1. The checkpoint file after CCSD calculation only contains information about HF reference wave function. The density associated with the CCSD correlated level must be generated separately.
2. Take the stationary structure's checkpoint file and start with the population analysis

```
%chk=RuP3HCl_mini_trans_CCSD_BS4
#p CCSD Chkbasis Guess(Check) Geom(NoDistance,AllCheck)
  Pop(NPA,Full,MKUFF) Density(Current) Punch(NaturalOrbitals) Output(WFX)

RuP3HCl_mini_trans_CCSD_BS4.wfx
```

   This will generate a FORT.7 file that need to be saved, because it has the natural orbital coefficients. Please note that from correlated electron density - we can only use natural orbitals (orbital energies are gone) with occupancy numbers. For example: HOMO and LUMO regions are as follows

```
                      36        37        38        39        40
    Eigenvalues --   1.95051   1.94893   1.94839   1.94432   1.94377
                      41        42        43        44        45
    Eigenvalues --   1.94236   1.93570   1.93379   1.93063   0.05744
                      46        47        48        49        50
    Eigenvalues --   0.05014   0.04590   0.04312   0.04006   0.03471
                      51        52        53        54        55
    Eigenvalues --   0.03392   0.03040   0.02283   0.02220   0.02174
```

   The lack of 2.0 occupation on the HOMOs and the presence of more than 0.00 electrons on the virtual orbitals (HOMO=MO44; LUMO=MO45) indicate multi-reference nature of the electronic structure. Some type of CAS/MRCI treatment may be required.

3. Now we have the density generated and saved into the checkpoint file; however, the density itself cannot be visualized from the MO coefficients, because they are still in the FORT.7 file. Rename FORT.7 to 'RuP3HCl_mini_trans_CCSD_BS4_gs.mo' and use it for

```
%oldchk=RuP3HCl_mini_trans_CCSD_BS4
%chk=RuP3HCl_mini_trans_CCSD_BS4_natorb
#p chkbasis geom(allcheck,nodistance)
   guess(cards,only,save,naturalorbitals) Pop(Full)

@RuP3HCl_mini_trans_CCSD_BS4_gs.mo
```

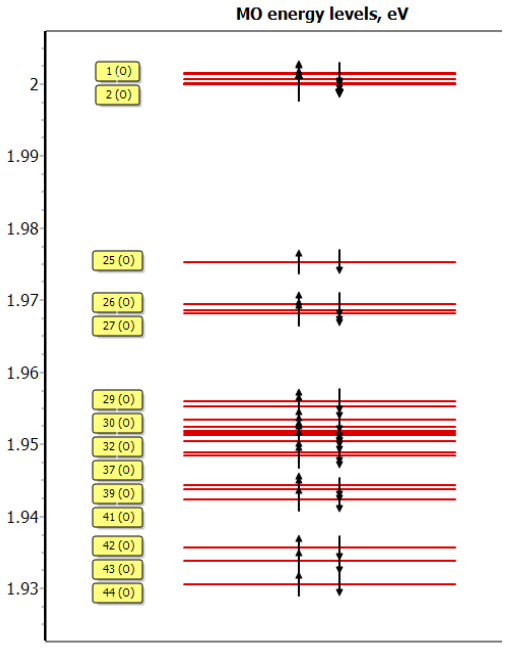
4. Generate the formatted checkpoint file to visualize the orbitals

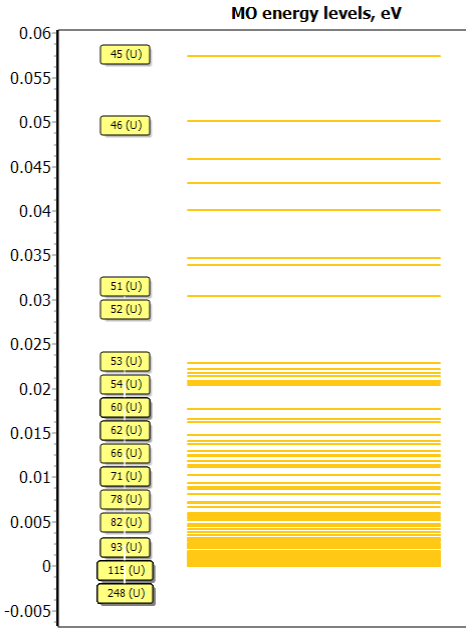
```
formchk RuP3HCl_mini_trans_CCSD_BS4_natorb.chk
```

5. In chemcraft/gaussview … open up the formatted checkpoint file
   a. Orbital energy diagrams (of course MO energies are no longer correct, it should read as MO occupations)

MO energies (A.U.)

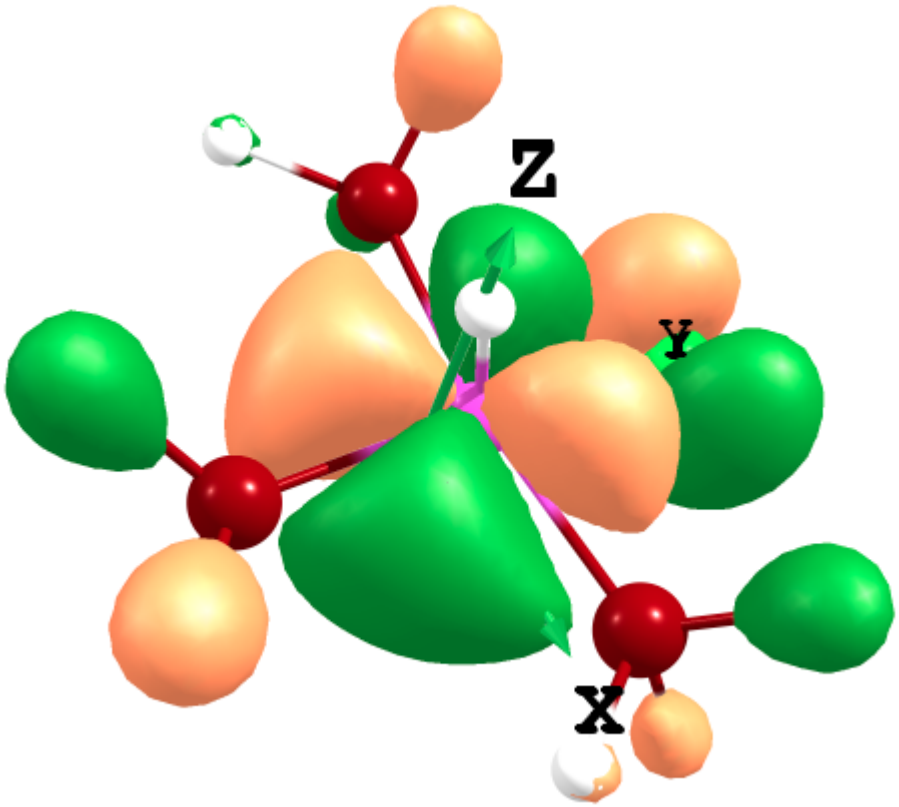
MO num	Energy	Occupancy
40	1.94376986	Occupied
41	1.94235804	Occupied
42	1.93569964	Occupied
43	1.93378796	Occupied
44	1.93063186	Occupied
45	0.0574368549	Unoccupied
46	0.0501357471	Unoccupied
47	0.0458959244	Unoccupied
48	0.0431249562	Unoccupied
49	0.0400610613	Unoccupied
50	0.0347137084	Unoccupied
51	0.0339181566	Unoccupied
52	0.03040215	Unoccupied
53	0.0228331953	Unoccupied
54	0.0222039278	Unoccupied



