

Supplementary Information

Peeling the onion: a revised model on the electron count for matryoshka clusters

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$K_{12}[Sn@Cu_{12}@Sn_{20}]$

Sn	0.000000	0.000000	0.000000
Cu	1.933043	-0.438122	1.725740
Cu	2.444115	-0.069360	-0.964389
Cu	1.157050	-2.357725	-0.103693
Cu	-0.534189	-1.659280	1.967110
Cu	-0.292298	1.061387	2.386009
Cu	1.548629	2.044364	0.574693
Cu	0.534188	1.659281	-1.967110
Cu	0.292298	-1.061387	-2.386009
Cu	-1.548629	-2.044363	-0.574693
Cu	-2.444115	0.069360	0.964389
Cu	-1.157051	2.357725	0.103693
Cu	-1.933043	0.438122	-1.725740
Sn	4.145774	1.075794	0.934863
Sn	3.871675	-2.004618	0.460111
Sn	1.787566	-3.117067	2.511244
Sn	0.773899	-0.724638	4.253522
Sn	2.231356	1.866542	3.279370
Sn	0.069537	3.823034	2.144708
Sn	0.648093	4.241138	-0.901095
Sn	3.167320	2.543342	-1.648664
Sn	2.288811	0.370253	-3.720349
Sn	2.723630	-2.440399	-2.417261
Sn	-0.069537	-3.823034	-2.144708
Sn	-0.648094	-4.241138	0.901095
Sn	-3.167320	-2.543342	1.648664
Sn	-2.288811	-0.370253	3.720349
Sn	-2.723630	2.440399	2.417261
Sn	-3.871675	2.004618	-0.460111
Sn	-1.787566	3.117067	-2.511245
Sn	-0.773899	0.724639	-4.253523
Sn	-2.231356	-1.866542	-3.279369
Sn	-4.145774	-1.075795	-0.934863
K	4.392389	-0.995550	3.922429
K	5.553964	-0.156169	-2.191224
K	2.628741	-5.357704	-0.236655
K	-1.214628	-3.771004	4.469532
K	-0.664917	2.411545	5.423321
K	3.518358	4.646040	1.306786
K	1.214629	3.771004	-4.469532
K	0.664917	-2.411545	-5.423321

K	-3.518358	-4.646040	-1.306786
K	-5.553964	0.156170	2.191223
K	-2.628741	5.357704	0.236655
K	-4.392389	0.995549	-3.922429

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
Sn 1	-2.44402	45.99781	6.38948	0.05673	52.44402
Cu 2	0.62316	17.99548	10.28898	0.09239	28.37684
Cu 3	0.62333	17.99547	10.28898	0.09222	28.37667
Cu 4	0.62347	17.99547	10.28898	0.09207	28.37653
Cu 5	0.62294	17.99547	10.28898	0.09261	28.37706
Cu 6	0.62332	17.99547	10.28891	0.09229	28.37668
Cu 7	0.62338	17.99547	10.28896	0.09218	28.37662
Cu 8	0.62294	17.99547	10.28898	0.09261	28.37706
Cu 9	0.62332	17.99547	10.28891	0.09229	28.37668
Cu 10	0.62338	17.99547	10.28896	0.09218	28.37662
Cu 11	0.62333	17.99547	10.28898	0.09222	28.37667
Cu 12	0.62347	17.99547	10.28898	0.09207	28.37653
Cu 13	0.62316	17.99548	10.28898	0.09239	28.37684
Sn 14	-0.83813	45.99629	4.77929	0.06255	50.83813
Sn 15	-0.83801	45.99628	4.77867	0.06306	50.83801
Sn 16	-0.83732	45.99629	4.77765	0.06337	50.83732
Sn 17	-0.83664	45.99629	4.78003	0.06032	50.83664
Sn 18	-0.83713	45.99629	4.77772	0.06312	50.83713
Sn 19	-0.83824	45.99628	4.77807	0.06388	50.83824
Sn 20	-0.83736	45.99629	4.77960	0.06147	50.83736
Sn 21	-0.83689	45.99629	4.77754	0.06306	50.83689
Sn 22	-0.83716	45.99629	4.77847	0.06240	50.83716
Sn 23	-0.83736	45.99629	4.77730	0.06378	50.83736
Sn 24	-0.83824	45.99628	4.77807	0.06388	50.83824
Sn 25	-0.83736	45.99629	4.77960	0.06147	50.83736
Sn 26	-0.83689	45.99629	4.77754	0.06306	50.83689
Sn 27	-0.83716	45.99629	4.77847	0.06240	50.83716
Sn 28	-0.83736	45.99629	4.77730	0.06378	50.83736
Sn 29	-0.83801	45.99628	4.77867	0.06306	50.83801
Sn 30	-0.83732	45.99629	4.77765	0.06337	50.83732
Sn 31	-0.83664	45.99629	4.78003	0.06032	50.83664
Sn 32	-0.83713	45.99629	4.77772	0.06312	50.83713
Sn 33	-0.83813	45.99629	4.77929	0.06255	50.83813
K 34	0.97606	17.97773	0.03622	0.00999	18.02394
K 35	0.97617	17.97773	0.03622	0.00987	18.02383
K 36	0.97613	17.97773	0.03622	0.00992	18.02387
K 37	0.97607	17.97774	0.03622	0.00998	18.02393
K 38	0.97614	17.97773	0.03623	0.00990	18.02386
K 39	0.97607	17.97773	0.03622	0.00998	18.02393
K 40	0.97607	17.97774	0.03622	0.00998	18.02393
K 41	0.97613	17.97773	0.03623	0.00990	18.02387
K 42	0.97607	17.97773	0.03622	0.00998	18.02393
K 43	0.97617	17.97773	0.03622	0.00987	18.02383
K 44	0.97613	17.97773	0.03622	0.00992	18.02387
K 45	0.97606	17.97773	0.03622	0.00999	18.02394
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* Total *	-0.00002	1397.60201	225.86042	2.53759	1626.00002

Natural Population	

Effective Core	588.00000
Core	809.60201 (99.9509% of 810)

Valence	225.86042 (99.0616% of 228)
Natural Minimal Basis	1623.46243 (99.8439% of 1626)
Natural Rydberg Basis	2.53759 (0.1561% of 1626)

