10.1071/CH16660_AC

Australian Journal of Chemistry 2017, 70(7), 797-805

Supplementary Material

A Theoretical Probe for Structures, Metal-Metal Bonding and Electronic Spectra of Paramagnetic Tetrapyrrolic Ru(II) Complex

Jin-Yu Lv,[A,B] *Yuan-Ru Guo,*[A,C] *and Qing-Jiang Pan*[B,C]

[A]Key Laboratory of Bio-based Material Science & Technology of Education Ministry, College of Material Science and Engineering, Northeast Forestry University, Harbin 150040, China.

[B]Key Laboratory of Functional Inorganic Material Chemistry of Education Ministry, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, China.

[C]Corresponding authors. Email: guoyrnefu@163.com; panqjitc@163.com

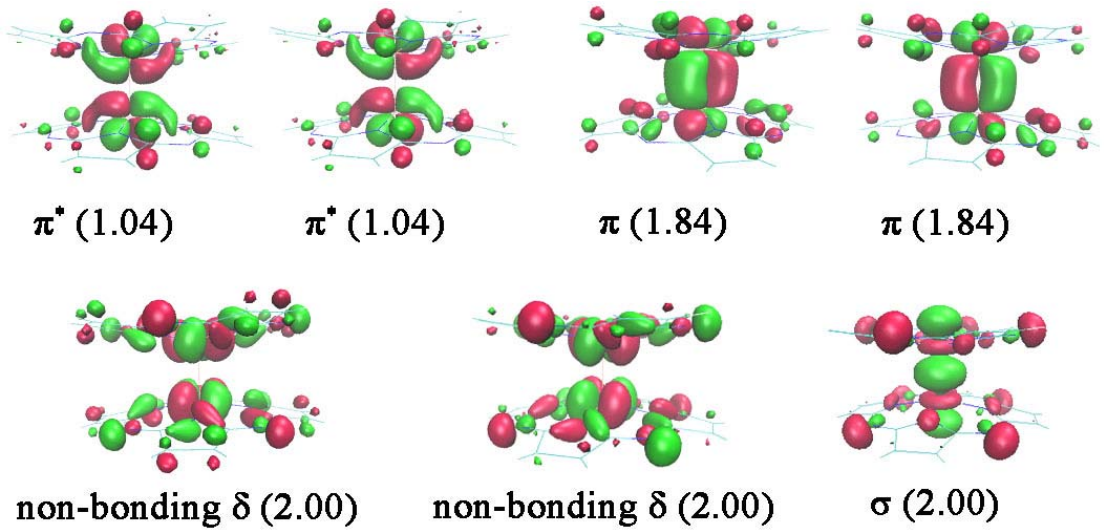

Figure S1. Orbitals and corresponding occupation numbers calculated by CASSCF.

Table S1. Calculated total energies (E in Hartree) and relative energies (ΔE in kcal/mol) of RuPz and $(RuPz)_2$ complexes with and without symmetry constraint.[a]

$(RuPz)_2$				RuPz		
Symm.	Configuration	E	ΔE	Symm.	E	ΔE
C_1	***s***taggered	-2292.5932269	0.00	C_1	-1146.274778	0.00
C_1	***e***clipsed	-2292.5893600	2.43	C_2	-1146.274596	0.11
C_2	***s***taggered	-2292.5932431	-0.01	C_i	-1146.274778	0.00
C_i	***e***clipsed	-2292.5884115	3.02			

[a] Only the triplet state of the complex was centered on.

Table S2. Optimized geometry parameters of monomeric RuPz and dimeric $(RuPz)_2$ complexes with and without symmetry constraint. (Distance in angstrom and angle in degree)

	Symm. (Configuration) [a]	Ru-Ru	Ru-N	Ru-N_4 [b]	α_1 [c]	α_2 [c]	h [c]
$(RuPz)_2$	C_2 (***s***)	2.383	2.021	0.342	99.7	88.4	33.3
	C_1 (***s***)	2.382	2.021	0.343	99.8	88.4	34.0
	C_i (***e***)	2.443	2.020	0.340	99.7	88.3	0.0
	C_1 (***e***)	2.446	2.021	0.342	99.8	88.4	0.3
RuPz	C_1	—	2.002	—	—	90.0	—
	C_2	—	2.002	—	—	90.0	—
	C_i	—	1.980	—	—	90.0	—
$(RuOEPor)_2$	Expt. [d]	2.408	2.050	0.30	98.4	88.8	23.8
$(RuPc)_2$	Expt. [d]	2.40	1.97	0.41	—	—	45

[a] The dimeric $(RuPz)_2$ correspond to eclipsed (***e***) and staggered (***s***) conformers; only the triplet state was centered on.

[b] The Ru-N_4 distance (mean value) is measured by the normal distance from the Ru atom to its N_4-donor plane.

[c] α_1 = Ru-Ru-N1, α_2 = N1-Ru-N2, and h = N1-Ru-Ru-N1′, where N1 and N2 are adjacent atoms in one porphyrazine ligand, and N1 and N1′ come from two different Pz ligands.

[d] Experimental values of $(RuOEPor)_2$ and $(RuPc)_2$ from Ref.s [5] and [19], respectively.

Table S3. CASSCF/NEVPT2 calculated relative energies of $(RuPz)_2$ using different active spaces.

Orbitals	Electrons	CASSCF [a]	NEVPT2 [a]
14	14	-2.21	— [b]
12	14	0.00	0.00
12	12	6.02	-0.30
12	10	4.37	10.26
12	8	10.23	— [b]
12	6	15.97	3.49

[b] Not converged.

Table S4. Optimized geometry parameters of the ground-state $(RuPz)_2$ (i.e. the staggered conformer in the triplet state), compared with experimental values. (Distance in angstrom and angle in degree)

	Complexes	Ru-Ru	Ru-N	Ru-N_4 [a]	α_1 [b]	α_2 [b]	h[b]	Refs.
Cal.	$(RuPz)_2$	2.383	2.021	0.342	99.7	88.4	33.3	This work
Expt. [c]	$(RuOEPor)_2$	2.408	2.050	0.30	98.4	88.8	23.8	[19]
	$(RuOEPor)_2$	2.40	2.05					[75]
	$(RuPc)_2$	2.40	1.97	0.41			45	[5]
	$(RuPc)_2$	2.42±0.03	2.01±0.02	0.40				[18]
	$(RuPc)_2$	2.39±0.01	1.98±0.01					[33]
	$(RuPc)_2$	2.41±0.01	2.03±0.01	0.28				[76]
	$(RuPc)_2$	2.40	1.97	0.41				[74]
	$(RuPc)_2(NO_2)$	2.411±0.01	2.002±0.01					[29]

[a] The Ru-N_4 distance means the normal distance from the Ru atom to its N_4-donor plane.

[b] α_1 = Ru-Ru-N1, α_2 = N1-Ru-N2, and h = N1-Ru-Ru-N1′, where N1 and N2 are adjacent atoms in one porphyrazine ligand, and N1 and N1′ come from two different Pz ligands.

Table S5. Calculated relative energies (kcal/mol) of various electron spin states using four levels of theory at the ground-state geometry of $(RuPz)_2$.

Code	Gaussian	Molpro		
Method	B3LYP	B3LYP	CASSCF	NEVPT2
Basis Sets [a]	B-II	B-III	B-III	B-III
Singlet	9.06	26.51	30.14	27.41
Triplet	0.00	0.00	0.00	0.00
Quintet	35.85	16.41	52.61	51.21
Septet	69.63	35.07	75.15	85.67
Nonet	98.19	115.51	159.13	180.02

[a] Basis sets were described in the text.