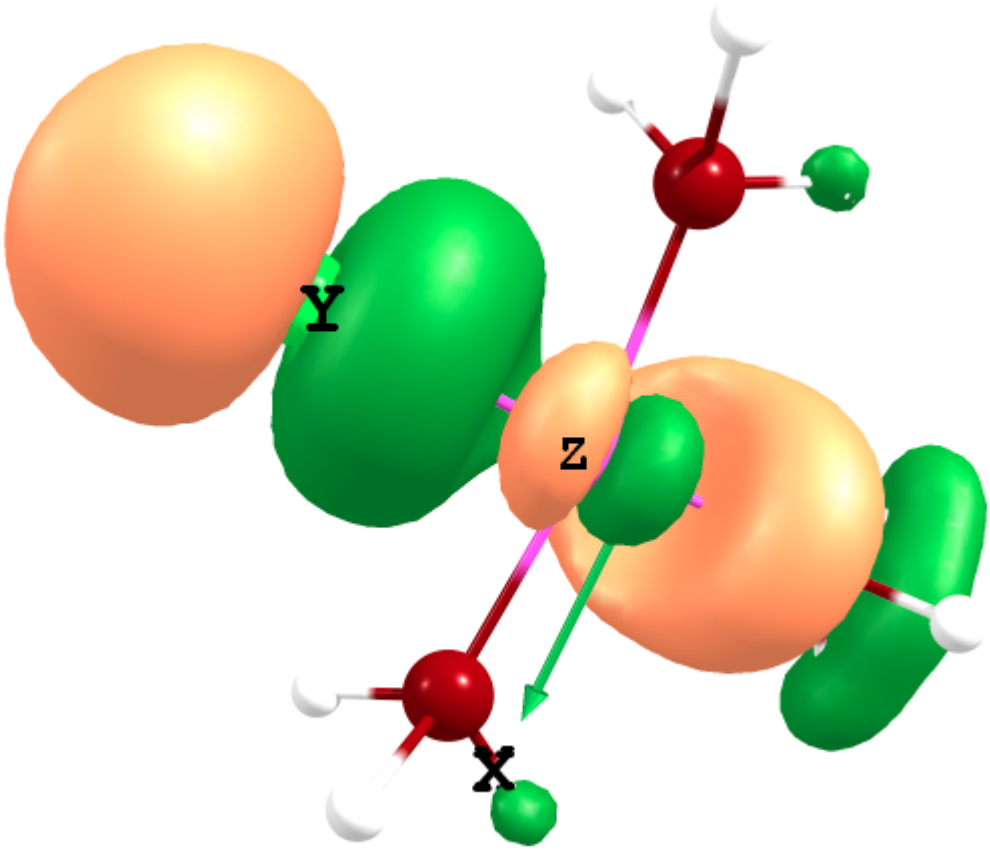


b. Render the virtual MOs for the highest 5 occupied = HOMO-4 … HOMO; MO40-MO44 and lowest 5 unoccupied orbitals = LUMO … LUMO+4; MO45-MO49
(Map points per Å is 5, Map size = 1 - check save cube file only if you really need the orbital plot contour value for orbitals 0.03)

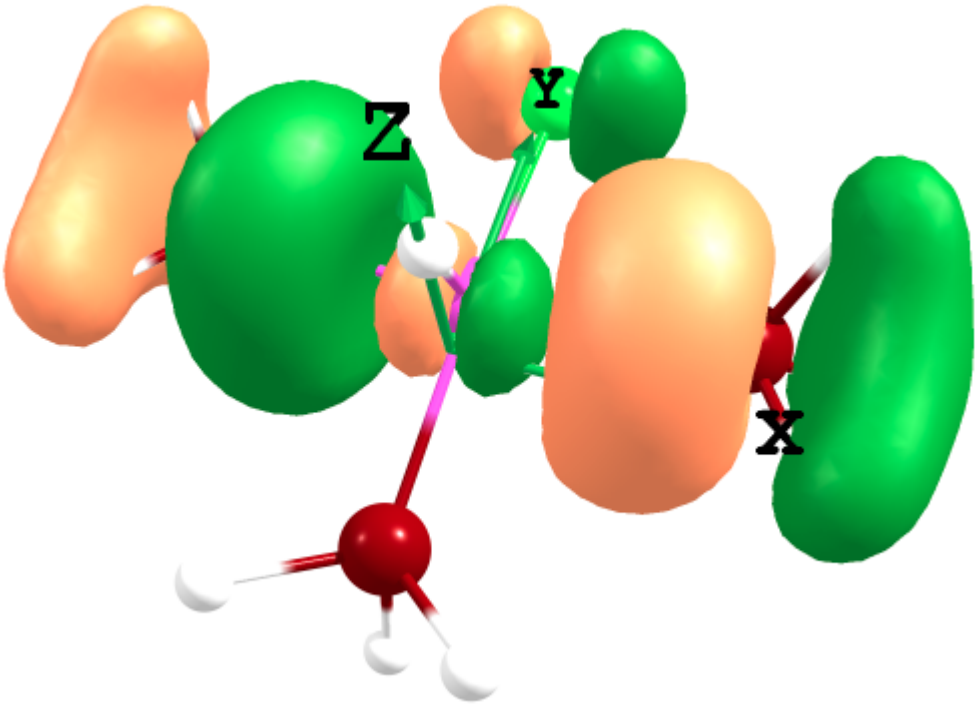
HOMO-4 MO40 Ru xy (slightly out of plane), Cl pi 3p and P-H sigma and



