

NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS:

Maximum off-diagonal element of DM in NLMO basis: 0.74927D-10

Hybridization/Polarization Analysis of NLMOs in NAO Basis:

NLMO/Occupancy/Percent from Parent NBO/ Atomic Hybrid Contributions

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1.	(2.00000)	99.6544%	BD ( 1) H 1- N 3
			28.951% H 1 s(100.00%)
			70.708% N 3 s( 30.18%)p 2.31( 69.82%)
			0.253% C 4 s( 5.84%)p16.14( 94.16%)
			0.076% O 5 s( 43.76%)p 1.29( 56.24%)
2.	(2.00000)	99.6610%	BD ( 1) H 2- N 3
			28.425% H 2 s(100.00%)
			71.242% N 3 s( 29.47%)p 2.39( 70.53%)
			0.196% C 4 s( 1.34%)p73.58( 98.66%)
			0.040% O 5 s( 19.63%)p 4.09( 80.37%)
			0.092% H 6 s(100.00%)
3.	(2.00000)	99.9141%	BD ( 1) N 3- C 4
			0.012% H 1 s(100.00%)
			0.016% H 2 s(100.00%)
			64.097% N 3 s( 37.96%)p 1.63( 62.04%)
			35.830% C 4 s( 32.46%)p 2.08( 67.54%)
			0.013% O 5 s( 2.79%)p34.84( 97.21%)
			0.033% H 6 s(100.00%)
4.	(2.00000)	99.9625%	BD ( 1) C 4- O 5
			0.037% N 3 s( 0.00%)p 1.00(100.00%)
			30.529% C 4 s( 0.00%)p 1.00(100.00%)
			69.434% O 5 s( 0.00%)p 1.00(100.00%)
5.	(2.00000)	99.9011%	BD ( 2) C 4- O 5
			0.056% H 1 s(100.00%)
			0.028% N 3 s( 10.43%)p 8.59( 89.57%)
			34.069% C 4 s( 32.20%)p 2.11( 67.80%)
			65.833% O 5 s( 41.38%)p 1.42( 58.62%)
6.	(2.00000)	99.4640%	BD ( 1) C 4- H 6
			0.296% H 2 s(100.00%)
			0.153% N 3 s( 43.44%)p 1.30( 56.56%)
			58.566% C 4 s( 36.27%)p 1.76( 63.73%)
			0.051% O 5 s( 2.05%)p47.81( 97.95%)
			40.930% H 6 s(100.00%)
7.	(2.00000)	99.9610%	CR ( 1) N 3
			99.963% N 3 s(100.00%)p 0.00( 0.00%)
			0.024% C 4 s( 17.87%)p 4.60( 82.13%)
8.	(2.00000)	99.9694%	CR ( 1) C 4
			99.974% C 4 s(100.00%)p 0.00( 0.00%)
			0.015% H 6 s(100.00%)
9.	(2.00000)	99.9814%	CR ( 1) O 5
			0.014% C 4 s( 15.50%)p 5.45( 84.50%)
			99.986% O 5 s(100.00%)p 0.00( 0.00%)
10.	(2.00000)	90.3414%	LP ( 1) N 3
			90.341% N 3 s( 0.00%)p 1.00(100.00%)
			6.702% C 4 s( 0.00%)p 1.00(100.00%)
			2.957% O 5 s( 0.00%)p 1.00(100.00%)
11.	(2.00000)	99.1301%	LP ( 1) O 5
			0.019% H 1 s(100.00%)
			0.030% H 2 s(100.00%)
			0.030% N 3 s( 9.83%)p 9.18( 90.17%)
			0.736% C 4 s( 15.34%)p 5.52( 84.66%)
			99.130% O 5 s( 58.64%)p 0.71( 41.36%)
			0.053% H 6 s(100.00%)

12. (2.00000) 94.2730% LP ( 2) O 5  
0.140% H 1 s(100.00%)  
0.070% H 2 s(100.00%)  
1.107% N 3 s( 63.37%)p 0.58( 36.63%)  
3.025% C 4 s( 1.57%)p62.67( 98.43%)  
94.273% O 5 s( 0.01%)p 1.00( 99.99%)  
1.384% H 6 s(100.00%)