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CMO: NBO Analysis of Canonical Molecular Orbitals

Leading (> 5%) NBO Contributions to Molecular Orbitals
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 MO    1 (occ): orbital energy = -20.424847 a.u.
                 0.991*[  9]: CR ( 1) O 5(cr)
 MO    2 (occ): orbital energy = -15.506132 a.u.
                 0.993*[  7]: CR ( 1) N 3(cr)
 MO    3 (occ): orbital energy = -11.301636 a.u.
                 0.993*[  8]: CR ( 1) C 4(cr)
 MO    4 (occ): orbital energy =  -1.392175 a.u.
                 0.841*[  5]: BD ( 2) C 4- O 5
                 0.388*[ 11]: LP ( 1) O 5(lp)
                 0.279*[  3]: BD ( 1) N 3- C 4
 MO    5 (occ): orbital energy =  -1.207576 a.u.
                 0.660*[  3]: BD ( 1) N 3- C 4
                -0.486*[  1]: BD ( 1) H 1- N 3
                -0.448*[  2]: BD ( 1) H 2- N 3
                -0.253*[  5]: BD ( 2) C 4- O 5
 MO    6 (occ): orbital energy =  -0.838823 a.u.
                 0.626*[  6]: BD ( 1) C 4- H 6
                 0.540*[  2]: BD ( 1) H 2- N 3
                 0.378*[  3]: BD ( 1) N 3- C 4
                -0.296*[ 11]: LP ( 1) O 5(lp)
                 0.273*[  1]: BD ( 1) H 1- N 3
 MO    7 (occ): orbital energy =  -0.742119 a.u.
                 0.735*[  1]: BD ( 1) H 1- N 3
                 0.378*[  3]: BD ( 1) N 3- C 4
                -0.371*[  6]: BD ( 1) C 4- H 6
                -0.267*[  2]: BD ( 1) H 2- N 3
                -0.262*[ 12]: LP ( 2) O 5(lp)
 MO    8 (occ): orbital energy =  -0.662887 a.u.
                 0.593*[  2]: BD ( 1) H 2- N 3
                -0.435*[  6]: BD ( 1) C 4- H 6
                 0.413*[ 11]: LP ( 1) O 5(lp)
                 0.371*[  3]: BD ( 1) N 3- C 4
                -0.282*[ 12]: LP ( 2) O 5(lp)
 MO    9 (occ): orbital energy =  -0.587833 a.u.
                 0.714*[ 11]: LP ( 1) O 5(lp)
                -0.424*[  5]: BD ( 2) C 4- O 5
                 0.348*[  6]: BD ( 1) C 4- H 6
                 0.310*[  1]: BD ( 1) H 1- N 3
                -0.240*[  2]: BD ( 1) H 2- N 3
 MO   10 (occ): orbital energy =  -0.566187 a.u.
                 0.798*[  4]: BD ( 1) C 4- O 5
                 0.572*[ 10]: LP ( 1) N 3(lp)
 MO   11 (occ): orbital energy =  -0.418463 a.u.
                 0.876*[ 12]: LP ( 2) O 5(lp)
                -0.339*[  6]: BD ( 1) C 4- H 6
 MO   12 (occ): orbital energy =  -0.401819 a.u.
                 0.759*[ 10]: LP ( 1) N 3(lp)
                -0.602*[  4]: BD ( 1) C 4- O 5
                 0.248*[ 31]: BD*( 1) C 4- O 5*
 MO   13 (vir): orbital energy =   0.212381 a.u.
                 0.943*[ 31]: BD*( 1) C 4- O 5*
                -0.307*[ 10]: LP ( 1) N 3(lp)
 MO   14 (vir): orbital energy =   0.260352 a.u.
                 0.671*[ 28]: BD*( 1) H 1- N 3*
                 0.472*[ 13]: RY*( 1) H 1(ry*)
                 0.395*[ 29]: BD*( 1) H 2- N 3*
                 0.265*[ 14]: RY*( 1) H 2(ry*)
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MO  15 (vir): orbital energy =   0.285963 a.u.