Table S6. Contributions (%) of β orbitals for $(RuPz)_2$ in pyridine solution.

Orbitals		Energy (eV)	Contributions (%)		Ru components (%)	Assignment
			2Ru	2Pz		
L+9	93a	0.109	92	8		
L+8	92a	-1.385		100		
L+7	91a	-1.764		100		
L+6	92b	-2.343	62	38	60 d_{xz}	
L+5	91b	-2.343	62	38	60 d_{yz}	
L+4	90a	-2.504	82	18	70 d_{z^2}	
L+3	90b	-2.951	11	89	4 d_{yz}, 4 d_{xz}	
L+2	89b	-2.951	10	90	4 d_{yz}, 4 d_{xz}	
L+1	88b	-3.746	21	79	14 d_{yz}, 3 d_{xz}	
LUMO	87b	-3.746	21	79	14 d_{xz}, 3 d_{yz}	
HOMO	89a	-5.613	2	98		L
H-1	86b	-5.861	52	48	44 d_{xz}	π
H-2	85b	-5.861	52	48	44 d_{yz}	π
H-3	88a	-6.038		100		L
H-4	87a	-6.144	72	28	41 d_{xy}, 30 $d_{x^2-y^2}$	δ (nonbonding)
H-5	86a	-6.273	67	33	38 d_{xy}, 28 $d_{x^2-y^2}$	δ (nonbonding)
H-6	85a	-7.110	3	97		L
H-7	84a	-7.127	2	98		L
H-8	83a	-7.293	47	53		L + σ*
H-9	82a	-7.324	1	99		L
H-10	84b	-7.354	8	92		L + π*
H-11	83b	-7.354	8	92		L + π*
H-12	81a	-7.455	44	56		L
H-13	80a	-7.792	33	67	10 d_{z^2}	σ + L
H-22	77a	-8.333	83	17	66d_{z^2}	σ

Table S7. The electron spin states of the whole molecule and fragments, their energies and the Ru_2 bond energy in the counterpoise calculations.

Spin states of Molecule / ***Fragments***	Triplet / ***Singlet***	Triplet / ***Triplet***	Triplet / ***Quintet***
System energies (Hartree)			
Molecule	-2295.072512	-2295.072512	-2295.072512
Fragment 1 (with BSSE)	-1147.480625	-1147.511891	-1147.468595
Fragment 2(with BSSE)	-1147.480468	-1147.511767	-1147.468487
Fragment 1	-1147.470078	-1147.503379	-1147.4609
Fragment 2	-1147.471895	-1147.503186	-1147.46074
Ru_2 bond energy (kcal/mol)			
Inclusion of BSSE	69.92	30.66	84.98
Exclusion of BSSE	81.91	41.38	94.67

Table S8. Electronic absorption maxima (nm) of (RuPz)·py_2 in pyridine calculated by various functionals, compared with available experimental values of analogous complex [Ru(OEPor)].

Functionals		Bands		
		Q_1	Q_2	Soret
LDA	SVWN	523	465	354
GGA	BLYP	532	471	349
	PBE	528	466	347
Meta-GGA	TPSS	516	450	347
	M06L	512	447	337
Hybrid	B3LYP″ (5% HF) [a]	512	448	345
	B3LYP′ (10%)	501	425	334
	O3LYP (12%)	499	409	329
	B3LYP* (15%)	496	404	326
	B3LYP (20%)	488	382	319
Meta-Hybrid	TPSSh	493	401	327
	M06	499	384	335
LC	CAM-B3	490	349	307
Expt. [80-81]		521	495	395

[a] The amount of HF exchange in hybrid functional is shown in parenthesis.

Table S9. Orbital contributions (%) of (RuPz)·py_2 calculated at the TD-BLYP/B-II/PCM level.

Orbitals		Energy	Contributions (%)			Ru components (%)
		(eV)	Ru	Pz	2py	
L+9	74a	0.071		99		
L+8	73a	0.011	93			
L+7	72a	-0.525	62	8	30	25 d_z^2
L+6	71a	-1.224			99	
L+5	70a	-1.324	8		89	8 $d_{x^2-y^2}$
L+4	69a	-1.777		100		
L+3	66b	-1.814	10		88	
L+2	65b	-1.814	10		88	
L+1	64b	-2.873	15	83		13 d_{xz}
LUMO	63b	-2.874	15	83		13 d_{yz}
HOMO	68a	-4.222	74	25		74 d_{xy}
H-1	62b	-4.251	55	39	6	45 d_{xz}, 6 d_{yz}
H-2	61b	-4.251	55	39	6	6 d_{xz}, 45 d_{yz}
H-3	67a	-4.911		100		
H-4	66a	-5.609		86	12	
H-5	65a	-5.752		95		
H-6	64a	-5.866	17	82		12 d_{xy}
H-7	60b	-6.000		98		
H-8	59b	-6.000		98		
H-9	63a	-6.044		93		
H-10	58b	-6.250	21	63	16	6 d_{xz}, 12 d_{yz}
H-11	57b	-6.250	21	63	16	12 d_{xz}, 6 d_{yz}
H-12	62a	-6.489		5	95	
H-13	61a	-6.493			96	
H-14	60a	-6.700		97		
H-22	58a	-8.206	18	12	70	7 d_z^2

Cartesian coordinates of optimized structures

RuPz: C_i symmetry in the Singlet state

Ru	0.00000000	0.00000000	0.00000000
N	2.00133300	0.00000000	0.00000000
N	-2.00133300	0.00000000	0.00000000
N	-0.00016100	-1.95806200	0.00000000
N	0.00016100	1.95806200	0.00000000
C	2.82837700	1.12787700	-0.00058800
C	-2.82837700	-1.12787700	0.00058800
C	2.82831300	-1.12792300	-0.00027000
C	-2.82831300	1.12792300	0.00027000
C	-1.14057600	-2.79579200	0.00161200
C	1.14057600	2.79579200	-0.00161200
C	1.14035600	-2.79565300	0.00019100
C	-1.14035600	2.79565300	-0.00019100
N	2.43537100	2.39922500	-0.00161300
N	-2.43537100	-2.39922500	0.00161300
N	2.43520100	-2.39923100	-0.00016100
N	-2.43520100	2.39923100	0.00016100
C	4.23675800	0.68290100	-0.00079600
C	-4.23675800	-0.68290100	0.00079600
C	4.23673800	-0.68300600	-0.00065900
C	-4.23673800	0.68300600	0.00065900
C	-0.70120200	-4.15690100	0.00245400
C	0.70120200	4.15690100	-0.00245400
C	0.70113200	-4.15681500	0.00146700
C	-0.70113200	4.15681500	-0.00146700
H	5.07481800	1.36501700	-0.00120700
H	-5.07481800	-1.36501700	0.00120700
H	5.07477200	-1.36514700	-0.00082500
H	-5.07477200	1.36514700	0.00082500
H	-1.36728600	-5.00807600	0.00344500
H	1.36728600	5.00807600	-0.00344500
H	1.36728000	-5.00793900	0.00176200
H	-1.36728000	5.00793900	-0.00176200

RuPz: C_i symmetry in the Triplet state

Ru	0.00000000	0.00000000	0.00000000
N	2.01045800	0.00000000	0.00000000
N	-2.01045800	0.00000000	0.00000000
N	0.00001600	-1.99293600	0.00000000

