Electronic supplementary information (ESI)

Glutathione binding to dirhodium tetraacetate: a spectroscopic, mass spectral and computational study of possible deactivation processes of an anti-tumour compound

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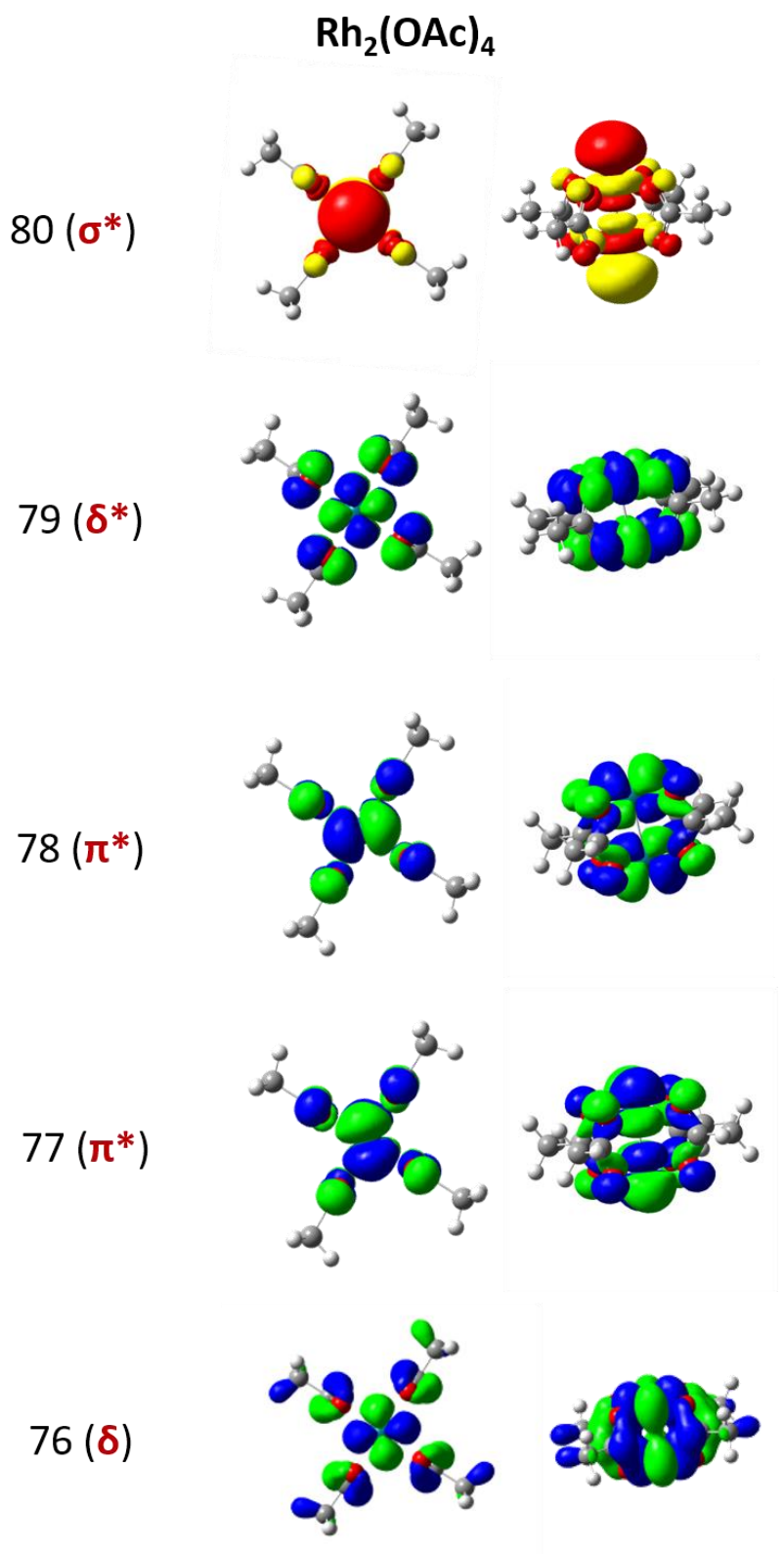

Fig S1. Expanded views of $Rh_2(OAc)_4$ molecular orbital surfaces, part 1.

