.91
448	-6.13	2.89	0.16	88.89	6.95	1.12
447	-6.20	0.65	0.02	99.06	0.23	0.04
446	-6.23	2.92	0.15	91.13	4.65	1.15
445	-6.25	2.99	0.15	90.51	5.26	1.08
444	-6.32	1.10	0.06	98.69	0.14	0.00
443	-6.33	3.03	0.15	91.05	4.46	1.31
442	-6.34	1.02	0.06	98.78	0.13	0.00
441	-6.42	1.03	0.06	98.77	0.14	0.00
440	-6.45	3.26	0.08	86.51	5.71	4.44
439	-6.52	3.27	0.06	88.43	4.49	3.75
438	-6.54	3.28	0.07	89.55	3.99	3.11
437	-6.55	1.89	0.11	74.19	13.31	10.50
436	-6.59	1.43	0.08	72.35	16.00	10.14
435	-6.62	1.14	0.05	97.81	0.69	0.31
434	-6.63	2.68	0.06	95.92	0.92	0.41
433	-6.63	1.83	0.07	88.07	6.27	3.76
432	-6.72	1.02	0.04	97.31	1.10	0.53
431	-7.79	0.42	0.02	17.13	7.89	74.54
430 (LUMO)	-7.85	0.69	0.03	25.90	12.56	60.82
429 (HOMO)	-12.02	67.53	8.62	17.40	4.10	2.36
428	-12.14	68.45	7.88	14.89	4.61	4.17
427	-12.18	73.42	8.62	13.72	3.55	0.69
426	-12.19	77.25	11.64	11.00	0.10	0.00
425	-12.25	71.32	8.44	14.28	3.66	2.29
424	-12.27	73.43	11.09	14.73	0.65	0.10