N	-0.00001600	1.99293600	0.00000000
C	2.82660900	1.12993700	-0.00000600
C	-2.82660900	-1.12993700	0.00000600
C	2.82661300	-1.12993500	0.00001300
C	-2.82661300	1.12993500	-0.00001300
C	-1.13448600	-2.81106700	-0.00015200
C	1.13448600	2.81106700	0.00015200
C	1.13450300	-2.81108100	0.00004700
C	-1.13450300	2.81108100	-0.00004700
N	2.42330600	2.40708600	0.00010600
N	-2.42330600	-2.40708600	-0.00010600
N	2.42332000	-2.40709000	0.00004800
N	-2.42332000	2.40709000	-0.00004800
C	4.23083900	0.68551700	-0.00003800
C	-4.23083900	-0.68551700	0.00003800
C	4.23084100	-0.68550700	-0.00003600
C	-4.23084100	0.68550700	0.00003600
C	-0.69316100	-4.19438600	-0.00021100
C	0.69316100	4.19438600	0.00021100
C	0.69316000	-4.19439400	-0.00007700
C	-0.69316000	4.19439400	0.00007700
H	5.07171400	1.36420100	-0.00006600
H	-5.07171400	-1.36420100	0.00006600
H	5.07172300	-1.36418200	-0.00006800
H	-5.07172300	1.36418200	0.00006800
H	-1.36499200	-5.04086400	-0.00035100
H	1.36499200	5.04086400	0.00035100
H	1.36498100	-5.04088100	-0.00000600
H	-1.36498100	5.04088100	0.00000600

RuPz: C_i symmetry in the Quintet state

Ru	0.00000000	0.00000000	0.00000000
N	1.99627900	0.00000000	0.00000000
N	-1.99627900	0.00000000	0.00000000
N	-0.00001500	-1.99018600	0.00000000
N	0.00001500	1.99018600	0.00000000
C	2.82444300	1.14441000	-0.00023200
C	-2.82444300	-1.14441000	0.00023200
C	2.82444500	-1.14437400	-0.00019900
C	-2.82444500	1.14437400	0.00019900
C	-1.13895400	-2.82775800	0.00019100

C	1.13895400	2.82775800	-0.00019100
C	1.13894700	-2.82771900	-0.00016900
C	-1.13894700	2.82771900	0.00016900
N	2.43585900	2.41052300	-0.00028900
N	-2.43585900	-2.41052300	0.00028900
N	2.43586200	-2.41049300	-0.00024900
N	-2.43586200	2.41049300	0.00024900
C	4.21393900	0.68752100	-0.00036600
C	-4.21393900	-0.68752100	0.00036600
C	4.21393700	-0.68748100	-0.00031900
C	-4.21393700	0.68748100	0.00031900
C	-0.70104100	-4.18878000	0.00013100
C	0.70104100	4.18878000	-0.00013100
C	0.70106500	-4.18875800	-0.00011900
C	-0.70106500	4.18875800	0.00011900
H	5.05789900	1.36253400	-0.00033500
H	-5.05789900	-1.36253400	0.00033500
H	5.05794100	-1.36243800	-0.00026900
H	-5.05794100	1.36243800	0.00026900
H	-1.36952300	-5.03727000	0.00032400
H	1.36952300	5.03727000	-0.00032400
H	1.36957300	-5.03722800	-0.00027200
H	-1.36957300	5.03722800	0.00027200

RuPz: C_2 symmetry in the Singlet state

Ru	0.00000000	0.00000000	0.02810500
N	1.95782500	-0.00033000	-0.00384000
N	-1.95782500	0.00033000	-0.00384000
N	0.00000000	2.00137000	0.01291500
N	0.00000000	-2.00137000	0.01291500
C	2.79552800	1.14013100	-0.00864600
C	-2.79552800	-1.14013100	-0.00864600
C	2.79549500	-1.14078900	-0.00849700
C	-2.79549500	1.14078900	-0.00849700
C	-1.12772700	2.82851200	-0.00174000
C	1.12772700	-2.82851200	-0.00174000
C	1.12797800	2.82820000	-0.00204800
C	-1.12797800	-2.82820000	-0.00204800
N	2.39921000	2.43495600	-0.00899000
N	-2.39921000	-2.43495600	-0.00899000
N	2.39907600	-2.43556200	-0.00869700

N	-2.39907600	2.43556200	-0.00869700
C	4.15670600	0.70083100	-0.01192500
C	-4.15670600	-0.70083100	-0.01192500
C	4.15666500	-0.70145600	-0.01211400
C	-4.15666500	0.70145600	-0.01211400
C	-0.68267900	4.23671700	-0.01711200
C	0.68267900	-4.23671700	-0.01711200
C	0.68325800	4.23654800	-0.01697600
C	-0.68325800	-4.23654800	-0.01697600
H	5.00773500	1.36701500	-0.01313100
H	-5.00773500	-1.36701500	-0.01313100
H	5.00772000	-1.36760700	-0.01208800
H	-5.00772000	1.36760700	-0.01208800
H	-1.36454900	5.07480300	-0.03030400
H	1.36454900	-5.07480300	-0.03030400
H	1.36536400	5.07447200	-0.02814600
H	-1.36536400	-5.07447200	-0.02814600

RuPz: C_2 symmetry in the Triplet state

Ru	0.00000000	0.00000000	0.00019600
N	-0.74640200	1.84840800	0.00002600
N	0.74640200	-1.84840800	0.00002600
N	1.86472900	0.75182200	0.00003300
N	-1.86472900	-0.75182200	0.00003300
C	0.00000000	3.03105700	-0.00000100
C	0.00000000	-3.03105700	-0.00000100
C	-2.10441100	2.18271900	0.00000400
C	2.10441100	-2.18271900	0.00000400
C	3.04448300	0.00925700	-0.00005100
C	-3.04448300	-0.00925700	-0.00005100
C	2.19845900	2.10514300	-0.00006400
C	-2.19845900	-2.10514300	-0.00006400
N	1.34646300	3.13825100	-0.00004000
N	-1.34646300	-3.13825100	-0.00004000
N	-3.14793100	1.32568700	-0.00002300
N	3.14793100	-1.32568700	-0.00002300
C	-0.92663800	4.14879800	-0.00001200
C	0.92663800	-4.14879800	-0.00001200
C	-2.21248200	3.63108200	-0.00004200
C	2.21248200	-3.63108200	-0.00004200
C	4.18029900	0.94711300	-0.00020800
C	-4.18029900	-0.94711300	-0.00020800

C	3.66712800	2.21843900	-0.00020300
C	-3.66712800	-2.21843900	-0.00020300
H	-0.61985000	5.18502400	-0.00002100
H	0.61985000	-5.18502400	-0.00002100
H	-3.15216700	4.16487000	-0.00017100
H	3.15216700	-4.16487000	-0.00017100
H	5.21407200	0.63243600	-0.00030600
H	-5.21407200	-0.63243600	-0.00030600
H	4.19276900	3.16256200	-0.00032700
H	-4.19276900	-3.16256200	-0.00032700

RuPz: C_2 symmetry in the Quintet state

Ru	0.00000000	0.00000000	0.00159400
N	0.00000000	1.99630300	0.00138800
N	0.00000000	-1.99630300	0.00138800
N	-1.99020400	0.00001700	0.00081100
N	1.99020400	-0.00001700	0.00081100
C	-1.14438400	2.82446900	-0.00017900
C	1.14438400	-2.82446900	-0.00017900
C	1.14441400	2.82444200	-0.00063300
C	-1.14441400	-2.82444200	-0.00063300
C	-2.82775100	-1.13896800	0.00006900
C	2.82775100	1.13896800	0.00006900
C	-2.82774000	1.13902000	0.00046300
C	2.82774000	-1.13902000	0.00046300
N	-2.41050100	2.43591900	-0.00004700
N	2.41050100	-2.43591900	-0.00004700
N	2.41052600	2.43586400	-0.00065500
N	-2.41052600	-2.43586400	-0.00065500
C	-0.68748200	4.21396100	-0.00232900
C	0.68748200	-4.21396100	-0.00232900
C	0.68755100	4.21394500	-0.00250900
C	-0.68755100	-4.21394500	-0.00250900
C	-4.18877100	-0.70104400	-0.00056900
C	4.18877100	0.70104400	-0.00056900
C	-4.18876500	0.70110700	-0.00031200
C	4.18876500	-0.70110700	-0.00031200
H	-1.36242400	5.05797800	-0.00321200
H	1.36242400	-5.05797800	-0.00321200
H	1.36250200	5.05795500	-0.00354800
H	-1.36250200	-5.05795500	-0.00354800
H	-5.03728000	-1.36950100	-0.00164100