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
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1. Sn	0.0000	0.1026	0.1025	0.1025	0.1026	0.1026	0.1026	0.1026	0.1026
2. Cu	0.1026	0.0000	0.0165	0.0165	0.0165	0.0165	0.0165	0.0020	0.0020
3. Cu	0.1025	0.0165	0.0000	0.0165	0.0020	0.0020	0.0165	0.0165	0.0165
4. Cu	0.1025	0.0165	0.0165	0.0000	0.0165	0.0020	0.0020	0.0020	0.0165
5. Cu	0.1026	0.0165	0.0020	0.0165	0.0000	0.0165	0.0020	0.0072	0.0020
6. Cu	0.1026	0.0165	0.0020	0.0020	0.0165	0.0000	0.0165	0.0020	0.0072
7. Cu	0.1026	0.0165	0.0165	0.0020	0.0020	0.0165	0.0000	0.0165	0.0020
8. Cu	0.1026	0.0020	0.0165	0.0020	0.0072	0.0020	0.0165	0.0000	0.0165
9. Cu	0.1026	0.0020	0.0165	0.0165	0.0020	0.0072	0.0020	0.0165	0.0000
10. Cu	0.1026	0.0020	0.0020	0.0165	0.0165	0.0020	0.0072	0.0020	0.0165
11. Cu	0.1025	0.0020	0.0072	0.0020	0.0165	0.0165	0.0020	0.0020	0.0020
12. Cu	0.1025	0.0020	0.0020	0.0072	0.0020	0.0165	0.0165	0.0165	0.0020
13. Cu	0.1026	0.0072	0.0020	0.0020	0.0020	0.0020	0.0020	0.0165	0.0165
14. Sn	0.0708	0.1072	0.1072	0.0104	0.0073	0.0104	0.1072	0.0103	0.0073
15. Sn	0.0708	0.1071	0.1071	0.1072	0.0103	0.0073	0.0104	0.0073	0.0103
16. Sn	0.0708	0.1072	0.0103	0.1072	0.1072	0.0103	0.0072	0.0045	0.0072
17. Sn	0.0708	0.1074	0.0073	0.0104	0.1075	0.1074	0.0104	0.0045	0.0045
18. Sn	0.0708	0.1071	0.0103	0.0073	0.0103	0.1071	0.1072	0.0073	0.0045
19. Sn	0.0708	0.0103	0.0073	0.0045	0.0073	0.1070	0.1070	0.0104	0.0045
20. Sn	0.0707	0.0073	0.0104	0.0045	0.0045	0.0103	0.1073	0.1073	0.0073
21. Sn	0.0707	0.0103	0.1071	0.0072	0.0045	0.0073	0.1072	0.1072	0.0103
22. Sn	0.0708	0.0073	0.1073	0.0103	0.0045	0.0045	0.0103	0.1073	0.1072
23. Sn	0.0708	0.0103	0.1070	0.1069	0.0073	0.0045	0.0072	0.0103	0.1070
24. Sn	0.0708	0.0073	0.0103	0.1070	0.0104	0.0045	0.0045	0.0073	0.1070
25. Sn	0.0707	0.0103	0.0073	0.1072	0.1073	0.0073	0.0045	0.0045	0.0103
26. Sn	0.0707	0.0073	0.0045	0.0103	0.1072	0.0103	0.0045	0.0045	0.0073
27. Sn	0.0708	0.0104	0.0045	0.0073	0.1073	0.1072	0.0073	0.0045	0.0045
28. Sn	0.0708	0.0073	0.0045	0.0045	0.0103	0.1070	0.0102	0.0073	0.0045
29. Sn	0.0708	0.0045	0.0045	0.0045	0.0073	0.0103	0.0073	0.0103	0.0073
30. Sn	0.0708	0.0045	0.0073	0.0045	0.0045	0.0072	0.0103	0.1072	0.0103
31. Sn	0.0708	0.0045	0.0104	0.0073	0.0045	0.0045	0.0073	0.1075	0.1074
32. Sn	0.0708	0.0045	0.0073	0.0103	0.0073	0.0045	0.0045	0.0103	0.1071
33. Sn	0.0708	0.0045	0.0045	0.0073	0.0103	0.0073	0.0045	0.0073	0.0104
34. K	0.0035	0.0092	0.0010	0.0010	0.0011	0.0011	0.0010	0.0001	0.0001
35. K	0.0035	0.0010	0.0092	0.0010	0.0001	0.0001	0.0010	0.0011	0.0011
36. K	0.0035	0.0011	0.0011	0.0092	0.0010	0.0001	0.0001	0.0001	0.0010
37. K	0.0035	0.0010	0.0001	0.0010	0.0092	0.0010	0.0001	0.0002	0.0001
38. K	0.0035	0.0010	0.0001	0.0001	0.0010	0.0092	0.0010	0.0001	0.0002
39. K	0.0035	0.0011	0.0010	0.0001	0.0001	0.0010	0.0092	0.0010	0.0001
40. K	0.0035	0.0001	0.0010	0.0001	0.0002	0.0001	0.0011	0.0092	0.0010
41. K	0.0035	0.0001	0.0010	0.0011	0.0001	0.0002	0.0001	0.0010	0.0092
42. K	0.0035	0.0001	0.0001	0.0010	0.0010	0.0001	0.0002	0.0001	0.0010
43. K	0.0035	0.0001	0.0002	0.0001	0.0011	0.0011	0.0001	0.0001	0.0001
44. K	0.0035	0.0001	0.0001	0.0002	0.0001	0.0010	0.0010	0.0010	0.0001
45. K	0.0035	0.0002	0.0001	0.0001	0.0001	0.0001	0.0001	0.0011	0.0011
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Atom	10	11	12	13	14	15	16	17	18
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1. Sn	0.1026	0.1025	0.1025	0.1026	0.0708	0.0708	0.0708	0.0708	0.0708
2. Cu	0.0020	0.0020	0.0020	0.0072	0.1072	0.1071	0.1072	0.1074	0.1071
3. Cu	0.0020	0.0072	0.0020	0.0020	0.1072	0.1071	0.0103	0.0073	0.0103
4. Cu	0.0165	0.0020	0.0072	0.0020	0.0104	0.1072	0.1072	0.0104	0.0073
5. Cu	0.0165	0.0165	0.0020	0.0020	0.0073	0.0103	0.1072	0.1075	0.0103
6. Cu	0.0020	0.0165	0.0165	0.0020	0.0104	0.0073	0.0103	0.1074	0.1071