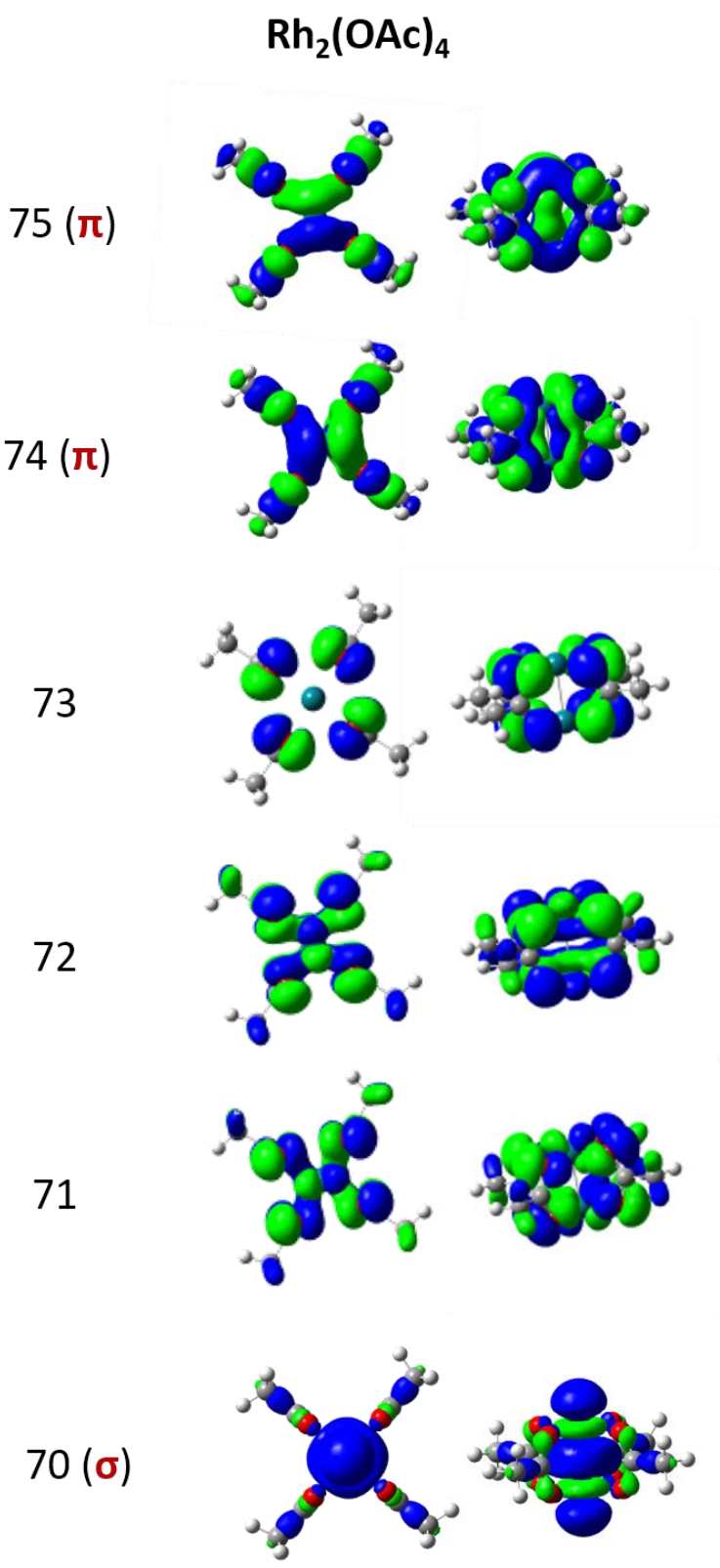

Fig S2. Expanded views of $Rh_2(OAc)_4$ molecular orbital surfaces, part 2.