H	5.03728000	1.36950100	-0.00164100
H	-5.03726900	1.36957000	-0.00116300
H	5.03726900	-1.36957000	-0.00116300

$(RuPz)_2$: C_i (*e*) symmetry in the Singlet state

Ru	0.00000000	0.00000000	-1.20608200
Ru	0.00000000	0.00000000	1.20608200
N	1.38333600	-1.38333600	-1.63511300
N	-1.38333600	1.38333600	1.63511300
N	-1.38419900	1.38340200	-1.63248300
N	1.38419900	-1.38340200	1.63248300
N	1.42041200	1.42110700	-1.51590200
N	-1.42041200	-1.42110700	1.51590200
N	-1.42098200	-1.42115300	-1.51214300
N	1.42098200	1.42115300	1.51214300
C	1.16568700	-2.76272200	-1.77731500
C	-1.16568700	2.76272200	1.77731500
C	-1.16692100	2.76268600	-1.77536400
C	1.16692100	-2.76268600	1.77536400
C	2.76244800	-1.16550200	-1.77927400
C	-2.76244800	1.16550200	1.77927400
C	-2.76360800	1.16548200	-1.77356500
C	2.76360800	-1.16548200	1.77356500
C	2.78449300	1.19966600	-1.71940000
C	-2.78449300	-1.19966600	1.71940000
C	-2.78552700	-1.19973300	-1.71236800
C	2.78552700	1.19973300	1.71236800
C	1.19833700	2.78537400	-1.71756200
C	-1.19833700	-2.78537400	1.71756200
C	-1.19941000	-2.78540600	-1.71390700
C	1.19941000	2.78540600	1.71390700
N	-0.01733000	-3.39948800	-1.79680000
N	0.01733000	3.39948800	1.79680000
N	3.39884100	0.01771700	-1.80150300
N	-3.39884100	-0.01771700	1.80150300
N	0.01611400	3.39942600	-1.79786700
N	-0.01611400	-3.39942600	1.79786700
N	-3.39997200	-0.01776300	-1.79373300
N	3.39997200	0.01776300	1.79373300
C	2.44178900	-3.41859900	-1.98070900
C	-2.44178900	3.41859900	1.98070900
C	-2.44349100	3.41855000	-1.97600200

C	2.44349100	-3.41855000	1.97600200
C	3.41844900	-2.44166700	-1.98186100
C	-3.41844900	2.44166700	1.98186100
C	-3.42012400	2.44161800	-1.97481300
C	3.42012400	-2.44161800	1.97481300
C	3.45127900	2.48521900	-1.96199700
C	-3.45127900	-2.48521900	1.96199700
C	-3.45298100	-2.48542100	-1.95247500
C	3.45298100	2.48542100	1.95247500
C	2.48340400	3.45277300	-1.96108700
C	-2.48340400	-3.45277300	1.96108700
C	-2.48513400	-3.45302800	-1.95325500
C	2.48513400	3.45302800	1.95325500
H	2.54838200	-4.48497400	-2.11750800
H	-2.54838200	4.48497400	2.11750800
H	-2.55038000	4.48489800	-2.11276400
H	2.55038000	-4.48489800	2.11276400
H	4.48466400	-2.54809800	-2.12002000
H	-4.48466400	2.54809800	2.12002000
H	-4.48665200	2.54799700	-2.11056900
H	4.48665200	-2.54799700	2.11056900
H	4.51220100	2.57802600	-2.14365800
H	-4.51220100	-2.57802600	2.14365800
H	-4.51427400	-2.57823000	-2.13196000
H	4.51427400	2.57823000	2.13196000
H	2.57569800	4.51391400	-2.14172500
H	-2.57569800	-4.51391400	2.14172500
H	-2.57781300	-4.51417300	-2.13368600
H	2.57781300	4.51417300	2.13368600

$(RuPz)_2$: C_i (*e*) symmetry in the Triplet state

Ru	0.00000000	0.00000000	-1.22151000
Ru	0.00000000	0.00000000	1.22151000
N	1.40817000	-1.40817000	-1.56190100
N	-1.40817000	1.40817000	1.56190100
N	-1.40813000	1.40822300	-1.56176200
N	1.40813000	-1.40822300	1.56176200
N	1.40820900	1.40822700	-1.56145800
N	-1.40820900	-1.40822700	1.56145800
N	-1.40818500	-1.40810000	-1.56209700
N	1.40818500	1.40810000	1.56209700
C	1.18562200	-2.77720900	-1.72973000

C	-1.18562200	2.77720900	1.72973000
C	-1.18561500	2.77740200	-1.72855500
C	1.18561500	-2.77740200	1.72855500
C	2.77726800	-1.18559900	-1.72939000
C	-2.77726800	1.18559900	1.72939000
C	-2.77725700	1.18578600	-1.72894000
C	2.77725700	-1.18578600	1.72894000
C	2.77729600	1.18572900	-1.72884600
C	-2.77729600	-1.18572900	1.72884600
C	-2.77728100	-1.18550500	-1.72954100
C	2.77728100	1.18550500	1.72954100
C	1.18569500	2.77736700	-1.72858900
C	-1.18569500	-2.77736700	1.72858900
C	-1.18567700	-2.77716800	-1.72974700
C	1.18567700	2.77716800	1.72974700
N	-0.00004100	-3.40074300	-1.77998800
N	0.00004100	3.40074300	1.77998800
N	3.40085100	0.00004000	-1.77924300
N	-3.40085100	-0.00004000	1.77924300
N	0.00004000	3.40095500	-1.77853300
N	-0.00004000	-3.40095500	1.77853300
N	-3.40081700	0.00013900	-1.77936000
N	3.40081700	-0.00013900	1.77936000
C	2.46856000	-3.44048200	-1.95040200
C	-2.46856000	3.44048200	1.95040200
C	-2.46861600	3.44083200	-1.94838500
C	2.46861600	-3.44083200	1.94838500
C	3.44055700	-2.46851300	-1.95017100
C	-3.44055700	2.46851300	1.95017100
C	-3.44061700	2.46884800	-1.94861300
C	3.44061700	-2.46884800	1.94861300
C	3.44064700	2.46872000	-1.94893100
C	-3.44064700	-2.46872000	1.94893100
C	-3.44060000	-2.46841900	-1.95025200
C	3.44060000	2.46841900	1.95025200
C	2.46866900	3.44071400	-1.94879500
C	-2.46866900	-3.44071400	1.94879500
C	-2.46864200	-3.44041600	-1.95036400
C	2.46864200	3.44041600	1.95036400
H	2.56933400	-4.50438900	-2.10927900
H	-2.56933400	4.50438900	2.10927900
H	-2.56945100	4.50486600	-2.10637500
H	2.56945100	-4.50486600	2.10637500
H	4.50450500	-2.56928500	-2.10878100