7.	Cu	0.0072	0.0020	0.0165	0.0020	0.1072	0.0104	0.0072	0.0104	0.1072
8.	Cu	0.0020	0.0020	0.0165	0.0165	0.0103	0.0073	0.0045	0.0045	0.0073
9.	Cu	0.0165	0.0020	0.0020	0.0165	0.0073	0.0103	0.0072	0.0045	0.0045
10.	Cu	0.0000	0.0165	0.0020	0.0165	0.0045	0.0073	0.0103	0.0073	0.0045
11.	Cu	0.0165	0.0000	0.0165	0.0165	0.0045	0.0045	0.0073	0.0104	0.0073
12.	Cu	0.0020	0.0165	0.0000	0.0165	0.0073	0.0045	0.0045	0.0073	0.0103
13.	Cu	0.0165	0.0165	0.0165	0.0000	0.0045	0.0045	0.0045	0.0045	0.0045
14.	Sn	0.0045	0.0045	0.0073	0.0045	0.0000	0.7793	0.0444	0.0444	0.7798
15.	Sn	0.0073	0.0045	0.0045	0.0045	0.7793	0.0000	0.7798	0.0443	0.0443
16.	Sn	0.0103	0.0073	0.0045	0.0045	0.0444	0.7798	0.0000	0.7795	0.0444
17.	Sn	0.0073	0.0104	0.0073	0.0045	0.0444	0.0443	0.7795	0.0000	0.7796
18.	Sn	0.0045	0.0073	0.0103	0.0045	0.7798	0.0443	0.0444	0.7796	0.0000
19.	Sn	0.0045	0.0103	0.1070	0.0073	0.0444	0.0220	0.0220	0.0444	0.7800
20.	Sn	0.0045	0.0073	0.1072	0.0103	0.0444	0.0220	0.0046	0.0220	0.0444
21.	Sn	0.0045	0.0045	0.0103	0.0073	0.7800	0.0444	0.0220	0.0220	0.0444
22.	Sn	0.0073	0.0045	0.0073	0.0104	0.0443	0.0444	0.0220	0.0046	0.0220
23.	Sn	0.0102	0.0045	0.0045	0.0073	0.0444	0.7799	0.0444	0.0220	0.0220
24.	Sn	0.1070	0.0073	0.0045	0.0103	0.0220	0.0444	0.0444	0.0220	0.0046
25.	Sn	0.1073	0.0104	0.0045	0.0073	0.0220	0.0444	0.7797	0.0444	0.0220
26.	Sn	0.1072	0.1071	0.0072	0.0103	0.0046	0.0220	0.0443	0.0444	0.0220
27.	Sn	0.0103	0.1073	0.0103	0.0073	0.0220	0.0220	0.0443	0.7791	0.0443
28.	Sn	0.0072	0.1070	0.1069	0.0103	0.0220	0.0046	0.0220	0.0443	0.0443
29.	Sn	0.0104	0.1071	0.1072	0.1071	0.0046	0.0039	0.0046	0.0221	0.0220
30.	Sn	0.0072	0.0103	0.1072	0.1072	0.0220	0.0046	0.0039	0.0046	0.0220
31.	Sn	0.0104	0.0073	0.0104	0.1074	0.0220	0.0221	0.0046	0.0039	0.0046
32.	Sn	0.1072	0.0103	0.0073	0.1071	0.0046	0.0220	0.0220	0.0046	0.0039
33.	Sn	0.1072	0.1072	0.0104	0.1072	0.0039	0.0046	0.0220	0.0220	0.0046
34.	K	0.0001	0.0001	0.0001	0.0002	0.0175	0.0176	0.0175	0.0177	0.0175
35.	K	0.0001	0.0002	0.0001	0.0001	0.0174	0.0174	0.0035	0.0003	0.0035
36.	K	0.0010	0.0001	0.0002	0.0001	0.0037	0.0177	0.0175	0.0035	0.0003
37.	K	0.0011	0.0010	0.0001	0.0001	0.0003	0.0036	0.0175	0.0175	0.0036
38.	K	0.0001	0.0010	0.0011	0.0001	0.0035	0.0003	0.0036	0.0174	0.0174
39.	K	0.0002	0.0001	0.0010	0.0001	0.0177	0.0037	0.0003	0.0036	0.0176
40.	K	0.0001	0.0001	0.0011	0.0010	0.0036	0.0003	0.0004	0.0004	0.0003
41.	K	0.0010	0.0001	0.0001	0.0010	0.0003	0.0036	0.0003	0.0004	0.0004
42.	K	0.0092	0.0010	0.0001	0.0011	0.0004	0.0003	0.0036	0.0003	0.0004
43.	K	0.0010	0.0092	0.0010	0.0010	0.0004	0.0004	0.0003	0.0037	0.0003
44.	K	0.0001	0.0011	0.0092	0.0011	0.0003	0.0004	0.0004	0.0003	0.0035
45.	K	0.0010	0.0010	0.0010	0.0092	0.0004	0.0004	0.0004	0.0004	0.0004

	Atom	19	20	21	22	23	24	25	26	27
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1.	Sn	0.0708	0.0707	0.0707	0.0708	0.0708	0.0708	0.0707	0.0707	0.0708
2.	Cu	0.0103	0.0073	0.0103	0.0073	0.0103	0.0073	0.0103	0.0073	0.0104
3.	Cu	0.0073	0.0104	0.1071	0.1073	0.1070	0.0103	0.0073	0.0045	0.0045
4.	Cu	0.0045	0.0045	0.0072	0.0103	0.1069	0.1070	0.1072	0.0103	0.0073
5.	Cu	0.0073	0.0045	0.0045	0.0045	0.0073	0.0104	0.1073	0.1072	0.1073
6.	Cu	0.1070	0.0103	0.0073	0.0045	0.0045	0.0045	0.0073	0.0103	0.1072
7.	Cu	0.1070	0.1073	0.1072	0.0103	0.0072	0.0045	0.0045	0.0045	0.0073
8.	Cu	0.0104	0.1073	0.1072	0.1073	0.0103	0.0073	0.0045	0.0045	0.0045
9.	Cu	0.0045	0.0073	0.0103	0.1072	0.1070	0.1070	0.0103	0.0073	0.0045
10.	Cu	0.0045	0.0045	0.0045	0.0073	0.0102	0.1070	0.1073	0.1072	0.0103
11.	Cu	0.0103	0.0073	0.0045	0.0045	0.0045	0.0073	0.0104	0.1071	0.1073
12.	Cu	0.1070	0.1072	0.0103	0.0073	0.0045	0.0045	0.0045	0.0072	0.0103
13.	Cu	0.0073	0.0103	0.0073	0.0104	0.0073	0.0103	0.0073	0.0103	0.0073
14.	Sn	0.0444	0.0444	0.7800	0.0443	0.0444	0.0220	0.0220	0.0046	0.0220
15.	Sn	0.0220	0.0220	0.0444	0.0444	0.7799	0.0444	0.0444	0.0220	0.0220
16.	Sn	0.0220	0.0046	0.0220	0.0220	0.0444	0.0444	0.7797	0.0443	0.0443
17.	Sn	0.0444	0.0220	0.0220	0.0046	0.0220	0.0220	0.0444	0.0444	0.7791
18.	Sn	0.7800	0.0444	0.0444	0.0220	0.0220	0.0046	0.0220	0.0220	0.0443
19.	Sn	0.0000	0.7798	0.0444	0.0220	0.0046	0.0039	0.0046	0.0220	0.0444
20.	Sn	0.7798	0.0000	0.7795	0.0444	0.0220	0.0046	0.0039	0.0046	0.0220
21.	Sn	0.0444	0.7795	0.0000	0.7799	0.0444	0.0220	0.0046	0.0039	0.0046