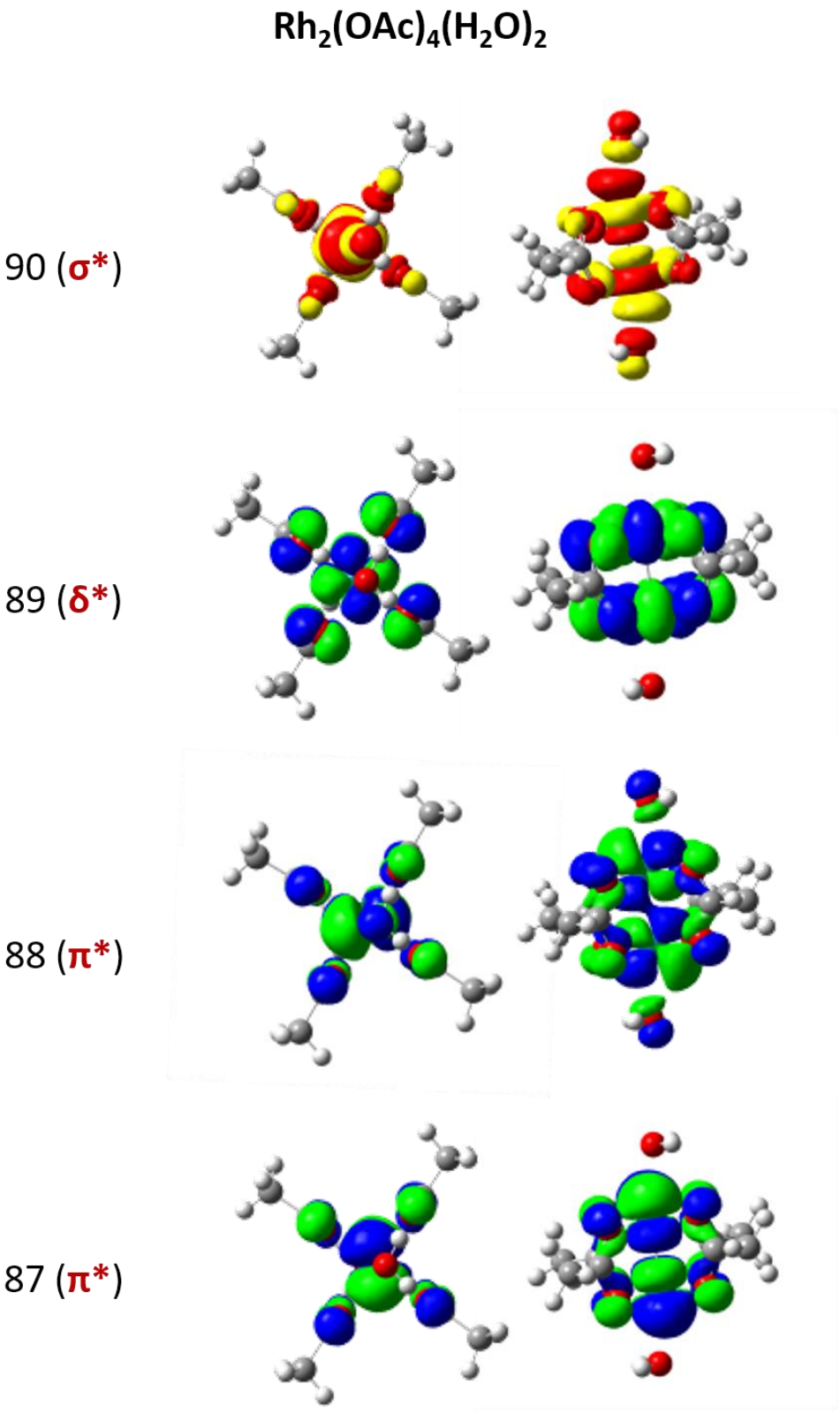

Fig S3. Expanded views of $Rh_2(OAc)_4(H_2O)_2$ molecular orbital surfaces, part 1.