H	-4.50450500	2.56928500	2.10878100
H	-4.50462100	2.56974400	-2.10676300
H	4.50462100	-2.56974400	2.10676300
H	4.50460500	2.56954100	-2.10743100
H	-4.50460500	-2.56954100	2.10743100
H	-4.50453600	-2.56916500	-2.10895300
H	4.50453600	2.56916500	2.10895300
H	2.56948700	4.50469300	-2.10716400
H	-2.56948700	-4.50469300	2.10716400
H	-2.56944500	-4.50432900	-2.10918300
H	2.56944500	4.50432900	2.10918300

$(RuPz)_2$: C_2 (*s*) symmetry in the Singlet state

Ru	0.00000000	0.00000000	-1.16908300
Ru	0.00000000	0.00000000	1.17048200
N	-1.82667400	0.72700100	-1.58330100
N	1.82667400	-0.72700100	-1.58330100
N	-1.92055900	-0.42006700	1.58427100
N	1.92055900	0.42006700	1.58427100
N	0.74238000	1.85728800	-1.48403600
N	-0.74238000	-1.85728800	-1.48403600
N	-0.42939300	1.95382900	1.48431200
N	0.42939300	-1.95382900	1.48431200
C	-2.16919700	2.08047200	-1.72839500
C	2.16919700	-2.08047200	-1.72839500
C	-2.96721100	0.50433000	1.68735100
C	2.96721100	-0.50433000	1.68735100
C	-3.00994400	-0.01436200	-1.68866000
C	3.00994400	0.01436200	-1.68866000
C	-2.47899300	-1.69952200	1.73014200
C	2.47899300	1.69952200	1.73014200
C	2.09174200	2.19470100	-1.64908300
C	-2.09174200	-2.19470100	-1.64908300
C	0.49294100	2.98535200	1.69560200
C	-0.49294100	-2.98535200	1.69560200
C	0.00000000	3.02523700	-1.69506200
C	0.00000000	-3.02523700	-1.69506200
C	-1.70599000	2.50620500	1.64789000
C	1.70599000	-2.50620500	1.64789000
N	-1.32620600	3.12935200	-1.77377200
N	1.32620600	-3.12935200	-1.77377200
N	-2.86248400	1.84764600	1.70085600

N	2.86248400	-1.84764600	1.70085600
N	-3.12554700	-1.35679600	-1.70272400
N	3.12554700	1.35679600	-1.70272400
N	-1.81830600	-2.87185800	1.77567000
N	1.81830600	2.87185800	1.77567000
C	-3.60220000	2.18292400	-1.89627900
C	3.60220000	-2.18292400	-1.89627900
C	-4.20891100	-0.21656900	1.87102700
C	4.20891100	0.21656900	1.87102700
C	-4.11732900	0.89930000	-1.87291500
C	4.11732900	-0.89930000	-1.87291500
C	-3.90975800	-1.56688200	1.89663500
C	3.90975800	1.56688200	1.89663500
C	2.19517800	3.64087600	-1.87778700
C	-2.19517800	-3.64087600	-1.87778700
C	-0.23575100	4.24069400	1.90796100
C	0.23575100	-4.24069400	1.90796100
C	0.92302600	4.14509400	-1.90916200
C	-0.92302600	-4.14509400	-1.90916200
C	-1.57300300	3.95011900	1.87552600
C	1.57300300	-3.95011900	1.87552600
H	-4.12305900	3.12023400	-2.02578200
H	4.12305900	-3.12023400	-2.02578200
H	-5.16998200	0.26596300	1.97575600
H	5.16998200	-0.26596300	1.97575600
H	-5.14400700	0.57975000	-1.97919500
H	5.14400700	-0.57975000	-1.97919500
H	-4.57646200	-2.40668300	2.02643100
H	4.57646200	2.40668300	2.02643100
H	3.13606600	4.15147100	-2.02344900
H	-3.13606600	-4.15147100	-2.02344900
H	0.25393700	5.18704300	2.08626300
H	-0.25393700	-5.18704300	2.08626300
H	0.59362300	5.15833400	-2.08803600
H	-0.59362300	-5.15833400	-2.08803600
H	-2.41838400	4.60721000	2.01955900
H	2.41838400	-4.60721000	2.01955900

$(RuPz)_2$: C_2 (*s*) symmetry in the Triplet state

Ru	0.00000000	0.00000000	-1.19095800
Ru	0.00000000	0.00000000	1.19203000
N	-1.99184800	-0.00030100	-1.53279200

N	1.99184800	0.00030100	-1.53279200
N	-1.66442500	-1.09498500	1.53361200
N	1.66442500	1.09498500	1.53361200
N	0.00000000	1.99188400	-1.53275000
N	0.00000000	-1.99188400	-1.53275000
N	-1.09500200	1.66445100	1.53354600
N	1.09500200	-1.66445100	1.53354600
C	-2.80355600	1.12484200	-1.69447500
C	2.80355600	-1.12484200	-1.69447500
C	-2.96066000	-0.59887500	1.69525100
C	2.96066000	0.59887500	1.69525100
C	-2.80216500	-1.12712600	-1.69501600
C	2.80216500	1.12712600	-1.69501600
C	-1.72387500	-2.48116700	1.69412600
C	1.72387500	2.48116700	1.69412600
C	1.12501100	2.80369500	-1.69440200
C	-1.12501100	-2.80369500	-1.69440200
C	-0.59890300	2.96068300	1.69518300
C	0.59890300	-2.96068300	1.69518300
C	-1.12692000	2.80207800	-1.69503500
C	1.12692000	-2.80207800	-1.69503500
C	-2.48117400	1.72391000	1.69405200
C	2.48117400	-1.72391000	1.69405200
N	-2.40655700	2.40444200	-1.74259400
N	2.40655700	-2.40444200	-1.74259400
N	-3.33197900	0.68877000	1.74150600
N	3.33197900	-0.68877000	1.74150600
N	-2.40467600	-2.40678000	-1.74252600
N	2.40467600	2.40678000	-1.74252600
N	-0.68876700	-3.33197700	1.74149100
N	0.68876700	3.33197700	1.74149100
C	-4.18075100	0.68543400	-1.90342300
C	4.18075100	-0.68543400	-1.90342300
C	-3.87086300	-1.72180300	1.90420800
C	3.87086300	1.72180300	1.90420800
C	-4.17965600	-0.68944800	-1.90455700
C	4.17965600	0.68944800	-1.90455700
C	-3.11607200	-2.87101400	1.90260200
C	3.11607200	2.87101400	1.90260200
C	0.68550300	4.18084400	-1.90337500
C	-0.68550300	-4.18084400	-1.90337500
C	-1.72181000	3.87088900	1.90409500
C	1.72181000	-3.87088900	1.90409500
C	-0.68940100	4.17959200	-1.90457000

C	0.68940100	-4.17959200	-1.90457000
C	-2.87103100	3.11609100	1.90249000
C	2.87103100	-3.11609100	1.90249000
H	-5.00751900	1.36526900	-2.04955100
H	5.00751900	-1.36526900	-2.04955100
H	-4.93471200	-1.60688900	2.05381400
H	4.93471200	1.60688900	2.05381400
H	-5.00513500	-1.37025300	-2.05430900
H	5.00513500	1.37025300	-2.05430900
H	-3.43319800	-3.89334900	2.04868400
H	3.43319800	3.89334900	2.04868400
H	1.36524300	5.00768200	-2.04952900
H	-1.36524300	-5.00768200	-2.04952900
H	-1.60691200	4.93473600	2.05372500
H	1.60691200	-4.93473600	2.05372500
H	-1.37027800	5.00499800	-2.05439400
H	1.37027800	-5.00499800	-2.05439400
H	-3.89335600	3.43323000	2.04860500
H	3.89335600	-3.43323000	2.04860500