22.	Sn	0.0220	0.0444	0.7799	0.0000	0.7798	0.0444	0.0220	0.0046	0.0039
23.	Sn	0.0046	0.0220	0.0444	0.7798	0.0000	0.7799	0.0443	0.0220	0.0046
24.	Sn	0.0039	0.0046	0.0220	0.0444	0.7799	0.0000	0.7798	0.0444	0.0220
25.	Sn	0.0046	0.0039	0.0046	0.0220	0.0443	0.7798	0.0000	0.7795	0.0444
26.	Sn	0.0220	0.0046	0.0039	0.0046	0.0220	0.0444	0.7795	0.0000	0.7799
27.	Sn	0.0444	0.0220	0.0046	0.0039	0.0046	0.0220	0.0444	0.7799	0.0000
28.	Sn	0.7799	0.0443	0.0220	0.0046	0.0039	0.0046	0.0220	0.0444	0.7798
29.	Sn	0.0444	0.0444	0.0220	0.0220	0.0046	0.0220	0.0220	0.0444	0.0444
30.	Sn	0.0444	0.7797	0.0443	0.0443	0.0220	0.0220	0.0046	0.0220	0.0220
31.	Sn	0.0220	0.0444	0.0444	0.7791	0.0443	0.0444	0.0220	0.0220	0.0046
32.	Sn	0.0046	0.0220	0.0220	0.0443	0.0443	0.7800	0.0444	0.0444	0.0220
33.	Sn	0.0220	0.0220	0.0046	0.0220	0.0220	0.0444	0.0444	0.7800	0.0443
34.	K	0.0036	0.0003	0.0036	0.0003	0.0036	0.0003	0.0036	0.0003	0.0037
35.	K	0.0003	0.0036	0.0175	0.0177	0.0176	0.0036	0.0003	0.0004	0.0004
36.	K	0.0004	0.0004	0.0003	0.0036	0.0176	0.0174	0.0174	0.0036	0.0003
37.	K	0.0003	0.0004	0.0004	0.0004	0.0003	0.0037	0.0177	0.0175	0.0175
38.	K	0.0177	0.0037	0.0003	0.0004	0.0004	0.0004	0.0003	0.0035	0.0174
39.	K	0.0176	0.0175	0.0175	0.0036	0.0003	0.0004	0.0004	0.0004	0.0003
40.	K	0.0037	0.0177	0.0175	0.0175	0.0036	0.0003	0.0004	0.0004	0.0004
41.	K	0.0004	0.0003	0.0035	0.0174	0.0176	0.0177	0.0037	0.0003	0.0004
42.	K	0.0004	0.0004	0.0004	0.0003	0.0036	0.0176	0.0175	0.0175	0.0036
43.	K	0.0036	0.0003	0.0004	0.0004	0.0004	0.0003	0.0036	0.0175	0.0177
44.	K	0.0174	0.0174	0.0036	0.0003	0.0004	0.0004	0.0004	0.0003	0.0036
45.	K	0.0003	0.0036	0.0003	0.0037	0.0003	0.0036	0.0003	0.0036	0.0003

	Atom	28	29	30	31	32	33	34	35	36
1.	Sn	0.0708	0.0708	0.0708	0.0708	0.0708	0.0708	0.0035	0.0035	0.0035
2.	Cu	0.0073	0.0045	0.0045	0.0045	0.0045	0.0045	0.0092	0.0010	0.0011
3.	Cu	0.0045	0.0045	0.0073	0.0104	0.0073	0.0045	0.0010	0.0092	0.0011
4.	Cu	0.0045	0.0045	0.0045	0.0073	0.0103	0.0073	0.0010	0.0010	0.0092
5.	Cu	0.0103	0.0073	0.0045	0.0045	0.0073	0.0103	0.0011	0.0001	0.0010
6.	Cu	0.1070	0.0103	0.0072	0.0045	0.0045	0.0073	0.0011	0.0001	0.0001
7.	Cu	0.0102	0.0073	0.0103	0.0073	0.0045	0.0045	0.0010	0.0010	0.0001
8.	Cu	0.0073	0.0103	0.1072	0.1075	0.0103	0.0073	0.0001	0.0011	0.0001
9.	Cu	0.0045	0.0073	0.0103	0.1074	0.1071	0.0104	0.0001	0.0011	0.0010
10.	Cu	0.0072	0.0104	0.0072	0.0104	0.1072	0.1072	0.0001	0.0001	0.0010
11.	Cu	0.1070	0.1071	0.0103	0.0073	0.0103	0.1072	0.0001	0.0002	0.0001
12.	Cu	0.1069	0.1072	0.1072	0.0104	0.0073	0.0104	0.0001	0.0001	0.0002
13.	Cu	0.0103	0.1071	0.1072	0.1074	0.1071	0.1072	0.0002	0.0001	0.0001
14.	Sn	0.0220	0.0046	0.0220	0.0220	0.0046	0.0039	0.0175	0.0174	0.0037
15.	Sn	0.0046	0.0039	0.0046	0.0221	0.0220	0.0046	0.0176	0.0174	0.0177
16.	Sn	0.0220	0.0046	0.0039	0.0046	0.0220	0.0220	0.0175	0.0035	0.0175
17.	Sn	0.0443	0.0221	0.0046	0.0039	0.0046	0.0220	0.0177	0.0003	0.0035
18.	Sn	0.0443	0.0220	0.0220	0.0046	0.0039	0.0046	0.0175	0.0035	0.0003
19.	Sn	0.7799	0.0444	0.0444	0.0220	0.0046	0.0220	0.0036	0.0003	0.0004
20.	Sn	0.0443	0.0444	0.7797	0.0444	0.0220	0.0220	0.0003	0.0036	0.0004
21.	Sn	0.0220	0.0220	0.0443	0.0444	0.0220	0.0046	0.0036	0.0175	0.0003
22.	Sn	0.0046	0.0220	0.0443	0.7791	0.0443	0.0220	0.0003	0.0177	0.0036
23.	Sn	0.0039	0.0046	0.0220	0.0443	0.0443	0.0220	0.0036	0.0176	0.0176
24.	Sn	0.0046	0.0220	0.0220	0.0444	0.7800	0.0444	0.0003	0.0036	0.0174
25.	Sn	0.0220	0.0220	0.0046	0.0220	0.0444	0.0444	0.0036	0.0003	0.0174
26.	Sn	0.0444	0.0444	0.0220	0.0220	0.0444	0.7800	0.0003	0.0004	0.0036
27.	Sn	0.7798	0.0444	0.0220	0.0046	0.0220	0.0443	0.0037	0.0004	0.0003
28.	Sn	0.0000	0.7799	0.0444	0.0220	0.0220	0.0444	0.0003	0.0004	0.0004
29.	Sn	0.7799	0.0000	0.7798	0.0443	0.0443	0.7793	0.0004	0.0004	0.0004
30.	Sn	0.0444	0.7798	0.0000	0.7795	0.0444	0.0444	0.0004	0.0003	0.0004
31.	Sn	0.0220	0.0443	0.7795	0.0000	0.7796	0.0444	0.0004	0.0037	0.0003
32.	Sn	0.0220	0.0443	0.0444	0.7796	0.0000	0.7798	0.0004	0.0003	0.0035
33.	Sn	0.0444	0.7793	0.0444	0.0444	0.7798	0.0000	0.0004	0.0004	0.0003
34.	K	0.0003	0.0004	0.0004	0.0004	0.0004	0.0004	0.0000	0.0004	0.0004
35.	K	0.0004	0.0004	0.0003	0.0037	0.0003	0.0004	0.0004	0.0000	0.0004
36.	K	0.0004	0.0004	0.0004	0.0003	0.0035	0.0003	0.0004	0.0004	0.0000

