

Table 1: continued

Mol. Orbital	Energy / eV	Ru ^{II}	Cl ⁻	Cl-Phen	Pyridyl	Porphyrin
423	-12.28	74.87	11.82	13.08	0.21	0.03
422	-12.37	74.71	11.75	13.01	0.22	0.30
421	-12.43	69.67	1.99	16.66	4.94	6.74
420	-12.51	68.26	0.54	18.51	5.46	7.23
419	-12.58	79.82	0.07	14.22	5.08	0.81
418	-12.65	73.94	0.16	16.09	5.30	4.51
417	-12.79	44.88	0.58	25.09	8.04	21.41
416	-12.92	0.70	0.02	0.97	2.10	96.20
415	-13.58	3.08	2.99	93.87	0.06	0.00
414	-13.69	3.52	2.67	93.67	0.13	0.01
413	-13.71	3.39	2.52	93.93	0.14	0.02
412	-13.79	3.46	2.53	93.86	0.14	0.02
411	-14.01	3.17	0.42	95.48	0.82	0.10
410	-14.09	4.54	0.88	94.19	0.36	0.03
409	-14.09	4.74	0.85	94.08	0.31	0.02
408	-14.18	4.70	0.83	94.14	0.30	0.03
407	-14.28	0.20	0.82	98.90	0.07	0.00
406	-14.38	0.31	1.48	98.13	0.08	0.01
405	-14.40	0.30	1.34	98.27	0.08	0.01
404	-14.48	0.33	1.32	98.26	0.08	0.01
403	-14.61	0.28	0.73	98.80	0.15	0.04
402	-14.68	0.25	0.90	98.67	0.12	0.05
401	-14.69	0.24	0.84	96.37	0.41	2.14
400	-14.71	0.13	0.25	2.79	8.87	87.96
399	-14.75	0.09	0.51	0.29	8.90	90.22
398	-14.78	0.28	0.77	98.81	0.10	0.05
397	-14.98	0.85	4.88	10.74	44.86	38.67
396	-15.11	1.38	20.09	7.60	51.56	19.37
395	-15.17	1.60	20.18	6.25	58.31	13.67
394	-15.21	1.64	24.19	7.92	59.35	6.90
393	-15.22	1.49	17.96	10.46	42.42	27.67
392	-15.33	0.68	8.60	4.48	4.70	81.53
391	-15.38	0.64	10.34	6.52	10.29	72.20
390	-15.42	4.91	52.27	28.13	9.92	4.77
389	-15.46	1.29	24.27	12.86	25.76	35.81