$(RuPz)_2$: C_2 (*s*) symmetry in the Quintet state

Ru	0.00000000	0.00000000	1.25574200
Ru	0.00000000	0.00000000	-1.18054600
N	0.00000000	1.99663400	1.53113300
N	0.00000000	-1.99663400	1.53113300
N	0.78890100	1.82342700	-1.53972600
N	-0.78890100	-1.82342700	-1.53972600
N	-1.99420100	-0.00052300	1.53575100
N	1.99420100	0.00052300	1.53575100
N	-1.82662000	0.78818400	-1.53487300
N	1.82662000	-0.78818400	-1.53487300
C	-1.13414600	2.81615900	1.66494400
C	1.13414600	-2.81615900	1.66494400
C	0.07351000	3.02199300	-1.69441100
C	-0.07351000	-3.02199300	-1.69441100
C	1.13828500	2.81376700	1.65349600
C	-1.13828500	-2.81376700	1.65349600
C	2.14570000	2.12908600	-1.67703300
C	-2.14570000	-2.12908600	-1.67703300
C	-2.81717700	-1.12962800	1.66190900
C	2.81717700	1.12962800	1.66190900
C	-3.02346600	0.07268000	-1.66832300

C	3.02346600	-0.07268000	-1.66832300
C	-2.81554000	1.13528800	1.67607200
C	2.81554000	-1.13528800	1.67607200
C	-2.12963400	2.14789600	-1.68440500
C	2.12963400	-2.14789600	-1.68440500
N	-2.40073200	2.42028500	1.71209200
N	2.40073200	-2.42028500	1.71209200
N	-1.26476600	3.16324300	-1.73817400
N	1.26476600	-3.16324300	-1.73817400
N	2.40514100	2.41826200	1.68968900
N	-2.40514100	-2.41826200	1.68968900
N	3.17222400	1.25369800	-1.70684400
N	-3.17222400	-1.25369800	-1.70684400
C	-0.68165500	4.19965600	1.82509400
C	0.68165500	-4.19965600	1.82509400
C	1.01615300	4.10542200	-1.88601900
C	-1.01615300	-4.10542200	-1.88601900
C	0.68912700	4.19857300	1.81724400
C	-0.68912700	-4.19857300	1.81724400
C	2.28661200	3.55894700	-1.87285300
C	-2.28661200	-3.55894700	-1.87285300
C	-4.17985500	-0.68976200	1.84540300
C	4.17985500	0.68976200	1.84540300
C	-4.11703100	1.02529200	-1.84784400
C	4.11703100	-1.02529200	-1.84784400
C	-4.17827500	0.69693600	1.85591400
C	4.17827500	-0.69693600	1.85591400
C	-3.57261300	2.28727400	-1.86003200
C	3.57261300	-2.28727400	-1.86003200
H	-1.36048700	5.03143400	1.94492900
H	1.36048700	-5.03143400	1.94492900
H	0.72247800	5.13466400	-2.03199700
H	-0.72247800	-5.13466400	-2.03199700
H	1.37036400	5.02903600	1.93268400
H	-1.37036400	-5.02903600	1.93268400
H	3.23875600	4.05241000	-2.00245200
H	-3.23875600	-4.05241000	-2.00245200
H	-5.01298300	-1.36566200	1.96991000
H	5.01298300	1.36566200	1.96991000
H	-5.14854000	0.72809000	-1.96947200
H	5.14854000	-0.72809000	-1.96947200
H	-5.00958500	1.37233300	1.99465400
H	5.00958500	-1.37233300	1.99465400
H	-4.06544700	3.23974300	-1.99084900

H	4.06544700	-3.23974300	-1.99084900

$(RuPz)_2$: C_2 (*s*) symmetry in the Septet state

Ru	0.00000000	0.00000000	-1.50389700
Ru	0.00000000	0.00000000	1.51550000
N	0.00000000	1.99462100	-1.70543900
N	0.00000000	-1.99462100	-1.70543900
N	-1.11998800	1.65135500	1.70955000
N	1.11998800	-1.65135500	1.70955000
N	1.99654200	-0.00118000	-1.72228600
N	-1.99654200	0.00118000	-1.72228600
N	1.65147800	1.12297800	1.72762800
N	-1.65147800	-1.12297800	1.72762800
C	1.13219900	2.81736800	-1.79583400
C	-1.13219900	-2.81736800	-1.79583400
C	-0.64549300	2.96748300	1.77851200
C	0.64549300	-2.96748300	1.77851200
C	-1.13189600	2.81671700	-1.78139000
C	1.13189600	-2.81671700	-1.78139000
C	-2.51930100	1.69558900	1.79414500
C	2.51930100	-1.69558900	1.79414500
C	2.81336300	-1.13430500	-1.80225100
C	-2.81336300	1.13430500	-1.80225100
C	2.96516900	0.64176100	1.81699800
C	-2.96516900	-0.64176100	1.81699800
C	2.81336900	1.13437700	-1.81625800
C	-2.81336900	-1.13437700	-1.81625800
C	1.69090400	2.51947600	1.80140400
C	-1.69090400	-2.51947600	1.80140400
N	2.42315900	2.41159000	-1.83679200
N	-2.42315900	-2.41159000	-1.83679200
N	0.65097300	3.36017000	1.80756200
N	-0.65097300	-3.36017000	1.80756200
N	-2.42494400	2.41369400	-1.81235800
N	2.42494400	-2.41369400	-1.81235800
N	-3.35925300	0.63438300	1.83472600
N	3.35925300	-0.63438300	1.83472600
C	0.69469800	4.19124700	-1.89053400
C	-0.69469800	-4.19124700	-1.89053400
C	-1.77986700	3.85949700	1.86996300
C	1.77986700	-3.85949700	1.86996300
C	-0.69487100	4.19138100	-1.88089600

C	0.69487100	-4.19138100	-1.88089600
C	-2.92939600	3.07853900	1.88072300
C	2.92939600	-3.07853900	1.88072300
C	4.20044700	-0.68885400	-1.91812500
C	-4.20044700	0.68885400	-1.91812500
C	3.86223200	1.78975900	1.92341600
C	-3.86223200	-1.78975900	1.92341600
C	4.19979700	0.68835200	-1.92840700
C	-4.19979700	-0.68835200	-1.92840700
C	3.08938400	2.92981800	1.91187800
C	-3.08938400	-2.92981800	1.91187800
H	1.36706000	5.03374600	-1.96191100
H	-1.36706000	-5.03374600	-1.96191100
H	-1.69621600	4.93501100	1.92945200
H	1.69621600	-4.93501100	1.92945200
H	-1.36861500	5.03334400	-1.94735900
H	1.36861500	-5.03334400	-1.94735900
H	-3.95909700	3.39847700	1.94664300
H	3.95909700	-3.39847700	1.94664300
H	5.04015600	-1.36540100	-1.98684600
H	-5.04015600	1.36540100	-1.98684600
H	4.93663400	1.70238000	2.00109700
H	-4.93663400	-1.70238000	2.00109700
H	5.03918100	1.36418400	-2.01007300
H	-5.03918100	-1.36418400	-2.01007300
H	3.40495900	3.96128900	1.97551500
H	-3.40495900	-3.96128900	1.97551500