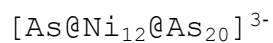
37.	K	0.0036	0.0003	0.0004	0.0004	0.0003	0.0036	0.0004	0.0000	0.0004
38.	K	0.0176	0.0036	0.0003	0.0004	0.0004	0.0003	0.0004	0.0000	0.0000
39.	K	0.0036	0.0003	0.0036	0.0003	0.0004	0.0004	0.0004	0.0004	0.0000
40.	K	0.0003	0.0036	0.0175	0.0175	0.0036	0.0003	0.0000	0.0004	0.0000
41.	K	0.0004	0.0003	0.0036	0.0174	0.0174	0.0035	0.0000	0.0004	0.0004
42.	K	0.0003	0.0037	0.0003	0.0036	0.0176	0.0177	0.0000	0.0000	0.0004
43.	K	0.0176	0.0174	0.0035	0.0003	0.0035	0.0174	0.0000	0.0000	0.0000
44.	K	0.0176	0.0177	0.0175	0.0035	0.0003	0.0037	0.0000	0.0000	0.0000
45.	K	0.0036	0.0176	0.0175	0.0177	0.0175	0.0175	0.0000	0.0000	0.0000

	Atom	37	38	39	40	41	42	43	44	45
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1.	Sn	0.0035	0.0035	0.0035	0.0035	0.0035	0.0035	0.0035	0.0035	0.0035
2.	Cu	0.0010	0.0010	0.0011	0.0001	0.0001	0.0001	0.0001	0.0001	0.0002
3.	Cu	0.0001	0.0001	0.0010	0.0010	0.0010	0.0001	0.0002	0.0001	0.0001
4.	Cu	0.0010	0.0001	0.0001	0.0001	0.0011	0.0010	0.0001	0.0002	0.0001
5.	Cu	0.0092	0.0010	0.0001	0.0002	0.0001	0.0010	0.0011	0.0001	0.0001
6.	Cu	0.0010	0.0092	0.0010	0.0001	0.0002	0.0001	0.0011	0.0010	0.0001
7.	Cu	0.0001	0.0010	0.0092	0.0011	0.0001	0.0002	0.0001	0.0010	0.0001
8.	Cu	0.0002	0.0001	0.0010	0.0092	0.0010	0.0001	0.0001	0.0010	0.0011
9.	Cu	0.0001	0.0002	0.0001	0.0010	0.0092	0.0010	0.0001	0.0001	0.0011
10.	Cu	0.0011	0.0001	0.0002	0.0001	0.0010	0.0092	0.0010	0.0001	0.0010
11.	Cu	0.0010	0.0010	0.0001	0.0001	0.0001	0.0010	0.0092	0.0011	0.0010
12.	Cu	0.0001	0.0011	0.0010	0.0011	0.0001	0.0001	0.0010	0.0092	0.0010
13.	Cu	0.0001	0.0001	0.0001	0.0010	0.0010	0.0011	0.0010	0.0011	0.0092
14.	Sn	0.0003	0.0035	0.0177	0.0036	0.0003	0.0004	0.0004	0.0003	0.0004
15.	Sn	0.0036	0.0003	0.0037	0.0003	0.0036	0.0003	0.0004	0.0004	0.0004
16.	Sn	0.0175	0.0036	0.0003	0.0004	0.0003	0.0036	0.0003	0.0004	0.0004
17.	Sn	0.0175	0.0174	0.0036	0.0004	0.0004	0.0003	0.0037	0.0003	0.0004
18.	Sn	0.0036	0.0174	0.0176	0.0003	0.0004	0.0004	0.0003	0.0035	0.0004
19.	Sn	0.0003	0.0177	0.0176	0.0037	0.0004	0.0004	0.0036	0.0174	0.0003
20.	Sn	0.0004	0.0037	0.0175	0.0177	0.0003	0.0004	0.0003	0.0174	0.0036
21.	Sn	0.0004	0.0003	0.0175	0.0175	0.0035	0.0004	0.0004	0.0036	0.0003
22.	Sn	0.0004	0.0004	0.0036	0.0175	0.0174	0.0003	0.0004	0.0003	0.0037
23.	Sn	0.0003	0.0004	0.0003	0.0036	0.0176	0.0036	0.0004	0.0004	0.0003
24.	Sn	0.0037	0.0004	0.0004	0.0003	0.0177	0.0176	0.0003	0.0004	0.0036
25.	Sn	0.0177	0.0003	0.0004	0.0004	0.0037	0.0175	0.0036	0.0004	0.0003
26.	Sn	0.0175	0.0035	0.0004	0.0004	0.0003	0.0175	0.0175	0.0003	0.0036
27.	Sn	0.0175	0.0174	0.0003	0.0004	0.0004	0.0036	0.0177	0.0036	0.0003
28.	Sn	0.0036	0.0176	0.0036	0.0003	0.0004	0.0003	0.0176	0.0176	0.0036
29.	Sn	0.0003	0.0036	0.0003	0.0036	0.0003	0.0037	0.0174	0.0177	0.0176
30.	Sn	0.0004	0.0003	0.0036	0.0175	0.0036	0.0003	0.0035	0.0175	0.0175
31.	Sn	0.0004	0.0004	0.0003	0.0175	0.0174	0.0036	0.0003	0.0035	0.0177
32.	Sn	0.0003	0.0004	0.0004	0.0036	0.0174	0.0176	0.0035	0.0003	0.0175
33.	Sn	0.0036	0.0003	0.0004	0.0003	0.0035	0.0177	0.0174	0.0037	0.0175
34.	K	0.0004	0.0004	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	K	0.0000	0.0000	0.0004	0.0004	0.0004	0.0000	0.0000	0.0000	0.0000
36.	K	0.0004	0.0000	0.0000	0.0000	0.0004	0.0004	0.0000	0.0000	0.0000
37.	K	0.0000	0.0004	0.0000	0.0000	0.0000	0.0004	0.0004	0.0000	0.0000
38.	K	0.0004	0.0000	0.0004	0.0000	0.0000	0.0000	0.0004	0.0004	0.0000
39.	K	0.0000	0.0004	0.0000	0.0004	0.0000	0.0000	0.0000	0.0004	0.0000
40.	K	0.0000	0.0000	0.0004	0.0000	0.0004	0.0000	0.0000	0.0004	0.0004
41.	K	0.0000	0.0000	0.0000	0.0004	0.0000	0.0004	0.0000	0.0000	0.0004
42.	K	0.0004	0.0000	0.0000	0.0000	0.0004	0.0000	0.0004	0.0000	0.0004
43.	K	0.0004	0.0004	0.0000	0.0000	0.0000	0.0004	0.0000	0.0004	0.0004
44.	K	0.0000	0.0004	0.0004	0.0004	0.0000	0.0000	0.0004	0.0000	0.0004
45.	K	0.0000	0.0000	0.0000	0.0004	0.0004	0.0004	0.0004	0.0004	0.0000