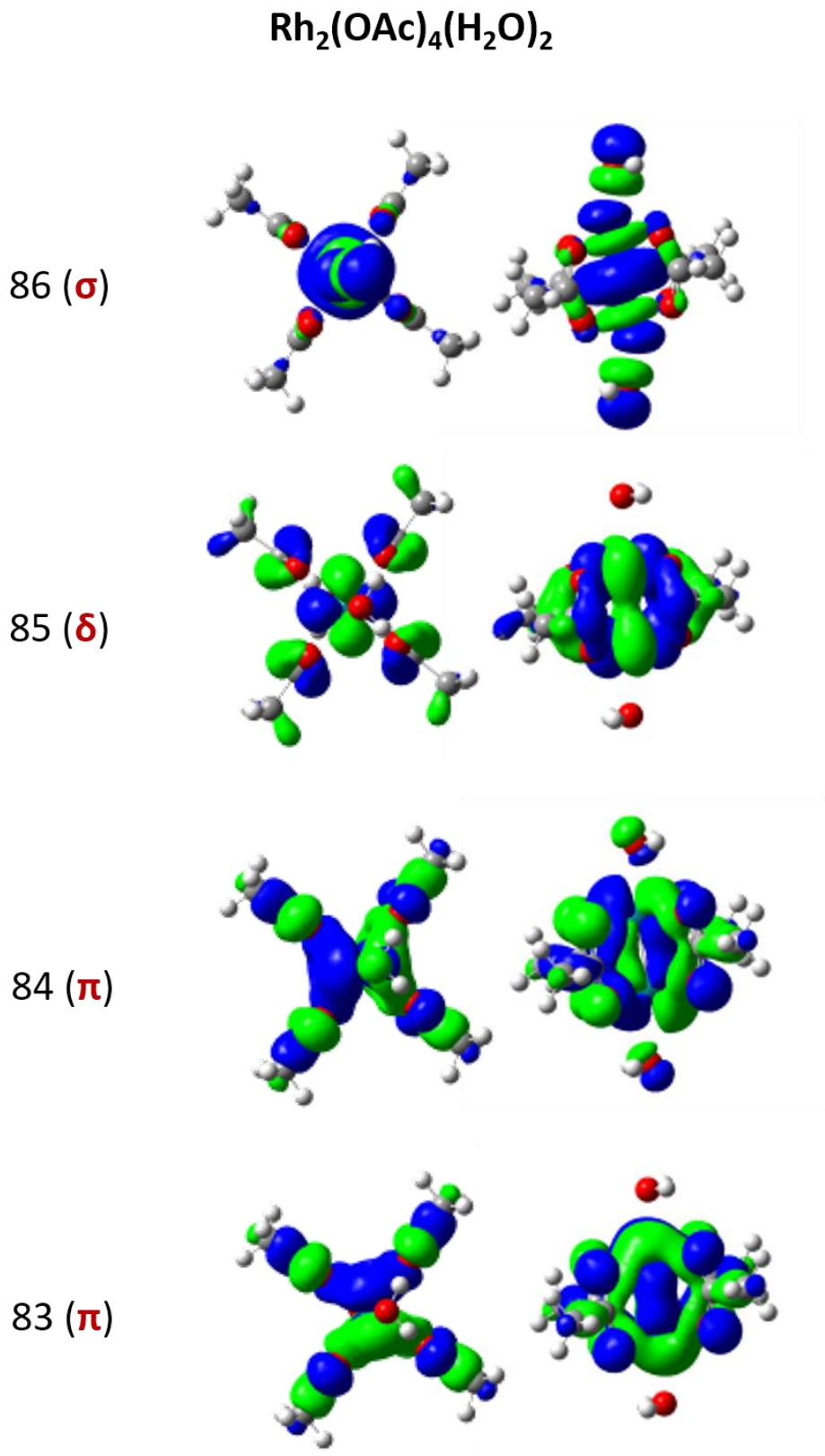

Fig S4. Expanded views of $Rh_2(OAc)_4(H_2O)_2$ molecular orbital surfaces, part 2.