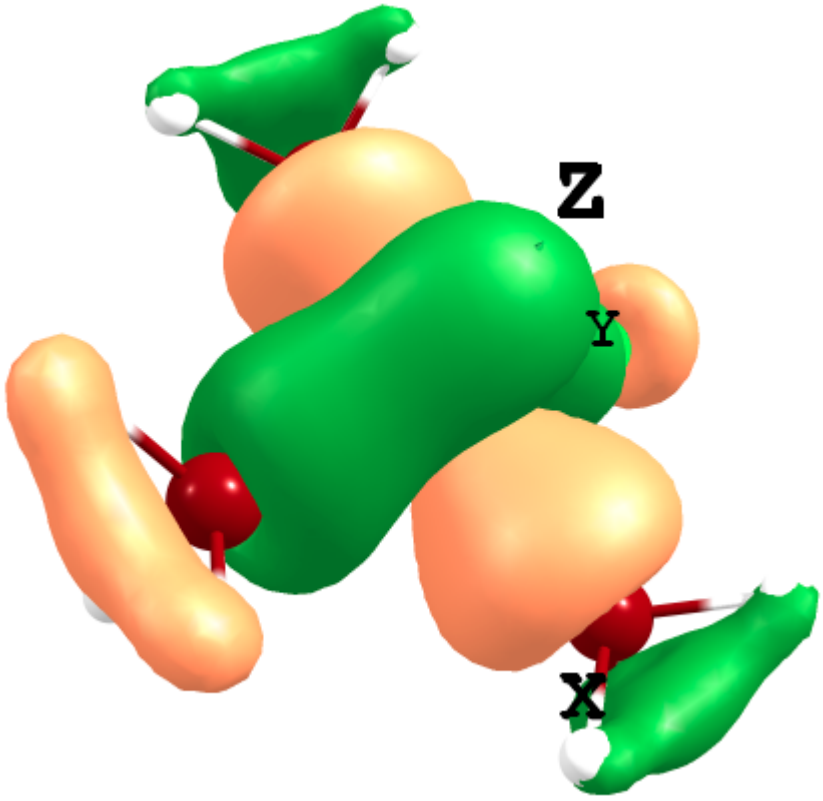
HOMO-3 MO41 Ru 5py sigma bonding interaction with Cl 3p



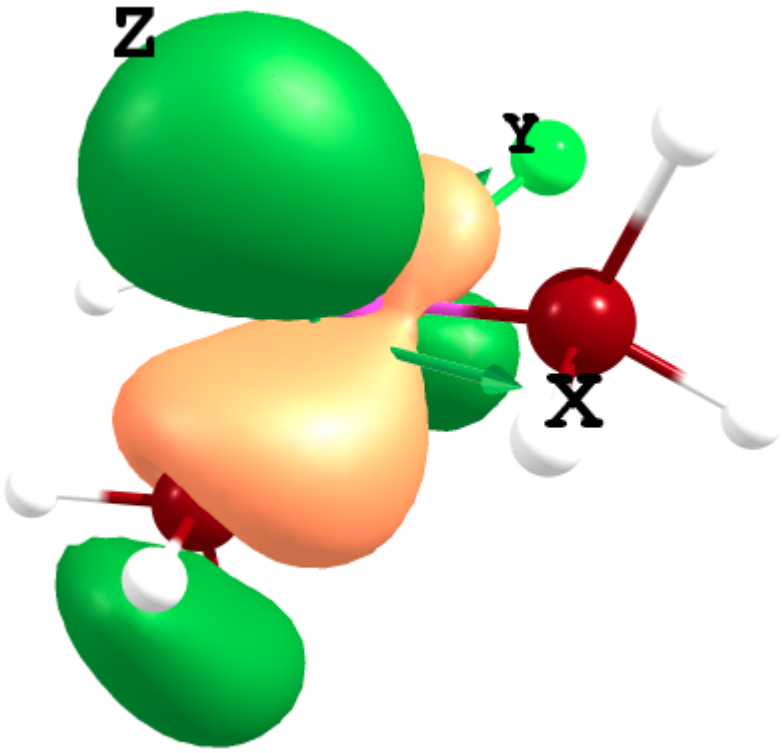
HOMO-2 MO42 Ru 5px sigma bonding interaction with the PH3 lone pairs