$(RuPz)_2$: C_2 (*s*) symmetry in the Nonet state

Ru	0.00000000	0.00000000	1.51831200
Ru	0.00000000	0.00000000	-1.39522600
N	-1.40964700	1.41689000	1.63769200
N	1.40964700	-1.41689000	1.63769200
N	0.00000000	2.00000300	-1.59680700
N	0.00000000	-2.00000300	-1.59680700
N	-1.38738100	-1.44175100	1.63642300
N	1.38738100	1.44175100	1.63642300
N	-1.99378600	0.00012000	-1.68912200
N	1.99378600	-0.00012000	-1.68912200
C	-2.81453400	1.16953100	1.70644600
C	2.81453400	-1.16953100	1.70644600
C	-1.13098900	2.81144500	-1.77634300

C	1.13098900	-2.81144500	-1.77634300
C	-1.21218200	2.78915700	1.70135900
C	1.21218200	-2.78915700	1.70135900
C	1.13153700	2.81119100	-1.77640300
C	-1.13153700	-2.81119100	-1.77640300
C	-1.16578700	-2.80997500	1.70060700
C	1.16578700	2.80997500	1.70060700
C	-2.81516200	-1.13607800	-1.68823700
C	2.81516200	1.13607800	-1.68823700
C	-2.79494100	-1.21735800	1.70614600
C	2.79494100	1.21735800	1.70614600
C	-2.81502100	1.13688900	-1.68829800
C	2.81502100	-1.13688900	-1.68829800
N	-3.40704700	-0.03113200	1.73813600
N	3.40704700	0.03113200	1.73813600
N	-2.43318400	2.40763900	-1.75265200
N	2.43318400	-2.40763900	-1.75265200
N	-0.02666500	3.43805400	1.71578300
N	0.02666500	-3.43805400	1.71578300
N	2.43336200	2.40721100	-1.75275800
N	-2.43336200	-2.40721100	-1.75275800
C	-3.48524800	2.44879300	1.79832400
C	3.48524800	-2.44879300	1.79832400
C	-0.69454900	4.16446200	-2.03646100
C	0.69454900	-4.16446200	-2.03646100
C	-2.51810600	3.43586600	1.79468000
C	2.51810600	-3.43586600	1.79468000
C	0.69523600	4.16433300	-2.03661000
C	-0.69523600	-4.16433300	-2.03661000
C	-2.46414900	-3.48009000	1.79429700
C	2.46414900	3.48009000	1.79429700
C	-4.21768800	-0.68400900	-1.66487600
C	4.21768800	0.68400900	-1.66487600
C	-3.44567600	-2.51173000	1.79833900
C	3.44567600	2.51173000	1.79833900
C	-4.21763700	0.68492300	-1.66479400
C	4.21763700	-0.68492300	-1.66479400
H	-4.55785500	2.55789100	1.86635700
H	4.55785500	-2.55789100	1.86635700
H	-1.36794600	4.99393700	-2.19516700
H	1.36794600	-4.99393700	-2.19516700
H	-2.64778400	4.50680200	1.85244100
H	2.64778400	-4.50680200	1.85244100
H	1.36875200	4.99366000	-2.19568400

H	-1.36875200	-4.99366000	-2.19568400
H	-2.57442300	-4.55323200	1.85238500
H	2.57442300	4.55323200	1.85238500
H	-5.05840600	-1.36272600	-1.66019700
H	5.05840600	1.36272600	-1.66019700
H	-4.51645300	-2.63763200	1.86636600
H	4.51645300	2.63763200	1.86636600
H	-5.05822700	1.36382600	-1.66031800
H	5.05822700	-1.36382600	-1.66031800

(RuPz)·py$_2$: C_2 (*s*) symmetry in the Singlet state

Ru	0.00000000	0.00000000	0.00020200
N	0.00000000	0.00000000	2.12540000
N	0.00000000	0.00000000	-2.12500400
N	0.00000000	2.00763100	0.00024500
N	0.00000000	-2.00763100	0.00024500
N	-2.00763300	0.00010800	0.00045700
N	2.00763300	-0.00010800	0.00045700
C	-1.12915200	2.82005800	0.03013000
C	1.12915200	-2.82005800	0.03013000
C	1.12925800	2.81990300	-0.02991500
C	-1.12925800	-2.81990300	-0.02991500
C	-2.81999300	-1.12907000	-0.03003300
C	2.81999300	1.12907000	-0.03003300
C	-2.81996400	1.12934000	0.02999900
C	2.81996400	-1.12934000	0.02999900
N	-2.41356800	2.41373400	0.05030700
N	2.41356800	-2.41373400	0.05030700
N	2.41363600	2.41348500	-0.05043500
N	-2.41363600	-2.41348500	-0.05043500
C	-0.68759500	4.21962100	0.02043000
C	0.68759500	-4.21962100	0.02043000
C	0.68787000	4.21953000	-0.02056100
C	-0.68787000	-4.21953000	-0.02056100
C	-4.21957900	-0.68755700	-0.02150500
C	4.21957900	0.68755700	-0.02150500
C	-4.21956400	0.68791400	0.01948300
C	4.21956400	-0.68791400	0.01948300
H	-1.36404400	5.06254300	0.04083900
H	1.36404400	-5.06254300	0.04083900
H	1.36442200	5.06236100	-0.04127800
H	-1.36442200	-5.06236100	-0.04127800

H	-5.06246700	-1.36401000	-0.04308600
H	5.06246700	1.36401000	-0.04308600
H	-5.06244200	1.36444400	0.03900500
H	5.06244200	-1.36444400	0.03900500
C	-0.82677300	-0.82771900	2.82803100
C	0.82677300	0.82771900	2.82803100
C	-0.85292600	-0.85385700	4.22840800
C	0.85292600	0.85385700	4.22840800
C	0.82792100	-0.82657300	-2.82765500
C	-0.82792100	0.82657300	-2.82765500
C	0.85414000	-0.85263700	-4.22803400
C	-0.85414000	0.85263700	-4.22803400
C	0.00000000	0.00000000	4.95002100
C	0.00000000	0.00000000	-4.94965800
H	0.00000000	0.00000000	6.03632200
H	0.00000000	0.00000000	-6.03596400
H	-1.47362300	-1.47532700	2.25422900
H	1.47362300	1.47532700	2.25422900
H	-1.53207800	-1.53371800	4.73280100
H	1.53207800	1.53371800	4.73280100
H	1.47569800	-1.47326200	-2.25386500
H	-1.47569800	1.47326200	-2.25386500
H	1.53429100	-1.53150100	-4.73242300
H	-1.53429100	1.53150100	-4.73242300

(RuPz)·py$_2$: C_2 (*e*) symmetry in the Singlet state

Ru	0.00000000	0.00000000	0.00045300
N	0.00000000	0.00000000	-2.12889000
N	0.00000000	0.00000000	2.12928400
N	-1.42178000	1.41736300	0.00012000
N	1.42178000	-1.41736300	0.00012000
N	1.42178000	1.41735800	0.00000000
N	-1.42178000	-1.41735800	0.00000000
C	-1.19448700	2.78834700	-0.00034400
C	1.19448700	-2.78834700	-0.00034400
C	-2.79734900	1.19670700	-0.00022400
C	2.79734900	-1.19670700	-0.00022400
C	2.79734600	1.19669700	0.00010900
C	-2.79734600	-1.19669700	0.00010900
C	1.19448700	2.78833000	-0.00008100
C	-1.19448700	-2.78833000	-0.00008100