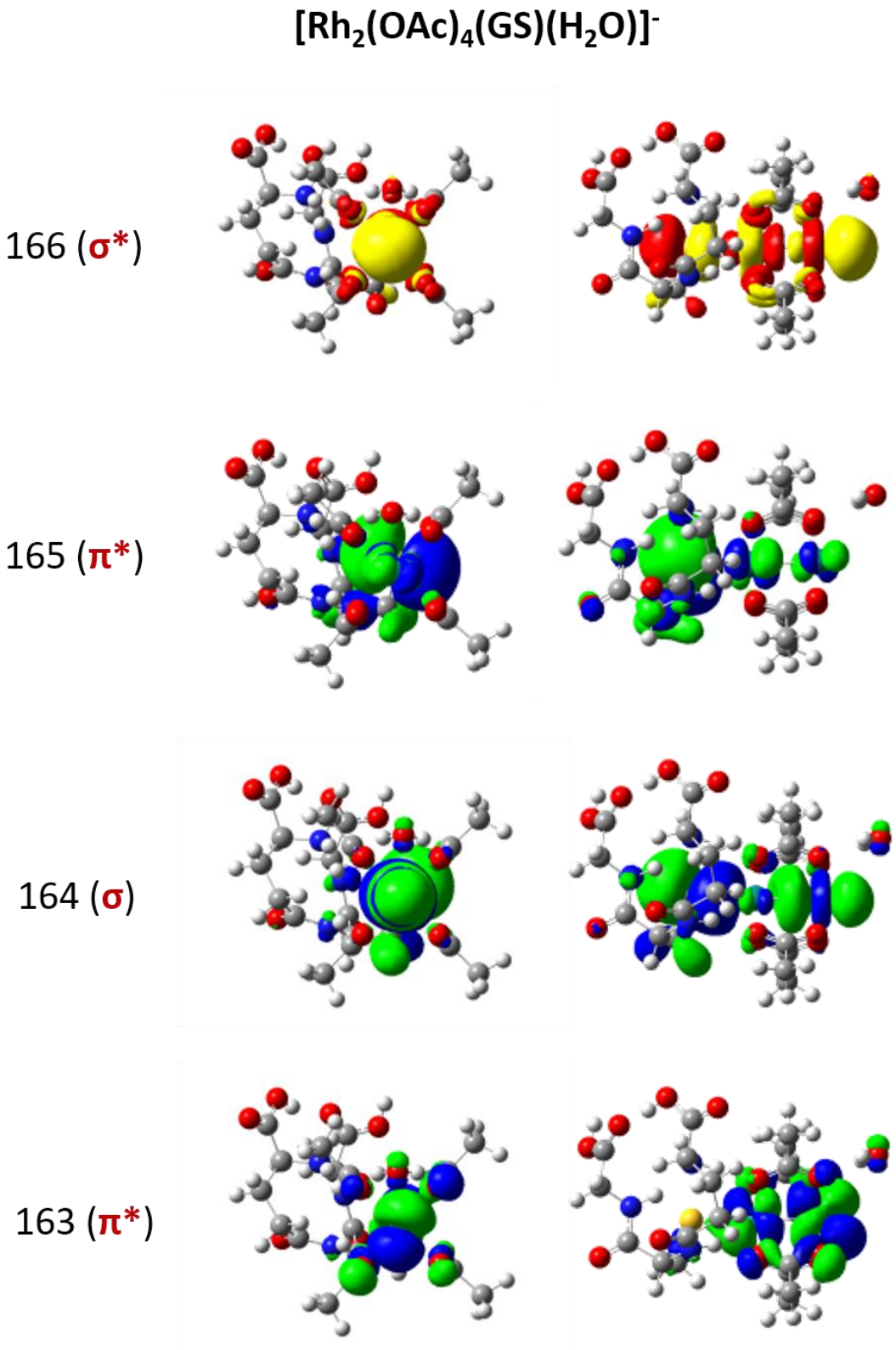

Fig S5. Expanded views of $[Rh_2(OAc)_4(GS)(H_2O)]^-$ molecular orbital surfaces, part 1.

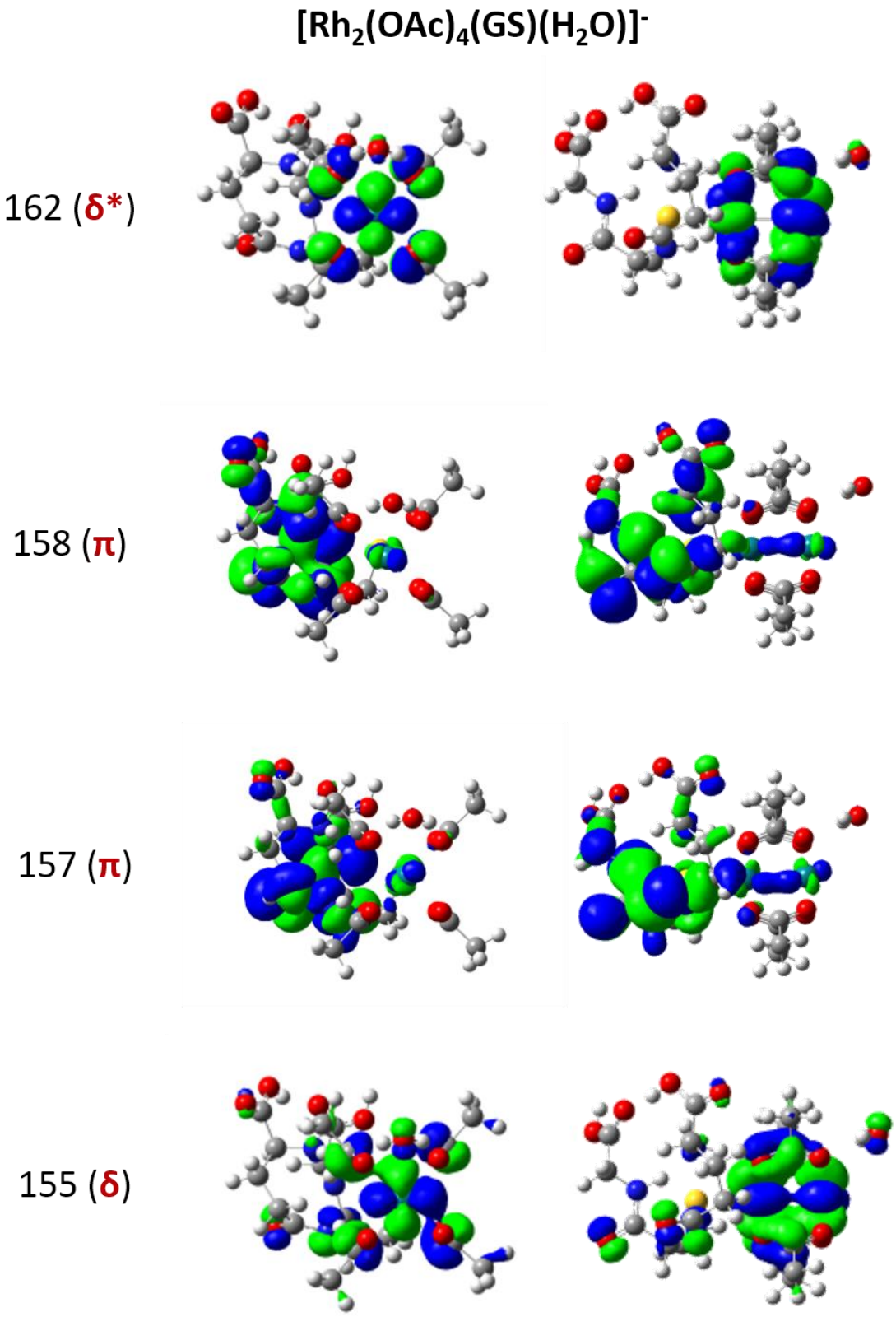

Fig S6. Expanded views of $[Rh_2(OAc)_4(GS)(H_2O)]^-$ molecular orbital surfaces, part 2.