              0.558*[ 33]: BD*( 1) C 4- H 6*
              0.543*[ 29]: BD*( 1) H 2- N 3*
             -0.405*[ 27]: RY*( 1) H 6(ry*)
              0.379*[ 14]: RY*( 1) H 2(ry*)
MO  16 (vir): orbital energy =   0.356943 a.u.
              0.484*[ 33]: BD*( 1) C 4- H 6*
             -0.424*[ 29]: BD*( 1) H 2- N 3*
             -0.384*[ 27]: RY*( 1) H 6(ry*)
              0.371*[ 28]: BD*( 1) H 1- N 3*
             -0.342*[ 14]: RY*( 1) H 2(ry*)
              0.309*[ 13]: RY*( 1) H 1(ry*)
MO  17 (vir): orbital energy =   0.516219 a.u.
              0.663*[ 32]: BD*( 2) C 4- O 5*
             -0.661*[ 19]: RY*( 1) C 4(ry*)
MO  18 (vir): orbital energy =   0.589231 a.u.
              0.786*[ 30]: BD*( 1) N 3- C 4*
             -0.381*[ 20]: RY*( 2) C 4(ry*)
MO  19 (vir): orbital energy =   0.952859 a.u.
              0.992*[ 22]: RY*( 4) C 4(ry*)
MO  20 (vir): orbital energy =   0.996171 a.u.
              0.775*[ 20]: RY*( 2) C 4(ry*)
              0.416*[ 30]: BD*( 1) N 3- C 4*
             -0.333*[ 19]: RY*( 1) C 4(ry*)
MO  21 (vir): orbital energy =   1.057986 a.u.
              0.432*[ 27]: RY*( 1) H 6(ry*)
              0.420*[ 21]: RY*( 3) C 4(ry*)
             -0.404*[ 32]: BD*( 2) C 4- O 5*
             -0.393*[ 19]: RY*( 1) C 4(ry*)
              0.303*[ 13]: RY*( 1) H 1(ry*)
             -0.262*[ 28]: BD*( 1) H 1- N 3*
              0.239*[ 33]: BD*( 1) C 4- H 6*
MO  22 (vir): orbital energy =   1.143603 a.u.
              0.429*[ 13]: RY*( 1) H 1(ry*)
              0.423*[ 32]: BD*( 2) C 4- O 5*
              0.398*[ 19]: RY*( 1) C 4(ry*)
              0.320*[ 14]: RY*( 1) H 2(ry*)
              0.297*[ 27]: RY*( 1) H 6(ry*)
             -0.280*[ 29]: BD*( 1) H 2- N 3*
             -0.253*[ 28]: BD*( 1) H 1- N 3*
              0.242*[ 33]: BD*( 1) C 4- H 6*
MO  23 (vir): orbital energy =   1.181781 a.u.
              0.460*[ 27]: RY*( 1) H 6(ry*)
             -0.442*[ 14]: RY*( 1) H 2(ry*)
              0.398*[ 33]: BD*( 1) C 4- H 6*
             -0.294*[ 13]: RY*( 1) H 1(ry*)
              0.263*[ 20]: RY*( 2) C 4(ry*)
              0.238*[ 29]: BD*( 1) H 2- N 3*
              0.228*[ 28]: BD*( 1) H 1- N 3*
MO  24 (vir): orbital energy =   1.395784 a.u.
              0.996*[ 16]: RY*( 2) N 3(ry*)
MO  25 (vir): orbital energy =   1.426162 a.u.
              0.489*[ 14]: RY*( 1) H 2(ry*)
             -0.425*[ 13]: RY*( 1) H 1(ry*)
             -0.398*[ 29]: BD*( 1) H 2- N 3*
              0.367*[ 28]: BD*( 1) H 1- N 3*
             -0.229*[ 20]: RY*( 2) C 4(ry*)
MO  26 (vir): orbital energy =   1.520435 a.u.