Wiberg bond index, Totals by atom:

Atom	1
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1. Sn 2.6889
2. Cu 0.8636
3. Cu 0.8633
4. Cu 0.8630
5. Cu 0.8640
6. Cu 0.8633
7. Cu 0.8632
8. Cu 0.8640
9. Cu 0.8633
10. Cu 0.8632
11. Cu 0.8633
12. Cu 0.8630
13. Cu 0.8636
14. Sn 3.2794
15. Sn 3.2792
16. Sn 3.2788
17. Sn 3.2791
18. Sn 3.2788
19. Sn 3.2796
20. Sn 3.2793
21. Sn 3.2788
22. Sn 3.2792
23. Sn 3.2790
24. Sn 3.2796
25. Sn 3.2793
26. Sn 3.2788
27. Sn 3.2792
28. Sn 3.2790
29. Sn 3.2792
30. Sn 3.2788
31. Sn 3.2791
32. Sn 3.2788
33. Sn 3.2794
34. K 0.1301
35. K 0.1299
36. K 0.1300
37. K 0.1301
38. K 0.1300
39. K 0.1301
40. K 0.1301
41. K 0.1300
42. K 0.1301
43. K 0.1299
44. K 0.1300
45. K 0.1301



As	0.000000	0.000000	0.000000
Ni	2.154602	-0.700180	-1.132794
Ni	1.331746	1.832932	-1.132908
Ni	0.000000	0.000120	-2.533186
Ni	0.000000	-2.265668	-1.132815
Ni	1.331746	-1.832931	1.132908
Ni	2.154602	0.700180	1.132794
Ni	0.000000	2.265667	1.132814
Ni	-1.331746	1.832932	-1.132908
Ni	-2.154602	-0.700180	-1.132794
Ni	-1.331746	-1.832932	1.132908
Ni	0.000000	-0.000120	2.533186
Ni	-2.154602	0.700180	1.132794
As	3.595638	1.168230	-0.722040

As	2.222300	0.722019	-3.058661
As	1.373404	-1.890329	-3.058661
As	2.222215	-3.058657	-0.721988
As	3.595638	-1.168230	0.722040
As	2.222300	-0.722018	3.058661
As	1.373405	1.890330	3.058662
As	2.222215	3.058657	0.721988
As	0.000000	3.780682	-0.722128
As	0.000000	2.336702	-3.058670
As	-2.222300	0.722019	-3.058661
As	-1.373404	-1.890329	-3.058662
As	-2.222215	-3.058657	-0.721988
As	0.000000	-3.780682	0.722128
As	0.000000	-2.336702	3.058670
As	-2.222300	-0.722018	3.058661
As	-1.373404	1.890330	3.058662
As	-2.222215	3.058658	0.721988
As	-3.595638	1.168230	-0.722040
As	-3.595638	-1.168230	0.722040

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
As 1	-0.71442	27.99898	5.68271	0.03273	33.71442
Ni 2	0.09641	17.99312	9.85219	0.05828	27.90359
Ni 3	0.09588	17.99312	9.85223	0.05876	27.90412
Ni 4	0.09643	17.99312	9.85232	0.05813	27.90357
Ni 5	0.09627	17.99312	9.85226	0.05835	27.90373
Ni 6	0.09544	17.99312	9.85234	0.05910	27.90456
Ni 7	0.09632	17.99312	9.85227	0.05829	27.90368
Ni 8	0.09627	17.99312	9.85226	0.05835	27.90373
Ni 9	0.09544	17.99312	9.85234	0.05910	27.90456
Ni 10	0.09632	17.99312	9.85227	0.05829	27.90368
Ni 11	0.09588	17.99312	9.85223	0.05876	27.90412
Ni 12	0.09643	17.99312	9.85232	0.05813	27.90357
Ni 13	0.09641	17.99312	9.85219	0.05828	27.90359
As 14	-0.17190	27.99855	5.08722	0.08613	33.17190
As 15	-0.17104	27.99855	5.08853	0.08396	33.17104
As 16	-0.17196	27.99855	5.08635	0.08706	33.17196
As 17	-0.17180	27.99855	5.08769	0.08556	33.17180
As 18	-0.17226	27.99855	5.08665	0.08706	33.17226
As 19	-0.17220	27.99855	5.08675	0.08689	33.17220
As 20	-0.17120	27.99855	5.08867	0.08397	33.17120
As 21	-0.17254	27.99855	5.08648	0.08752	33.17254
As 22	-0.17255	27.99855	5.08658	0.08741	33.17255
As 23	-0.17210	27.99855	5.08664	0.08691	33.17210
As 24	-0.17220	27.99855	5.08675	0.08689	33.17220
As 25	-0.17120	27.99855	5.08867	0.08397	33.17120
As 26	-0.17254	27.99855	5.08648	0.08752	33.17254
As 27	-0.17255	27.99855	5.08658	0.08741	33.17255
As 28	-0.17210	27.99855	5.08664	0.08691	33.17210
As 29	-0.17104	27.99855	5.08853	0.08396	33.17104
As 30	-0.17196	27.99855	5.08635	0.08706	33.17196
As 31	-0.17180	27.99855	5.08769	0.08556	33.17180
As 32	-0.17226	27.99855	5.08665	0.08706	33.17226
As 33	-0.17190	27.99855	5.08722	0.08613	33.17190
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* Total *	-2.99999	803.88747	225.65304	2.45949	1031.99999

Natural Population	
Core	803.88747 (99.9860% of 804)
Valence	225.65304 (98.9706% of 228)
Natural Minimal Basis	1029.54051 (99.7617% of 1032)
Natural Rydberg Basis	2.45949 (0.2383% of 1032)