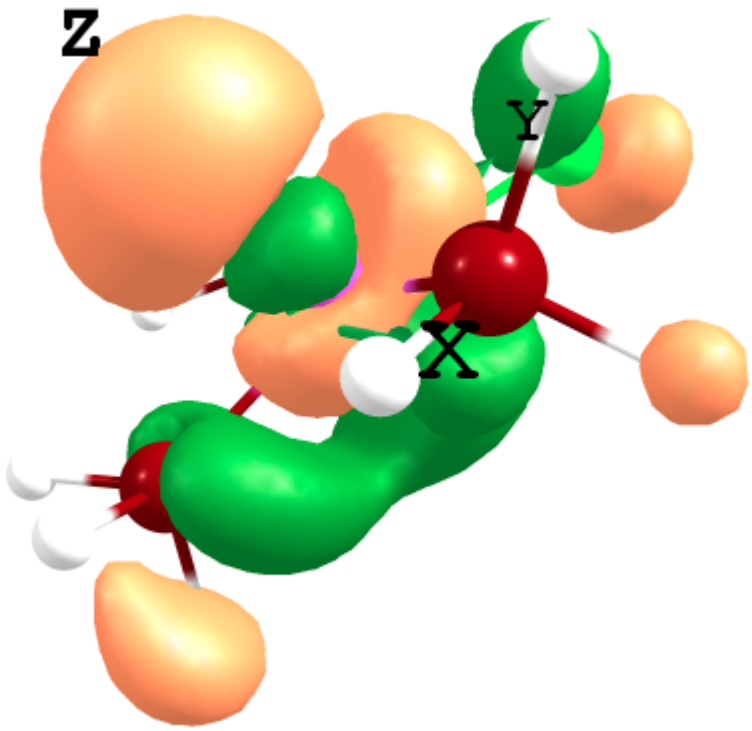
HOMO-1 MO43 Ru 4dx2-y2 + Cl 3px + P-H s



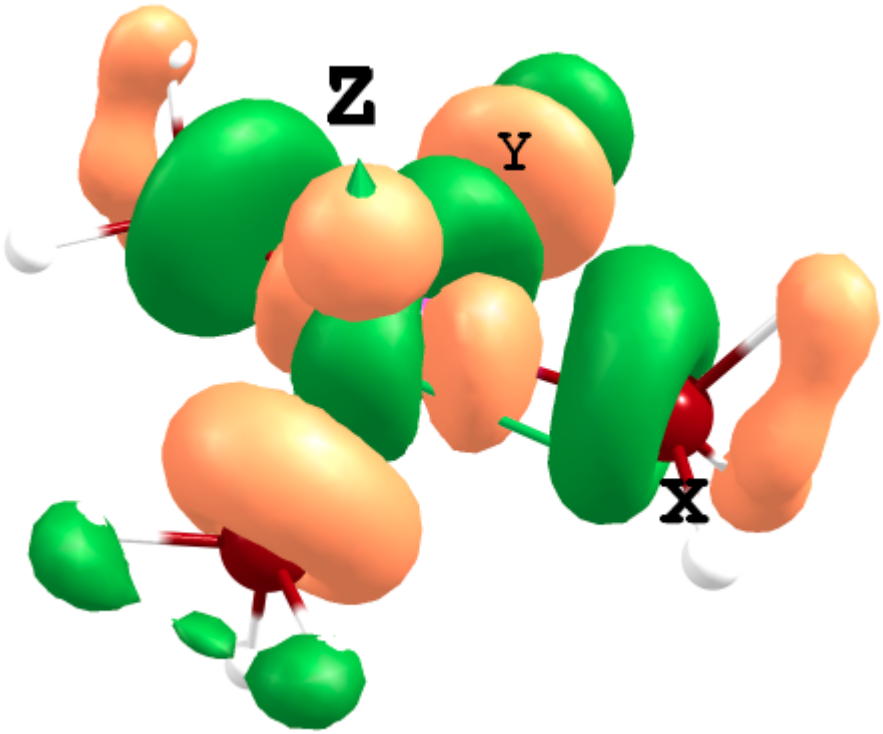
HOMO MO44 Ru 4dyz + Cl 3py + P-H s



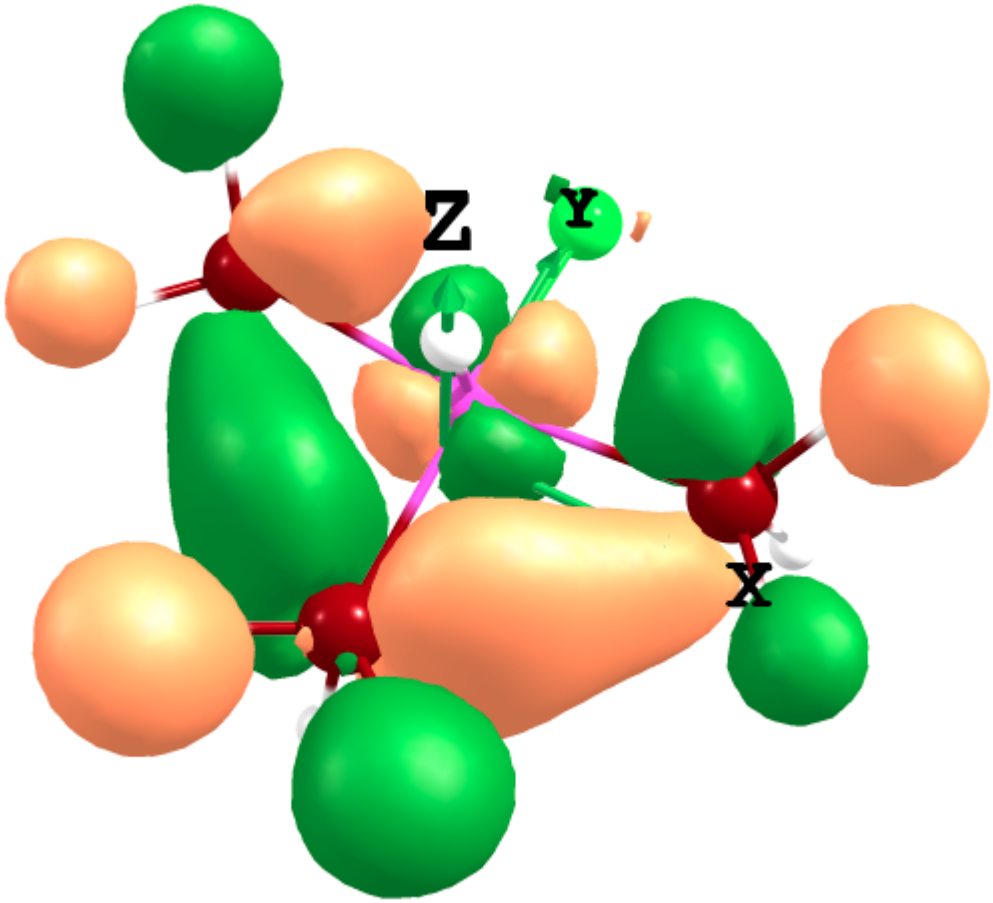
LUMO MO45 Ru 4dyz antibonding with H s + Cl 3pz + P-H s



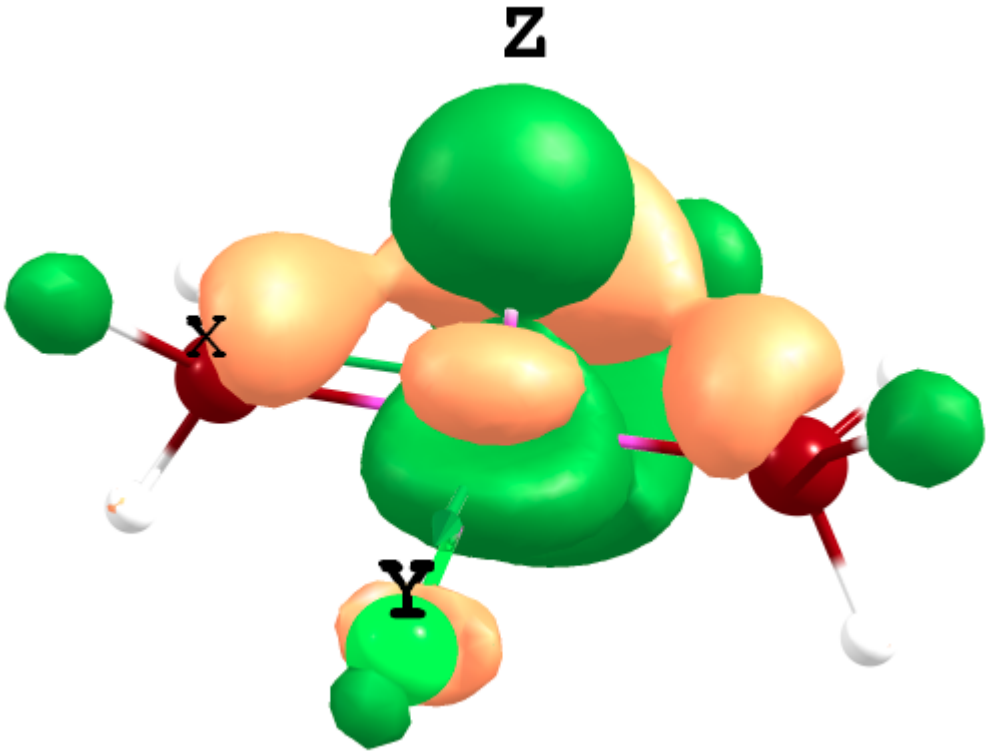
LUMO+1 MO46 Ru 4dx2-y2 antibonding with P 3px/3py + Cl 3py