N	0.00000000	3.40810800	-0.00032000
N	0.00000000	-3.40810800	-0.00032000
N	-3.41996400	0.00001000	-0.00006500
N	3.41996400	-0.00001000	-0.00006500
C	-2.49498500	3.46915200	-0.00091500
C	2.49498500	-3.46915200	-0.00091500
C	-3.47162200	2.49972900	-0.00075100
C	3.47162200	-2.49972900	-0.00075100
C	3.47162000	2.49972100	-0.00000800
C	-3.47162000	-2.49972100	-0.00000800
C	2.49498000	3.46914300	-0.00007200
C	-2.49498000	-3.46914300	-0.00007200
H	-2.60875300	4.54412700	-0.00126600
H	2.60875300	-4.54412700	-0.00126600
H	-4.54582800	2.62053600	-0.00094400
H	4.54582800	-2.62053600	-0.00094400
H	4.54582400	2.62053900	-0.00020800
H	-4.54582400	-2.62053900	-0.00020800
H	2.60875500	4.54411500	-0.00029700
H	-2.60875500	-4.54411500	-0.00029700
C	1.16988000	0.00109200	-2.83160400
C	-1.16988000	-0.00109200	-2.83160400
C	1.20695300	0.00111100	-4.23192300
C	-1.20695300	-0.00111100	-4.23192300
C	1.16990200	-0.00006500	2.83200900
C	-1.16990200	0.00006500	2.83200900
C	1.20695400	-0.00006400	4.23231800
C	-1.20695400	0.00006400	4.23231800
C	0.00000000	0.00000000	-4.95345600
C	0.00000000	0.00000000	4.95385400
H	0.00000000	0.00000000	-6.03978000
H	0.00000000	0.00000000	6.04017700
H	2.08447600	0.00197300	-2.25700500
H	-2.08447600	-0.00197300	-2.25700500
H	2.16791200	0.00199200	-4.73630200
H	-2.16791200	-0.00199200	-4.73630200
H	2.08448000	-0.00014000	2.25736900
H	-2.08448000	0.00014000	2.25736900
H	2.16791200	-0.00012200	4.73670200
H	-2.16791200	0.00012200	4.73670200

(RuPz)·py$_2$: C_2 (*s*) symmetry in the Triplet state

Ru	0.00000000	0.00000000	0.00054800
N	0.00000000	0.00000000	-2.12840700
N	0.00000000	0.00000000	2.12900900
N	0.00000000	2.03193600	0.00033700
N	0.00000000	-2.03193600	0.00033700
N	1.99563800	-0.00002200	-0.00014100
N	-1.99563800	0.00002200	-0.00014100
C	1.13415900	2.83977900	-0.03726500
C	-1.13415900	-2.83977900	-0.03726500
C	-1.13416000	2.83980000	0.03701900
C	1.13416000	-2.83980000	0.03701900
C	2.81973000	-1.13816200	0.03469600
C	-2.81973000	1.13816200	0.03469600
C	2.81971500	1.13812600	-0.03529400
C	-2.81971500	-1.13812600	-0.03529400
N	2.40677600	2.44789800	-0.05866100
N	-2.40677600	-2.44789800	-0.05866100
N	-2.40680300	2.44798400	0.05807400
N	2.40680300	-2.44798400	0.05807400
C	0.68439400	4.24775900	-0.02639700
C	-0.68439400	-4.24775900	-0.02639700
C	-0.68438900	4.24777300	0.02506400
C	0.68438900	-4.24777300	0.02506400
C	4.18117600	-0.70431900	0.02296600
C	-4.18117600	0.70431900	0.02296600
C	4.18116800	0.70426200	-0.02414400
C	-4.18116800	-0.70426200	-0.02414400
H	1.36313400	5.08896400	-0.05212300
H	-1.36313400	-5.08896400	-0.05212300
H	-1.36313900	5.08899700	0.04986800
H	1.36313900	-5.08899700	0.04986800
H	5.03196800	-1.37054300	0.04538000
H	-5.03196800	1.37054300	0.04538000
H	5.03195100	1.37048400	-0.04694200
H	-5.03195100	-1.37048400	-0.04694200
C	0.82439600	-0.83298600	-2.82442400
C	-0.82439600	0.83298600	-2.82442400
C	0.85223000	-0.85616500	-4.22461900
C	-0.85223000	0.85616500	-4.22461900
C	0.82396400	0.83339900	2.82510600
C	-0.82396400	-0.83339900	2.82510600
C	0.85149700	0.85685700	4.22532800
C	-0.85149700	-0.85685700	4.22532800

C	0.00000000	0.00000000	-4.94423400
C	0.00000000	0.00000000	4.94504200
H	0.00000000	0.00000000	-6.03059300
H	0.00000000	0.00000000	6.03145200
H	1.46783100	-1.48181500	-2.24802100
H	-1.46783100	1.48181500	-2.24802100
H	1.53029600	-1.53623300	-4.72961500
H	-1.53029600	1.53623300	-4.72961500
H	1.46713000	1.48249700	2.24869300
H	-1.46713000	-1.48249700	2.24869300
H	1.52880400	1.53772200	4.73027400
H	-1.52880400	-1.53772200	4.73027400

(RuPz)·py$_2$: C_2 (*e*) symmetry in the Triple state

Ru	0.00000000	0.00000000	0.00029000
N	0.00000000	0.00000000	2.13020600
N	0.00000000	0.00000000	-2.12976100
N	0.00000000	2.03028200	0.00004800
N	0.00000000	-2.03028200	0.00004800
N	-1.99633400	-0.01722000	-0.00041700
N	1.99633400	0.01722000	-0.00041700
C	-1.14776500	2.83190000	-0.00108200
C	1.14776500	-2.83190000	-0.00108200
C	1.12177400	2.84662800	-0.00071800
C	-1.12177400	-2.84662800	-0.00071800
C	-2.81750300	-1.15263700	0.00069200
C	2.81750300	1.15263700	0.00069200
C	-2.82381100	1.12403000	0.00035500
C	2.82381100	-1.12403000	0.00035500
N	-2.41263500	2.42985000	-0.00049900
N	2.41263500	-2.42985000	-0.00049900
N	2.40445400	2.46452900	0.00014300
N	-2.40445400	-2.46452900	0.00014300
C	-0.70928100	4.24009100	-0.00279400
C	0.70928100	-4.24009100	-0.00279400
C	0.66138400	4.25075400	-0.00246600
C	-0.66138400	-4.25075400	-0.00246600
C	-4.18276400	-0.71866000	0.00240700
C	4.18276400	0.71866000	0.00240700
C	-4.18359700	0.68925200	0.00217300
C	4.18359700	-0.68925200	0.00217300
H	-1.39448800	5.07635800	-0.00409500

H	1.39448800	-5.07635800	-0.00409500
H	1.33401200	5.09725400	-0.00359200
H	-1.33401200	-5.09725400	-0.00359200
H	-5.03250100	-1.38668600	0.00403800
H	5.03250100	1.38668600	0.00403800
H	-5.03468300	1.35538000	0.00345700
H	5.03468300	-1.35538000	0.00345700
C	-0.82094200	-0.83663300	2.82686600
C	0.82094200	0.83663300	2.82686600
C	-0.84809000	-0.85986600	4.22699400
C	0.84809000	0.85986600	4.22699400
C	-0.82174000	-0.83578800	-2.82649700
C	0.82174000	0.83578800	-2.82649700
C	-0.84872000	-0.85920200	-4.22664600
C	0.84872000	0.85920200	-4.22664600
C	0.00000000	0.00000000	4.94671600
C	0.00000000	0.00000000	-4.94644200
H	0.00000000	0.00000000	6.03301300
H	0.00000000	0.00000000	-6.03276900
H	-1.46202100	-1.48848000	2.25171000
H	1.46202100	1.48848000	2.25171000
H	-1.52304000	-1.54318100	4.73177700
H	1.52304000	1.54318100	4.73177700
H	-1.46354500	-1.48695800	-2.25139500
H	1.46354500	1.48695800	-2.25139500
H	-1.52407800	-1.54215800	-4.73137300
H	1.52407800	1.54215800	-4.73137300