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
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1. As	0.0000	0.0986	0.0985	0.0987	0.0986	0.0985	0.0986	0.0986	0.0985
2. Ni	0.0986	0.0000	0.0278	0.0278	0.0278	0.0278	0.0278	0.0050	0.0049
3. Ni	0.0985	0.0278	0.0000	0.0278	0.0050	0.0050	0.0278	0.0278	0.0278
4. Ni	0.0987	0.0278	0.0278	0.0000	0.0278	0.0050	0.0049	0.0050	0.0278
5. Ni	0.0986	0.0278	0.0050	0.0278	0.0000	0.0278	0.0049	0.0055	0.0049
6. Ni	0.0985	0.0278	0.0050	0.0050	0.0278	0.0000	0.0279	0.0049	0.0055
7. Ni	0.0986	0.0278	0.0278	0.0049	0.0049	0.0279	0.0000	0.0278	0.0050
8. Ni	0.0986	0.0050	0.0278	0.0050	0.0055	0.0049	0.0278	0.0000	0.0278
9. Ni	0.0985	0.0049	0.0278	0.0278	0.0049	0.0055	0.0050	0.0278	0.0000
10. Ni	0.0986	0.0050	0.0050	0.0278	0.0278	0.0050	0.0055	0.0049	0.0279
11. Ni	0.0985	0.0049	0.0055	0.0050	0.0278	0.0278	0.0050	0.0050	0.0050
12. Ni	0.0987	0.0050	0.0050	0.0055	0.0050	0.0278	0.0278	0.0278	0.0050
13. Ni	0.0986	0.0055	0.0049	0.0050	0.0050	0.0049	0.0050	0.0278	0.0278
14. As	0.1021	0.2067	0.2067	0.0161	0.0106	0.0161	0.2065	0.0161	0.0106
15. As	0.1020	0.2064	0.2068	0.2062	0.0161	0.0107	0.0161	0.0107	0.0161
16. As	0.1020	0.2067	0.0162	0.2065	0.2069	0.0162	0.0105	0.0040	0.0106
17. As	0.1020	0.2062	0.0107	0.0161	0.2063	0.2066	0.0161	0.0040	0.0041
18. As	0.1020	0.2065	0.0161	0.0106	0.0161	0.2069	0.2063	0.0106	0.0040
19. As	0.1020	0.0161	0.0106	0.0041	0.0106	0.2069	0.2065	0.0161	0.0040
20. As	0.1020	0.0107	0.0161	0.0040	0.0040	0.0161	0.2066	0.2063	0.0107
21. As	0.1019	0.0161	0.2066	0.0106	0.0041	0.0106	0.2064	0.2065	0.0161
22. As	0.1020	0.0106	0.2063	0.0161	0.0041	0.0041	0.0161	0.2066	0.2066
23. As	0.1021	0.0161	0.2069	0.2062	0.0106	0.0040	0.0106	0.0161	0.2069
24. As	0.1020	0.0106	0.0161	0.2063	0.0161	0.0040	0.0041	0.0106	0.2069
25. As	0.1020	0.0161	0.0107	0.2064	0.2063	0.0107	0.0041	0.0040	0.0161
26. As	0.1019	0.0106	0.0040	0.0161	0.2065	0.0161	0.0040	0.0041	0.0106
27. As	0.1020	0.0161	0.0040	0.0106	0.2066	0.2066	0.0106	0.0041	0.0041
28. As	0.1021	0.0106	0.0041	0.0041	0.0161	0.2069	0.0161	0.0106	0.0040
29. As	0.1020	0.0040	0.0040	0.0040	0.0107	0.0161	0.0107	0.0161	0.0107
30. As	0.1020	0.0040	0.0106	0.0040	0.0040	0.0106	0.0161	0.2069	0.0162
31. As	0.1020	0.0040	0.0161	0.0106	0.0040	0.0041	0.0106	0.2063	0.2066
32. As	0.1020	0.0041	0.0106	0.0161	0.0106	0.0040	0.0040	0.0161	0.2069
33. As	0.1021	0.0041	0.0041	0.0106	0.0161	0.0106	0.0040	0.0106	0.0161

Atom	10	11	12	13	14	15	16	17	18
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1. As	0.0986	0.0985	0.0987	0.0986	0.1021	0.1020	0.1020	0.1020	0.1020
2. Ni	0.0050	0.0049	0.0050	0.0055	0.2067	0.2064	0.2067	0.2062	0.2065
3. Ni	0.0050	0.0055	0.0050	0.0049	0.2067	0.2068	0.0162	0.0107	0.0161
4. Ni	0.0278	0.0050	0.0055	0.0050	0.0161	0.2062	0.2065	0.0161	0.0106
5. Ni	0.0278	0.0278	0.0050	0.0050	0.0106	0.0161	0.2069	0.2063	0.0161
6. Ni	0.0050	0.0278	0.0278	0.0049	0.0161	0.0107	0.0162	0.2066	0.2069
7. Ni	0.0055	0.0050	0.0278	0.0050	0.2065	0.0161	0.0105	0.0161	0.2063
8. Ni	0.0049	0.0050	0.0278	0.0278	0.0161	0.0107	0.0040	0.0040	0.0106
9. Ni	0.0279	0.0050	0.0050	0.0278	0.0106	0.0161	0.0106	0.0041	0.0040
10. Ni	0.0000	0.0278	0.0049	0.0278	0.0040	0.0107	0.0161	0.0106	0.0040
11. Ni	0.0278	0.0000	0.0278	0.0278	0.0041	0.0040	0.0106	0.0161	0.0106
12. Ni	0.0049	0.0278	0.0000	0.0278	0.0106	0.0040	0.0040	0.0106	0.0161
13. Ni	0.0278	0.0278	0.0278	0.0000	0.0041	0.0040	0.0040	0.0040	0.0041
14. As	0.0040	0.0041	0.0106	0.0041	0.0000	0.6748	0.0335	0.0335	0.6748
15. As	0.0107	0.0040	0.0040	0.0040	0.6748	0.0000	0.6757	0.0335	0.0335

16.	As	0.0161	0.0106	0.0040	0.0040	0.0335	0.6757	0.0000	0.6748	0.0336
17.	As	0.0106	0.0161	0.0106	0.0040	0.0335	0.0335	0.6748	0.0000	0.6755
18.	As	0.0040	0.0106	0.0161	0.0041	0.6748	0.0335	0.0336	0.6755	0.0000
19.	As	0.0041	0.0161	0.2063	0.0106	0.0335	0.0166	0.0166	0.0336	0.6753
20.	As	0.0041	0.0107	0.2064	0.0161	0.0335	0.0166	0.0049	0.0166	0.0335
21.	As	0.0040	0.0040	0.0161	0.0106	0.6753	0.0335	0.0166	0.0166	0.0335
22.	As	0.0106	0.0040	0.0106	0.0161	0.0336	0.0335	0.0166	0.0049	0.0166
23.	As	0.0161	0.0041	0.0041	0.0106	0.0335	0.6749	0.0335	0.0166	0.0166
24.	As	0.2065	0.0106	0.0041	0.0161	0.0166	0.0335	0.0335	0.0166	0.0049
25.	As	0.2066	0.0161	0.0040	0.0107	0.0166	0.0335	0.6749	0.0336	0.0166
26.	As	0.2064	0.2066	0.0106	0.0161	0.0049	0.0166	0.0336	0.0336	0.0166
27.	As	0.0161	0.2063	0.0161	0.0106	0.0166	0.0166	0.0336	0.6756	0.0336
28.	As	0.0106	0.2069	0.2062	0.0161	0.0166	0.0049	0.0166	0.0336	0.0336
29.	As	0.0161	0.2068	0.2062	0.2064	0.0049	0.0069	0.0049	0.0165	0.0166
30.	As	0.0105	0.0162	0.2065	0.2067	0.0166	0.0049	0.0069	0.0049	0.0166
31.	As	0.0161	0.0107	0.0161	0.2062	0.0166	0.0165	0.0049	0.0069	0.0049
32.	As	0.2063	0.0161	0.0106	0.2065	0.0049	0.0166	0.0166	0.0049	0.0069
33.	As	0.2065	0.2067	0.0161	0.2067	0.0069	0.0049	0.0166	0.0166	0.0049