              0.796*[ 21]: RY*( 3) C 4(ry*)
             -0.227*[ 27]: RY*( 1) H 6(ry*)
MO  27 (vir): orbital energy =   1.580318 a.u.
              0.627*[ 18]: RY*( 4) N 3(ry*)
             -0.526*[ 17]: RY*( 3) N 3(ry*)
             -0.401*[ 15]: RY*( 1) N 3(ry*)
MO  28 (vir): orbital energy =   1.842857 a.u.
              0.557*[ 25]: RY*( 3) O 5(ry*)
              0.500*[ 17]: RY*( 3) N 3(ry*)
             -0.465*[ 15]: RY*( 1) N 3(ry*)
              0.324*[ 21]: RY*( 3) C 4(ry*)
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MO  29 (vir): orbital energy =   1.921433 a.u.
              0.997*[ 24]: RY*( 2) O 5(ry*)
MO  30 (vir): orbital energy =   1.998941 a.u.
              0.691*[ 25]: RY*( 3) O 5(ry*)
              0.492*[ 23]: RY*( 1) O 5(ry*)
             -0.373*[ 17]: RY*( 3) N 3(ry*)
              0.252*[ 15]: RY*( 1) N 3(ry*)
MO  31 (vir): orbital energy =   2.043110 a.u.
              0.842*[ 23]: RY*( 1) O 5(ry*)
             -0.341*[ 25]: RY*( 3) O 5(ry*)
             -0.290*[ 15]: RY*( 1) N 3(ry*)
MO  32 (vir): orbital energy =   2.730328 a.u.
              0.701*[ 18]: RY*( 4) N 3(ry*)
              0.586*[ 15]: RY*( 1) N 3(ry*)
              0.363*[ 17]: RY*( 3) N 3(ry*)
MO  33 (vir): orbital energy =   3.564190 a.u.
              0.962*[ 26]: RY*( 4) O 5(ry*)
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Molecular Orbital Atom-Atom Bonding Character

MO	bonding (2c, 3c)	nonbonding (1c, 1c*)	antibonding (2c*, 3c*)
1(o)		0.983 O 5	
	0.008(b)	0.992(n)	0.000(a) total
2(o)		0.987 N 3	
	0.013(b)	0.987(n)	0.000(a) total
3(o)		0.987 C 4	
	0.013(b)	0.987(n)	0.000(a) total
4(o)	0.707 C 4- O 5 0.078 N 3- C 4	0.150 O 5	
	0.827(b)	0.172(n)	0.001(a) total
5(o)	0.436 N 3- C 4 0.236 H 1- N 3 0.201 H 2- N 3 0.064 C 4- O 5		
	0.948(b)	0.051(n)	0.001(a) total
6(o)	0.392 C 4- H 6 0.291 H 2- N 3 0.143 N 3- C 4 0.075 H 1- N 3	0.087 O 5	
	0.901(b)	0.096(n)	0.003(a) total
7(o)	0.540 H 1- N 3 0.143 N 3- C 4 0.138 C 4- H 6 0.072 H 2- N 3	0.069 O 5	
	0.896(b)	0.098(n)	0.006(a) total
8(o)	0.352 H 2- N 3 0.189 C 4- H 6 0.138 N 3- C 4	0.250 O 5	
	0.745(b)	0.253(n)	0.002(a) total
9(o)	0.180 C 4- O 5 0.121 C 4- H 6 0.096 H 1- N 3	0.510 O 5	

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        0.058  H 2- N 3

        _____          _____          _____
        0.459(b)       0.538(n)       0.003(a)  total
-------------------------------------------------------
 10(o)  0.637  C 4- O 5  0.327  N 3
        _____          _____          _____
        0.637(b)       0.328(n)       0.035(a)  total
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 11(o)  0.115  C 4- H 6  0.768  O 5
        _____          _____          _____
        0.178(b)       0.774(n)       0.049(a)  total
-------------------------------------------------------
 12(o)  0.362  C 4- O 5  0.576  N 3  0.061  C 4- O 5
        _____          _____          _____
        0.362(b)       0.576(n)       0.061(a)  total
-------------------------------------------------------
 13(v)                 0.094  N 3  0.889  C 4- O 5
        _____          _____          _____
        0.000(b)       0.111(n)       0.889(a)  total
-------------------------------------------------------
 14(v)                 0.223  H 1  0.450  H 1- N 3