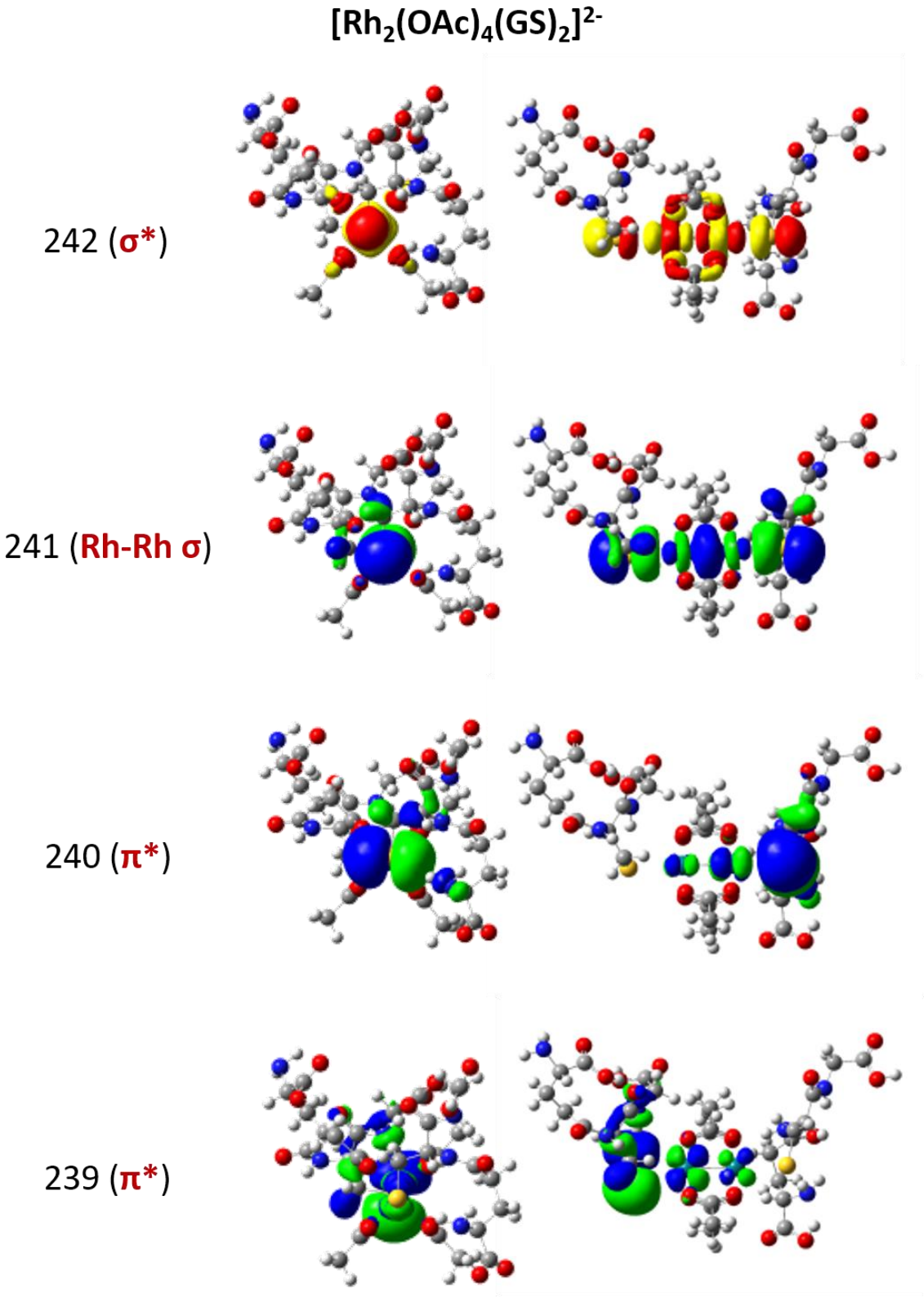

Fig S7. Expanded views of $[Rh_2(OAc)_4(GS)_2]^{2-}$ molecular orbital surfaces, part 1.