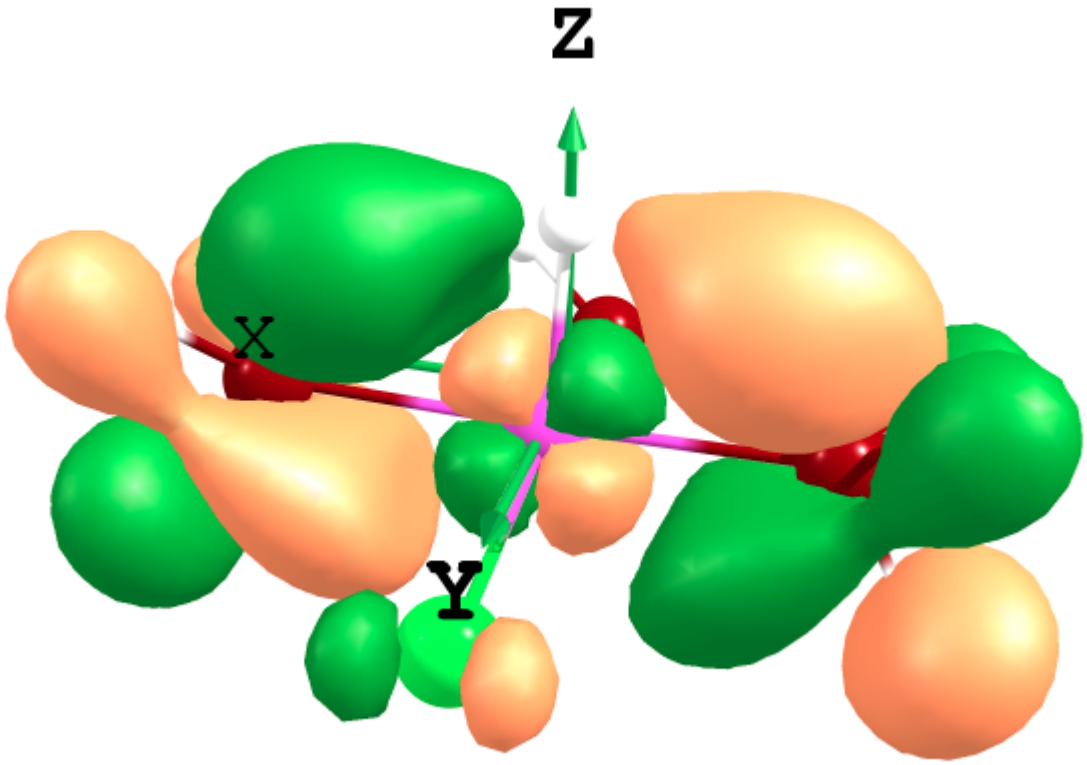
LUMO+2 MO47 Ru 4dxy + P-H s/s* back-donation orbital



LUMO+3 MO48 Ru 4dz2 + P-H s/s* back-donation orbital



LUMO+4 MO49 Ru 4xz + P-H s/s* back-donation



6. The focus is on the covalent bonding i.e. Ru-H (LUMO) Ru-P/Cl (LUMO+1)
7. Let's compare and contrast atomic point charges (AIM analysis - need to use AIMQB)

```
/AIMAll/aimqb.ish -nogui -nproc=8 $1.wfx >& $1_aimqb.out
```

Check for minimal basis set definitions:	core orbitals Ru [core potential] 4s4p	2.0 e^- enforced
	valence orbitals 4d 5s 5p	varied 0-2.0 e^-
	Rydberg orbitals 5d 6s 6p … rest	minimized ~ 0 e^-

```
 [ 28 electrons found in the effective core potential]
 WARNING:  4 low occupancy (<1.9990e) core orbitals found on Ru    1

     1   Ru    1  S      Cor( 4S)     1.98988          maybe the ECP basis set
     7   Ru    1  px     Cor( 4p)     1.99399          is not enough for this.
    11   Ru    1  py     Cor( 4p)     1.99324          3s3p3d should be the core!
    15   Ru    1  pz     Cor( 4p)     1.98459

           1 low occupancy (<1.9990e) core orbital  found on  P    4
           1 low occupancy (<1.9990e) core orbital  found on  P    8
           1 low occupancy (<1.9990e) core orbital  found on  P   12
```

Must check that you are using the correct (NON HF reference) density

```
 ***********************************************************************

            Population analysis using the QCI/CC density.

 ***********************************************************************
```

Atom	No	Charge	Core	Valence	Rydberg	Total
Ru	1	-1.34020	35.96171	9.25439	0.12410	45.34020
H	2	0.18338	0.00000	0.80691	0.00971	0.81662
Cl	3	-0.41339	9.99935	7.26269	0.15134	17.41339
P	4	0.65523	9.99589	4.21952	0.12935	14.34477
H	5	-0.04170	0.00000	1.02620	0.01550	1.04170
H	6	-0.04154	0.00000	1.02607	0.01547	1.04154
H	7	-0.04083	0.00000	1.02565	0.01518	1.04083
P	8	0.56854	9.99659	4.31373	0.12115	14.43146
H	9	-0.03641	0.00000	1.02181	0.01460	1.03641
H	10	0.00054	0.00000	0.98554	0.01392	0.99946
H	11	-0.01311	0.00000	0.99888	0.01423	1.01311
P	12	0.56847	9.99659	4.31381	0.12114	14.43153
H	13	0.00055	0.00000	0.98553	0.01392	0.99945
H	14	-0.01318	0.00000	0.99895	0.01423	1.01318
H	15	-0.03635	0.00000	1.02175	0.01460	1.03635
* Total *		0.00000	75.95013	39.26143	0.78844	116.00000

If Rydberg occupation is big (not sure how big though) indication of inappropriate single determinant electronic structure, excited state mixing, need to use multi-reference treatment

Atom	No	Natural Electron Configuration	
Ru	1	[core]5S(0.46)4d(7.92)5p(0.87)4f(0.03)5d(0.07)6p(0.01)6d(0.01)	covalent+ionic bonding Ru-1.34 effectively
(Ru	1	[core]5S(0.00)4d(8.00)5p(0.00)5d(0.00)	ionic only bonding Ru+2 theoretically)
H	2	1S(0.81)2p(0.01)	
Cl	3	[core]3S(1.85)3p(5.41)4S(0.01)3d(0.10)4p(0.03)4f(0.01)	
P	4	[core]3S(1.25)3p(2.97)3d(0.09)4p(0.02)4f(0.01)	
H	5	1S(1.03)2S(0.01)2p(0.01)	
H	6	1S(1.03)2S(0.01)2p(0.01)	
H	7	1S(1.03)2p(0.01)	
P	8	[core]3S(1.30)3p(3.01)3d(0.08)4p(0.02)4f(0.01)	
H	9	1S(1.02)2p(0.01)	
H	10	1S(0.99)2p(0.01)	
H	11	1S(1.00)2p(0.01)	
P	12	[core]3S(1.30)3p(3.01)3d(0.08)4p(0.02)4f(0.01)	
H	13	1S(0.99)2p(0.01)	
H	14	1S(1.00)2p(0.01)	
H	15	1S(1.02)2p(0.01)	

Mulliken:

1	Ru	0.147552
2	H	0.005798
3	Cl	-0.536799
4	P	-0.112567
5	H	0.054957
6	H	0.054838
7	H	0.058871
8	P	-0.057899
9	H	0.052568
10	H	0.091368
11	H	0.077658
12	P	-0.057939
13	H	0.091385
14	H	0.077582
15	H	0.052627

ESP charges:

1	Ru	0.312242
2	H	-0.167805
3	Cl	-0.476891
4	P	0.109525
5	H	0.009667
6	H	0.009294
7	H	-0.031880
8	P	-0.051974
9	H	0.036445
10	H	0.080801
11	H	0.053556
12	P	-0.061121
13	H	0.083696
14	H	0.056573
15	H	0.037873