                       0.070  H 2  0.156  H 2- N 3
        _____          _____          _____
        0.001(b)       0.340(n)       0.659(a)  total
-------------------------------------------------------
 15(v)                 0.164  H 6  0.311  C 4- H 6
                       0.144  H 2  0.295  H 2- N 3
        _____          _____          _____
        0.003(b)       0.336(n)       0.661(a)  total
-------------------------------------------------------
 16(v)                 0.147  H 6  0.234  C 4- H 6
                       0.117  H 2  0.180  H 2- N 3
                       0.096  H 1  0.138  H 1- N 3
        _____          _____          _____
        0.002(b)       0.386(n)       0.613(a)  total
-------------------------------------------------------
 17(v)                 0.437  C 4  0.440  C 4- O 5
        _____          _____          _____
        0.001(b)       0.541(n)       0.457(a)  total
-------------------------------------------------------
 18(v)                 0.145  C 4  0.618  N 3- C 4
        _____          _____          _____
        0.001(b)       0.298(n)       0.701(a)  total
-------------------------------------------------------
 19(v)                 0.984  C 4
        _____          _____          _____
        0.000(b)       0.991(n)       0.009(a)  total
-------------------------------------------------------
 20(v)                 0.712  C 4  0.173  N 3- C 4
        _____          _____          _____
        0.000(b)       0.779(n)       0.221(a)  total
-------------------------------------------------------
 21(v)                 0.331  C 4  0.163  C 4- O 5
                       0.187  H 6  0.069  H 1- N 3
                       0.092  H 1  0.057  C 4- H 6
        _____          _____          _____
        0.001(b)       0.677(n)       0.322(a)  total
-------------------------------------------------------
 22(v)                 0.184  H 1  0.179  C 4- O 5
                       0.158  C 4  0.078  H 2- N 3
                       0.102  H 2  0.064  H 1- N 3
                       0.088  H 6  0.059  C 4- H 6
        _____          _____          _____
        0.002(b)       0.616(n)       0.382(a)  total
-------------------------------------------------------
 23(v)                 0.212  H 6  0.158  C 4- H 6
                       0.195  H 2  0.057  H 2- N 3
                       0.086  H 1  0.052  H 1- N 3
                       0.069  C 4
        _____          _____          _____
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	0.001(b)	0.687(n)	0.312(a) total
24(v)		0.992 N 3	
	0.000(b)	0.998(n)	0.001(a) total
25(v)		0.239 H 2	0.159 H 2- N 3
		0.181 H 1	0.135 H 1- N 3
		0.052 C 4	
	0.000(b)	0.659(n)	0.340(a) total
26(v)		0.634 C 4	
		0.051 H 6	
	0.000(b)	0.872(n)	0.128(a) total
27(v)		0.831 N 3	
	0.000(b)	0.908(n)	0.092(a) total
28(v)		0.467 N 3	
		0.310 O 5	
		0.105 C 4	
	0.000(b)	0.995(n)	0.005(a) total
29(v)		0.993 O 5	
	0.000(b)	0.996(n)	0.004(a) total
30(v)		0.720 O 5	
		0.203 N 3	
	0.000(b)	0.990(n)	0.009(a) total
31(v)		0.825 O 5	
		0.084 N 3	
	0.001(b)	0.993(n)	0.006(a) total
32(v)		0.966 N 3	
	0.000(b)	0.987(n)	0.013(a) total
33(v)		0.926 O 5	
	0.000(b)	0.986(n)	0.014(a) total
	6.000(b)	21.000(n)	6.000(a) Sum total for MOs