

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	H	1	s	Val(1s)	0.58340	0.20603
2	H	1	s	Ryd(2s)	0.00054	0.92481
3	H	2	s	Val(1s)	0.57541	0.21608
4	H	2	s	Ryd(2s)	0.00173	0.95408
5	N	3	s	Cor(1s)	1.99922	-15.31889
6	N	3	s	Val(2s)	1.34827	-0.73528
7	N	3	s	Ryd(3s)	0.00040	2.67615
8	N	3	px	Val(2p)	1.37478	-0.29723
9	N	3	px	Ryd(3p)	0.00095	1.56735
10	N	3	py	Val(2p)	1.42212	-0.29288
11	N	3	py	Ryd(3p)	0.00095	1.73705
12	N	3	pz	Val(2p)	1.80657	-0.39400
13	N	3	pz	Ryd(3p)	0.00101	1.39224
14	C	4	s	Cor(1s)	1.99939	-11.16959
15	C	4	s	Val(2s)	0.87473	-0.19294
16	C	4	s	Ryd(3s)	0.00577	1.41667
17	C	4	px	Val(2p)	0.72398	0.08603
18	C	4	px	Ryd(3p)	0.02003	0.86683
19	C	4	py	Val(2p)	1.02077	-0.01580
20	C	4	py	Ryd(3p)	0.00907	1.08911
21	C	4	pz	Val(2p)	0.74070	-0.04746
22	C	4	pz	Ryd(3p)	0.00391	0.93036
23	O	5	s	Cor(1s)	1.99963	-20.09029
24	O	5	s	Val(2s)	1.70820	-1.18275
25	O	5	s	Ryd(3s)	0.00015	3.45878
26	O	5	px	Val(2p)	1.66996	-0.40024
27	O	5	px	Ryd(3p)	0.00052	1.94714
28	O	5	py	Val(2p)	1.80863	-0.40792
29	O	5	py	Ryd(3p)	0.00100	1.99892
30	O	5	pz	Val(2p)	1.44750	-0.27972
31	O	5	pz	Ryd(3p)	0.00031	1.91304
32	H	6	s	Val(1s)	0.84667	0.07560
33	H	6	s	Ryd(2s)	0.00375	0.89527

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
H 1	0.41606	0.00000	0.58340	0.00054	0.58394
H 2	0.42286	0.00000	0.57541	0.00173	0.57714
N 3	-0.95426	1.99922	5.95174	0.00331	7.95426
C 4	0.60165	1.99939	3.36018	0.03878	5.39835
O 5	-0.63589	1.99963	6.63428	0.00198	8.63589
H 6	0.14959	0.00000	0.84667	0.00375	0.85041
* Total *	0.00000	5.99824	17.95168	0.05008	24.00000

Natural Population

Core	5.99824	(99.9706%	of	6)
Valence	17.95168	(99.7316%	of	18)
Natural Minimal Basis	23.94992	(99.7913%	of	24)
Natural Rydberg Basis	0.05008	(0.2087%	of	24)

Atom No	Natural Electron Configuration
H 1	1s(0.58)
H 2	1s(0.58)
N 3	[core]2s(1.35)2p(4.60)
C 4	[core]2s(0.87)2p(2.49)3s(0.01)3p(0.03)
O 5	[core]2s(1.71)2p(4.93)
H 6	1s(0.85)