NPA charges:

Ru	1	-1.34020
H	2	0.18338
Cl	3	-0.41339
P	4	0.65523
H	5	-0.04170
H	6	-0.04154
H	7	-0.04083
P	8	0.56854
H	9	-0.03641
H	10	0.00054
H	11	-0.01311
P	12	0.56847
H	13	0.00055
H	14	-0.01318
H	15	-0.03635

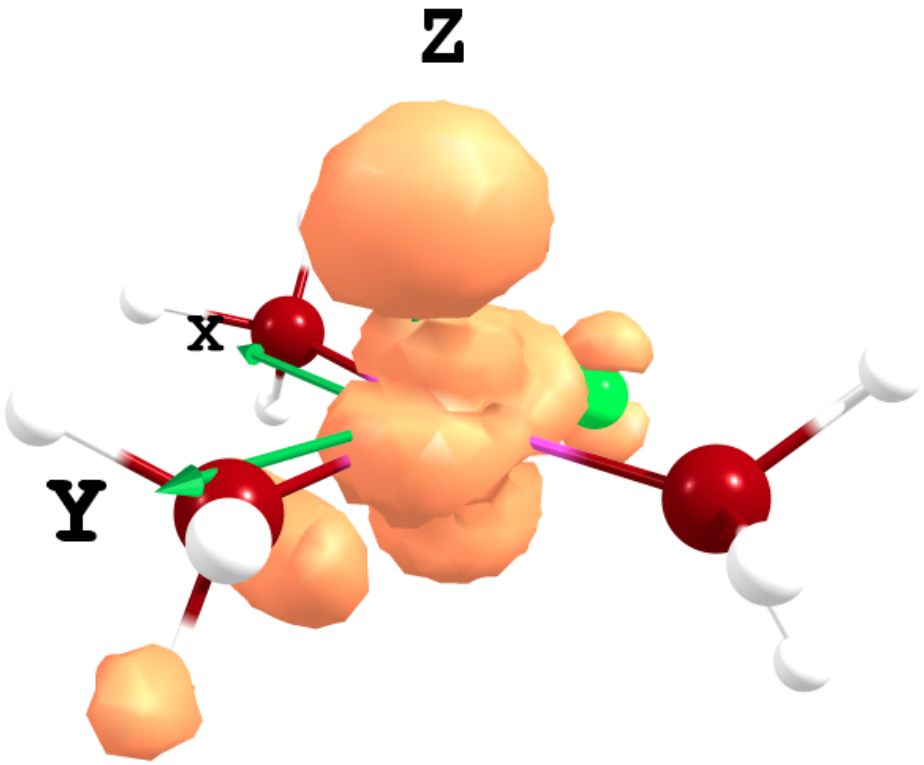
AIM charges (from .int):

Ru	1	0.368
H	2	-0.145
Cl	3	-0.688
P	4	1.886
H	5	-0.587
H	6	-0.587
H	7	-0.587
P	8	1.865
H	9	-0.584
H	10	-0.549
H	11	-0.562
P	12	1.865
H	13	-0.549
H	14	-0.562
H	15	-0.584

8. Looking at LUMO - same machinery, but must not use “NaturalOrbitals” keyword in guess

```
%oldchk=RuP3HCl_mini_trans_CCSD_BS4_natorb
%chk=RuP3HCl_mini_trans_CCSD_BS4_LUMO
#p uhf chkbasis geom(check,nodistance)
   guess(check,only,save) Pop(Full,NPA,MKUFF)
   Output(WFX)

LUMO orbital

-1 2

RuP3HCl_mini_trans_CCSD_BS4_LUMO.wfx
```

Render the SPIN DENSITY (considerably slower process - map points per Å is 5, Map size = 1 - check save cube file only if you really need the orbital plot - contour value for spin density plot 0.003 - 1/10 of orbital contour)



Ru 4dyz + H s + Cl 3pz + P-H s

Spin densities describe the single unoccupied/occupied orbital composition

Mulliken:

1	Ru	0.560938
2	H	0.235051
3	Cl	0.049962
4	P	0.083378
5	H	-0.000079
6	H	-0.000067
7	H	0.017620
8	P	0.019881
9	H	0.000250
10	H	0.002375
11	H	0.004076
12	P	0.019908
13	H	0.002368
14	H	0.004094
15	H	0.000246

ESP:

1	Ru	0.784
2	H	0.192
3	Cl	0.041
4	P	0.124
5	H	-0.028
6	H	-0.028
7	H	0.009
8	P	-0.098
9	H	0.016
10	H	0.013
11	H	0.025
12	P	-0.130
13	H	0.021
14	H	0.034
15	H	0.024

from difference to GS

NPA:

Ru	1	0.507
H	2	0.337
Cl	3	0.061
P	4	0.078
H	5	-0.002
H	6	-0.002
H	7	0.023
P	8	-0.009
H	9	-0.001
H	10	0.004
H	11	0.005
P	12	-0.009
H	13	0.004
H	14	0.005
H	15	-0.001

from difference to GS

AIM:

Ru	1	0.594
H	2	0.258
Cl	3	0.049
P	4	-0.008
H	5	0.020
H	6	0.020
H	7	0.039
P	8	-0.064
H	9	0.023
H	10	0.027
H	11	0.028
P	12	-0.063
H	13	0.027
H	14	0.029
H	15	0.023

from difference to GS

	1 Ru -0.472040 2 H -0.359975 3 Cl -0.517935 4 P -0.014866 5 H 0.037536 6 H 0.037497 7 H -0.040561 8 P 0.046265 9 H 0.019987 10 H 0.067694 11 H 0.028850 12 P 0.068725 13 H 0.062458 14 H 0.022162 15 H 0.014202	Ru 1 -1.84761 H 2 -0.15319 Cl 3 -0.47420 P 4 0.57758 H 5 -0.04012 H 6 -0.03993 H 7 -0.06428 P 8 0.57771 H 9 -0.03557 H 10 -0.00304 H 11 -0.01817 P 12 0.57762 H 13 -0.00302 H 14 -0.01827 H 15 -0.03551	Ru 1 -0.226 H 2 -0.403 Cl 3 -0.737 P 4 1.894 H 5 -0.607 H 6 -0.607 H 7 -0.626 P 8 1.929 H 9 -0.606 H 10 -0.576 H 11 -0.590 P 12 1.929 H 13 -0.576 H 14 -0.590 H 15 -0.606