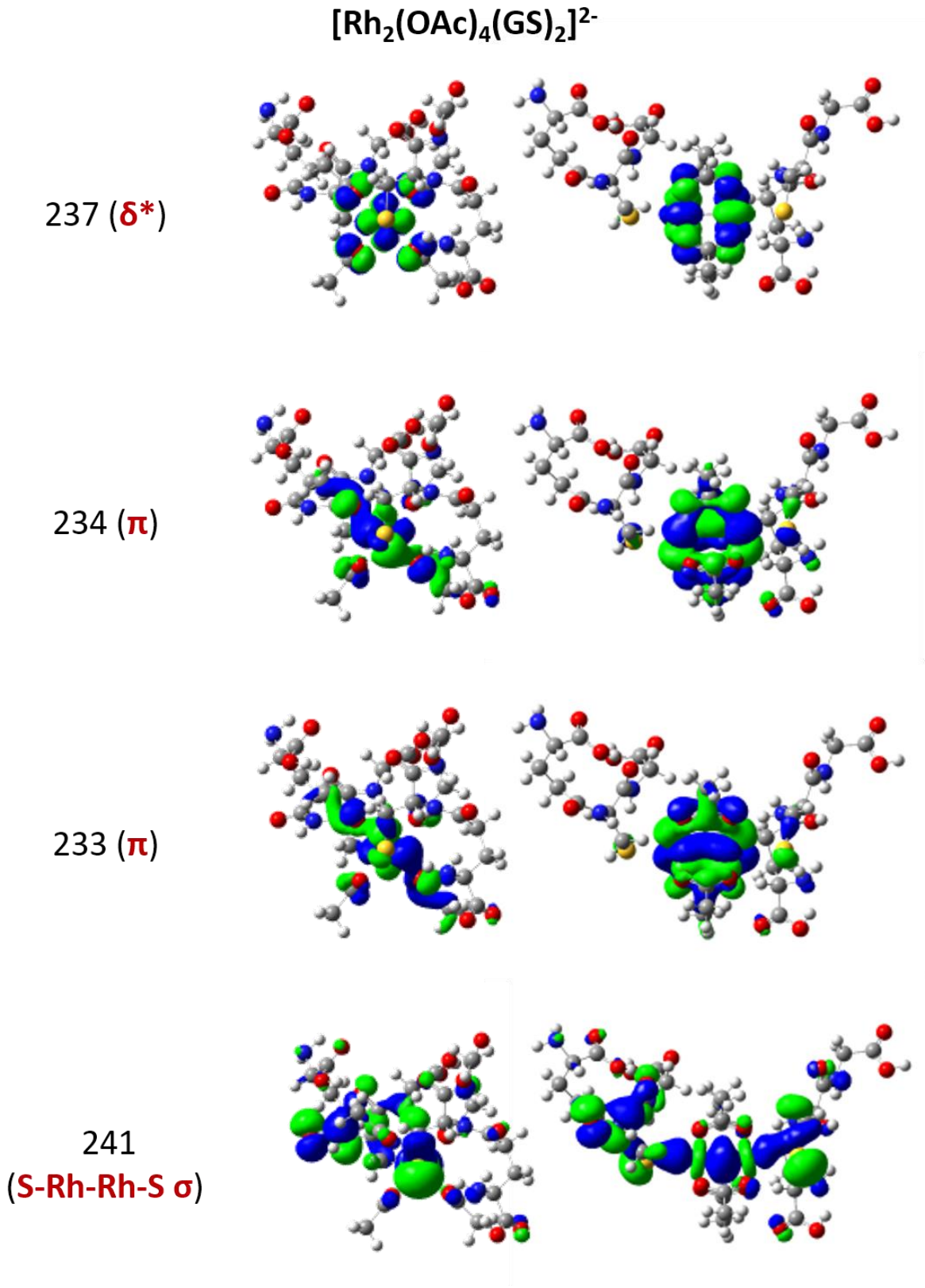

Fig S8. Expanded views of $[Rh_2(OAc)_4(GS)_2]^{2-}$ molecular orbital surfaces, part 2.

Table S1. Transition contributions for excited states (ES) with oscillator strength (f) greater than 0.001

$Rh_2(OAc)_4$				
ES	**Transition**	**Contribution**	**Energy [eV (nm)]**	**f**
1	72 -> 80	0.12995	1.5418 (804.16)	0.0037
	78 -> 80	0.67953		
2	71 -> 80	0.13086	1.5426 (803.75)	0.0037
	77 -> 80	0.67956		
14	72 -> 80	0.68665	4.7555 (260.72)	0.0229
	78 -> 80	-0.12489		
15	71 -> 80	0.68635	4.7676 (260.06)	0.232
	77 -> 80	-0.12557		
16	69 -> 80	0.69654	5.1009 (243.06)	0.0140
17	68 -> 80	0.69633	5.1094 (242.66)	0.0142
20	62 -> 81	0.14182	5.3426 (232.07)	0.0643
	63 -> 80	-0.14773		
	66 -> 82	-0.12428		
	70 -> 80	0.61243		
	79 -> 87	-0.11805		
	79 -> 88	0.14491		