Atom	No	Natural Electron Configuration
Ru	1	[core]5s(-0.01)4d(0.49)5p(0.10)5d(-0.04)4f(-0.03)6p(-0.01)6d(-0.01)
(Ru	1	[core]5S(0.00)4d(2.00)5p(0.00)5d(0.00) Ru(0) effectively ionic only bonding Ru+2 theoretically)
H	2	1s(0.34)2s(-0.01)
Cl	3	[core]3s(0.02)3p(0.06)3d(-0.09)4s(-0.01)4p(-0.02)4f(0.01)
P	4	[core]3p(0.04)3d(0.09)3d(-0.03)4p(-0.01)4f(-0.01)
H	5	1S(0.01)2S(-0.01)2p(-0.01)
H	6	1S(0.01)2S(-0.01)2p(-0.01)
H	7	1S(0.03)2p(-0.01)
P	8	[core]3S(0.01)3p(0.04)3d(-0.03)4p(-0.01)4f(-0.01)
H	9	1S(-0.01)2p(-0.01)
H	10	1S(-0.01)2p(-0.01)
H	11	1S(-0.02)2p(-0.01)
P	12	[core]3S(0.01)3p(0.04)3d(-0.03)4p(-0.01)4f(-0.01)
H	13	1S(-0.01)2p(-0.01)
H	14	1S(0.00)2p(-0.01)
H	15	1S(-0.01)2p(-0.01)

The ground state NPA electron configuration is pretty messed up that results in lots of small negative values.

From difference between the reduced below and the ground state from above

Atom	No	Natural Electron Configuration
Ru	1	[core]5S(0.45)4d(8.41)5p(0.97)5d(0.03)
H	2	1S(1.15)
Cl	3	[core]3S(1.87)3p(5.59)3d(0.01)4p(0.01)
P	4	[core]3S(1.29)3p(3.06)3d(0.06)4p(0.01)
H	5	1S(1.04)
H	6	1S(1.04)
H	7	1S(1.06)
P	8	[core]3S(1.31)3p(3.05)3d(0.05)4p(0.01)
H	9	1S(1.03)
H	10	1S(1.00)
H	11	1S(1.02)
P	12	[core]3S(1.31)3p(3.05)3d(0.05)4p(0.01)
H	13	1S(1.00)
H	14	1S(1.02)
H	15	1S(1.03)

Workaround - is to take the NPA Spin alpha/Spin 1 density and subtract from it the NPA Spin beta/Spin 2 density

Atom	No	Natural Alpha Electron Configuration
Ru	1	[core]4d(1.95)6S(0.23)5d(0.96)6p(0.51)6d(1.52)
H	2	1S(0.73)
Cl	3	[core]3p(0.98)4S(0.94)3d(0.01)4p(1.84)
P	4	[core]3p(0.94)4S(0.66)4p(0.62)4d(0.03)
H	5	3S(0.52)
H	6	3S(0.52)
H	7	3S(0.54)
P	8	[core]3p(0.93)4S(0.66)4d(0.02)5p(0.60)
H	9	3S(0.52)
H	10	3S(0.50)
H	11	3S(0.51)
P	12	[core]3p(0.93)4S(0.66)4d(0.02)5p(0.60)
H	13	3S(0.50)
H	14	3S(0.51)
H	15	3S(0.52)

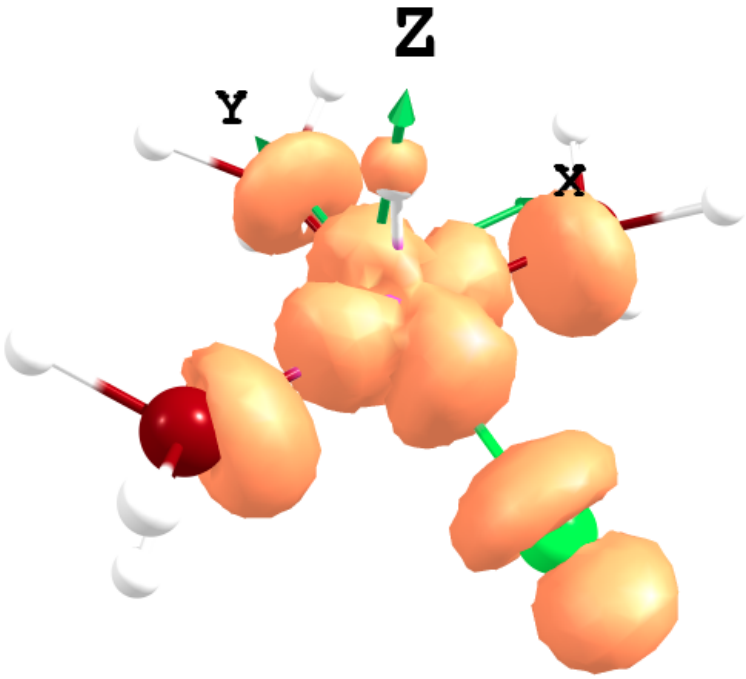
Atom	No	Natural Beta Electron Configuration
Ru	1	[core]4d(1.82)6S(0.23)5d(0.95)6p(0.46)6d(1.26)
H	2	1S(0.42)
Cl	3	[core]3p(0.95)4S(0.93)4p(1.82)
P	4	[core]3p(0.93)4S(0.63)4p(0.57)4d(0.03)
H	5	3S(0.52)
H	6	3S(0.52)
H	7	3S(0.52)
P	8	[core]3p(0.93)4S(0.65)4d(0.02)5p(0.59)
H	9	3S(0.52)
H	10	3S(0.50)
H	11	3S(0.50)
P	12	[core]3p(0.93)4S(0.65)4d(0.02)5p(0.60)
H	13	3S(0.50)
H	14	3S(0.50)
H	15	3S(0.52)

Atom	No	Natural Electron Configuration
Ru	1	[core]4d(0.13)5d(0.01)6p(0.05)6d(0.26)
(Ru	1	[core]5S(0.00)4d(2.00)5p(0.00)5d(0.00) ionic only bonding Ru(0) effectively Ru+2 theoretically)
H	2	1s(0.31)
Cl	3	[core]3p(0.01)4s(0.01)3d(0.01)4p(0.02)
P	4	[core]3p(0.01)4s(0.03)4p(0.05)
H	5	1S(0.00)
H	6	1S(0.00)
H	7	1S(0.02)
P	8	[core]4s(0.01)5p(0.01)
H	9	1S(0.00)
H	10	1S(0.00)
H	11	1S(0.01)
P	12	[core]4s(0.01)
H	13	1S(0.00)
H	14	1S(0.01)
H	15	1S(0.00)

9. Looking at LUMO+1 - same machinery, , but must not use “NaturalOrbitals” keyword in guess note that orbital rotations need to be minimized to avoid artifacts in total density (in AIM analysis)

```
%oldchk=RuP3HCl_mini_trans_CCSD_BS4_natorb
%chk=RuP3HCl_mini_trans_CCSD_BS4_LUMO+1
#p uhf chkbasis geom(check,nodistance)
   guess(check,only,alter,save) Pop(Full,NPA,MKUFF) Output(WFX)

LUMO+1 orbital

-1 2

45 46

45 46

RuP3HCl_mini_trans_CCSD_BS4_LUMO+1.wfx
```

Render the SPIN DENSITY (considerably slower process - map points per Å is 5, Map size = 1 - check save cube file only if you really need the orbital plot - contour value for spin density plot 0.003 - 1/10 of orbital contour)