$Rh_2(OAc)_4 2H_2O$				
ES	**Transition**	**Contribution**	**Energy [eV (nm)]**	**f**
1	86 -> 90	0.10876	2.2561 (549.55)	0.0034
	87 -> 91	0.17148		
	88 -> 90	0.65326		
2	80 -> 90	0.10439	2.3078 (537.23)	0.0027
	87 -> 90	0.65256		
	88 -> 91	0.19584		
6	76 -> 92	-0.11427	3.1246 (396.80)	0.0018
	84 -> 92	-0.20679		
	87 -> 90	-0.22219		
	88 -> 91	0.61712		
7	74 -> 92	-0.12927	3.1860 (389.15)	0.0019
	83 -> 92	0.20788		
	87 -> 91	0.62609		
	88 -> 90	-0.19353		
15	72 -> 91	0.13910	5.2099 (237.98)	0.1489
	75 -> 92	-0.11732		
	86 -> 90	0.61760		
	88 -> 90	-0.10257		
	89 -> 99	0.20974		

$[Rh_2(OAc)_4 1GS]^-$				
ES	**Transition**	**Contribution**	**Energy [eV (nm)]**	**f**
1	153 ->166	-0.12239	2.0002 (619.85)	0.0013
	161 ->166	-0.30150		
	165 ->166	0.57168		

	165 ->167	-0.11791		
2	153 ->167	-0.12419	2.3540 (526.69)	0.0029
	161 ->167	-0.20202		
	161 ->169	0.10319		
	163 ->166	0.44851		
	163 ->167	0.12743		
	165 ->167	0.35148		
4	153 ->167	-0.13409	2.5712 (482.20)	0.0013
	161 ->167	-0.15160		
	162 ->169	0.14879		
	163 ->166	-0.37276		
	163 ->167	-0.12279		
	163 ->169	0.14540		
	165 ->166	0.13916		
	165 ->167	0.43725		
6	161 ->166	0.23994	2.7976 (443.18)	0.0016
	161 ->169	0.32872		
	162 ->169	-0.10429		
	163 ->166	0.10738		
	163 ->167	-0.24660		
	163 ->169	0.34638		
	165 ->166	0.20374		
	165 ->169	-0.13194		
13	153 ->167	0.19539	3.8002 (326.26)	0.0704
	154 ->166	-0.10185		
	156 ->166	-0.16372		
	161 ->167	0.42275		
	163 ->166	0.12060		
	164 ->166	0.26718		
	165 ->167	0.31264		
14	153 ->167	-0.10584	3.8639 (320.88)	0.3938
	161 ->167	-0.24010		
	164 ->166	0.58547		
	165 ->167	-0.15724		
15	138 ->166	0.13137	4.0651 (305.00)	0.0569
	152 ->166	0.22820		
	154 ->166	0.23745		
	156 ->166	0.46218		
	157 ->166	0.12203		
	160 ->166	-0.10821		
	161 ->167	0.15066		
	163 ->166	-0.10670		
	164 ->166	0.19565		

$[Rh_2(OAc)_4 2GS]^{2-}$

ES	Transition	Contribution	Energy [eV (nm)]	f
1	232 -> 245	-0.12926	2.3396 (529.93)	0.0029
	235 -> 242	0.13289		

	235 -> 244	-0.14224		
	236 -> 242	0.42475		
	236 -> 244	-0.21641		
	239 -> 242	-0.21184		
	239 -> 244	0.15268		
	240 -> 242	0.29186		
	240 -> 244	-0.11257		
2	234 -> 245	-0.12280	2.3866 (519.50)	0.0021
	235 -> 242	0.31121		
	235 -> 244	0.16534		
	236 -> 244	-0.17550		
	238 -> 242	0.28945		
	238 -> 244	0.22085		
	239 -> 242	-0.23043		
	240 -> 242	-0.19450		
	240 -> 244	-0.20986		
9	232 -> 245	0.12454	2.9522 (419.98)	0.0035
	233 -> 244	0.14644		
	234 -> 244	-0.14958		
	235 -> 244	0.17043		
	235 -> 245	0.22699		
	236 -> 242	0.15648		
	236 -> 244	0.33913		
	236 -> 245	-0.15082		
	238 -> 245	0.25701		
	239 -> 242	-0.11774		
	239 -> 244	-0.13665		
	240 -> 245	-0.10547		
	241 -> 244	-0.11128		
12	241 -> 242	0.67072	3.4198 (362.55)	0.7178