Ru $4dx^2$-y^2 + P 3px + Cl 3py

Spin densities describe the single unoccupied/occupied orbital composition

Mulliken:			ESP:			NPA:			AIM:		
1	Ru	0.566541	1	Ru	0.539	Ru	1	0.444	Ru	1	0.673
2	H	0.016167	2	H	0.026	H	2	0.026	H	2	0.021
3	Cl	0.128054	3	Cl	0.156	Cl	3	0.152	Cl	3	0.111
4	P	0.070502	4	P	0.055	P	4	0.092	P	4	-0.020
5	H	0.005051	5	H	0.010	H	5	0.003	H	5	0.023
6	H	0.005046	6	H	0.010	H	6	0.003	H	6	0.023
7	H	0.001229	7	H	-0.004	H	7	-0.001	H	7	0.020
8	P	0.090547	8	P	0.114	P	8	0.130	P	8	0.003
9	H	0.000837	9	H	-0.011	H	9	0.000	H	9	0.021
10	H	0.005763	10	H	0.000	H	10	0.005	H	10	0.025
11	H	0.006595	11	H	0.003	H	11	0.006	H	11	0.026
12	P	0.090482	12	P	0.096	P	12	0.130	P	12	0.004
13	H	0.005774	13	H	0.005	H	13	0.005	H	13	0.025
14	H	0.006578	14	H	0.008	H	14	0.006	H	14	0.026
15	H	0.000834	15	H	-0.007	H	15	0.000	H	15	0.021

	from difference to GS			from difference to GS			from difference to GS		
	1	Ru	-0.226859	Ru	1	-1.78441	Ru	1	-0.305
	2	H	-0.193328	H	2	0.15722	H	2	-0.166
	3	Cl	-0.633154	Cl	3	-0.56503	Cl	3	-0.800
	4	P	0.054634	P	4	0.56361	P	4	1.906
	5	H	-0.000101	H	5	-0.04460	H	5	-0.610
	6	H	-0.000456	H	6	-0.04446	H	6	-0.610
	7	H	-0.028352	H	7	-0.04005	H	7	-0.607
	8	P	-0.166204	P	8	0.43823	P	8	1.862
	9	H	0.047078	H	9	-0.03663	H	9	-0.604
	10	H	0.080907	H	10	-0.00400	H	10	-0.574
	11	H	0.051012	H	11	-0.01875	H	11	-0.587
	12	P	-0.156666	P	12	0.43825	P	12	1.862
	13	H	0.078212	H	13	-0.00400	H	13	-0.574
	14	H	0.048485	H	14	-0.01881	H	14	-0.588
	15	H	0.044794	H	15	-0.03657	H	15	-0.604

Skipping total density based analysis dye to the ground state electron configuration issues

Workaround - is to take the NPA Spin alpha/Spin 1 density and subtract from it the NPA Spin beta/Spin 2 density

Atom	No	Natural Alpha Electron Configuration
Ru	1	[core]4d(1.82)5p(0.17)6S(0.23)5d(0.95)6p(0.28)6d(1.67)
H	2	1S(0.43)
Cl	3	[core]3S(0.01)3p(0.95)4S(0.96)3d(0.01)4p(1.92)
P	4	[core]3p(0.93)4S(0.68)4p(0.63)4d(0.03)
H	5	3S(0.52)
H	6	3S(0.52)
H	7	3S(0.52)
P	8	[core]3p(0.93)4S(0.72)4d(0.02)5p(0.68)
H	9	2S(0.52)
H	10	3S(0.50)
H	11	3S(0.51)
P	12	[core]3p(0.93)4S(0.72)4d(0.02)5p(0.68)
H	13	3S(0.50)
H	14	3S(0.51)
H	15	2S(0.52)

Atom	No	Natural Electron Configuration
Ru	1	[core]4d(1.82)5p(0.16)6S(0.23)5d(0.95)6p(0.27)6d(1.26)
H	2	1S(0.41)
Cl	3	[core]3p(0.95)4S(0.94)4p(1.83)
P	4	[core]3p(0.93)4S(0.63)4p(0.58)4d(0.03)
H	5	3S(0.52)
H	6	3S(0.52)
H	7	3S(0.52)
P	8	[core]3p(0.93)4S(0.66)4d(0.02)5p(0.60)
H	9	2S(0.52)
H	10	3S(0.50)
H	11	3S(0.50)
P	12	[core]3p(0.93)4S(0.66)4d(0.02)5p(0.60)
H	13	3S(0.50)
H	14	3S(0.50)
H	15	2S(0.52)

Atom	No	Natural Electron Configuration
Ru	1	[core]5p(0.01)6p(0.01)6d(0.41)
(Ru	1	[core]5S(0.00)4d(2.00)5p(0.00)5d(0.00) ionic only bonding Ru(0) effectively Ru+2 theoretically)
H	2	1s(0.02)
Cl	3	[core]3s(0.01)3p(0.01)4s(0.02)3d(0.01)4p(0.09)
P	4	[core]4s(0.05)4p(0.05)
H	5	1S(0.00)
H	6	1S(0.00)
H	7	1S(0.00)
P	8	[core]4s(0.06)5p(0.08)
H	9	1S(0.00)
H	10	1S(0.00)
H	11	1S(0.00)
P	12	[core]4s(0.06)5p(0.08)
H	13	1S(0.00)
H	14	1S(0.01)
H	15	1S(0.00)

Summary of electronic structure analysis

Total density-based properties (atomic charges)

	MPA	ESP	NPA	**AIM**
Ru	0.15	0.31	-1.34	**0.37**
H (hydride)	0.01	-0.17	0.18	**-0.15**
Cl	-0.54	-0.48	-0.41	**-0.69**
P trans to Cl	-0.11	0.11	0.66	**1.89**
P trans to P	-0.06	-0.06	0.57	**1.87**

Component of the density-based properties (orbital composition)

LUMO	MPA	ESP	NPA		**AIM**
Ru	56%	78%	51%	4d(0.40)5p(0.05)	**59%**
H (hydride)	24%	19%	34%	1s(0.31)	**26%**
Cl	5%	4%	6%	3s(0.01)3p(0.03)3d(0.01)	**5%**
P trans to Cl	8%	12%	8%	3s(0.03)3p(0.06)	**-1%**
P trans to P	2%	-19%	-1%	3s(0.01)3p(0.01)	**-6%**

LUMO+1	MPA	ESP	NPA		**AIM**
Ru	56%	54%	44%	4d(0.)5p(0.)6p(0.)	**67%**
H (hydride)	2%	3%	3%	1s(0.)2s(0.)	**2%**
Cl	13%	16%	15%	3s(0.)3p(0.)	**11%**
P trans to Cl	7%	6%	1%	3s(0.)3p(0.)3d(0.)	**-2%**
P trans to P	9%	10%	13%	3s(0.)3p(0.)3d(0.)	**0%**