Atom	19	20	21	22	23	24	25	26	27
1. As	0.1020	0.1020	0.1019	0.1020	0.1021	0.1020	0.1020	0.1019	0.1020
2. Ni	0.0161	0.0107	0.0161	0.0106	0.0161	0.0106	0.0161	0.0106	0.0161
3. Ni	0.0106	0.0161	0.2066	0.2063	0.2069	0.0161	0.0107	0.0040	0.0040
4. Ni	0.0041	0.0040	0.0106	0.0161	0.2062	0.2063	0.2064	0.0161	0.0106
5. Ni	0.0106	0.0040	0.0041	0.0041	0.0106	0.0161	0.2063	0.2065	0.2066
6. Ni	0.2069	0.0161	0.0106	0.0041	0.0040	0.0040	0.0107	0.0161	0.2066
7. Ni	0.2065	0.2066	0.2064	0.0161	0.0106	0.0041	0.0041	0.0040	0.0106
8. Ni	0.0161	0.2063	0.2065	0.2066	0.0161	0.0106	0.0040	0.0041	0.0041
9. Ni	0.0040	0.0107	0.0161	0.2066	0.2069	0.2069	0.0161	0.0106	0.0041
10. Ni	0.0041	0.0041	0.0040	0.0106	0.0161	0.2065	0.2066	0.2064	0.0161
11. Ni	0.0161	0.0107	0.0040	0.0040	0.0041	0.0106	0.0161	0.2066	0.2063
12. Ni	0.2063	0.2064	0.0161	0.0106	0.0041	0.0041	0.0040	0.0106	0.0161
13. Ni	0.0106	0.0161	0.0106	0.0161	0.0106	0.0161	0.0107	0.0161	0.0106
14. As	0.0335	0.0335	0.6753	0.0336	0.0335	0.0166	0.0166	0.0049	0.0166
15. As	0.0166	0.0166	0.0335	0.0335	0.6749	0.0335	0.0335	0.0166	0.0166
16. As	0.0166	0.0049	0.0166	0.0166	0.0335	0.0335	0.6749	0.0336	0.0336
17. As	0.0336	0.0166	0.0166	0.0049	0.0166	0.0166	0.0336	0.0336	0.6756
18. As	0.6753	0.0335	0.0335	0.0166	0.0166	0.0049	0.0166	0.0166	0.0336
19. As	0.0000	0.6749	0.0336	0.0166	0.0049	0.0069	0.0049	0.0166	0.0336
20. As	0.6749	0.0000	0.6755	0.0335	0.0166	0.0049	0.0069	0.0049	0.0166
21. As	0.0336	0.6755	0.0000	0.6753	0.0336	0.0166	0.0049	0.0069	0.0049
22. As	0.0166	0.0335	0.6753	0.0000	0.6749	0.0336	0.0166	0.0049	0.0069
23. As	0.0049	0.0166	0.0336	0.6749	0.0000	0.6754	0.0335	0.0166	0.0049
24. As	0.0069	0.0049	0.0166	0.0336	0.6754	0.0000	0.6749	0.0336	0.0166
25. As	0.0049	0.0069	0.0049	0.0166	0.0335	0.6749	0.0000	0.6755	0.0335
26. As	0.0166	0.0049	0.0069	0.0049	0.0166	0.0336	0.6755	0.0000	0.6753
27. As	0.0336	0.0166	0.0049	0.0069	0.0049	0.0166	0.0335	0.6753	0.0000
28. As	0.6754	0.0335	0.0166	0.0049	0.0069	0.0049	0.0166	0.0336	0.6749
29. As	0.0335	0.0335	0.0166	0.0166	0.0049	0.0166	0.0166	0.0335	0.0335
30. As	0.0335	0.6749	0.0336	0.0336	0.0166	0.0166	0.0049	0.0166	0.0166
31. As	0.0166	0.0336	0.0336	0.6756	0.0336	0.0336	0.0166	0.0166	0.0049
32. As	0.0049	0.0166	0.0166	0.0336	0.0336	0.6753	0.0335	0.0335	0.0166
33. As	0.0166	0.0166	0.0049	0.0166	0.0166	0.0335	0.0335	0.6753	0.0336

Atom	28	29	30	31	32	33
1.	As	0.1021	0.1020	0.1020	0.1020	0.1021
2.	Ni	0.0106	0.0040	0.0040	0.0040	0.0041
3.	Ni	0.0041	0.0040	0.0106	0.0161	0.0106
4.	Ni	0.0041	0.0040	0.0040	0.0106	0.0161
5.	Ni	0.0161	0.0107	0.0040	0.0040	0.0106
6.	Ni	0.2069	0.0161	0.0106	0.0041	0.0106

7.	Ni	0.0161	0.0107	0.0161	0.0106	0.0040	0.0040
8.	Ni	0.0106	0.0161	0.2069	0.2063	0.0161	0.0106
9.	Ni	0.0040	0.0107	0.0162	0.2066	0.2069	0.0161
10.	Ni	0.0106	0.0161	0.0105	0.0161	0.2063	0.2065
11.	Ni	0.2069	0.2068	0.0162	0.0107	0.0161	0.2067
12.	Ni	0.2062	0.2062	0.2065	0.0161	0.0106	0.0161
13.	Ni	0.0161	0.2064	0.2067	0.2062	0.2065	0.2067
14.	As	0.0166	0.0049	0.0166	0.0166	0.0049	0.0069
15.	As	0.0049	0.0069	0.0049	0.0165	0.0166	0.0049
16.	As	0.0166	0.0049	0.0069	0.0049	0.0166	0.0166
17.	As	0.0336	0.0165	0.0049	0.0069	0.0049	0.0166
18.	As	0.0336	0.0166	0.0166	0.0049	0.0069	0.0049
19.	As	0.6754	0.0335	0.0335	0.0166	0.0049	0.0166
20.	As	0.0335	0.0335	0.6749	0.0336	0.0166	0.0166
21.	As	0.0166	0.0166	0.0336	0.0336	0.0166	0.0049
22.	As	0.0049	0.0166	0.0336	0.6756	0.0336	0.0166
23.	As	0.0069	0.0049	0.0166	0.0336	0.0336	0.0166
24.	As	0.0049	0.0166	0.0166	0.0336	0.6753	0.0335
25.	As	0.0166	0.0166	0.0049	0.0166	0.0335	0.0335
26.	As	0.0336	0.0335	0.0166	0.0166	0.0335	0.6753
27.	As	0.6749	0.0335	0.0166	0.0049	0.0166	0.0336
28.	As	0.0000	0.6749	0.0335	0.0166	0.0166	0.0335
29.	As	0.6749	0.0000	0.6757	0.0335	0.0335	0.6748
30.	As	0.0335	0.6757	0.0000	0.6748	0.0336	0.0335
31.	As	0.0166	0.0335	0.6748	0.0000	0.6756	0.0335
32.	As	0.0166	0.0335	0.0336	0.6756	0.0000	0.6748
33.	As	0.0335	0.6748	0.0335	0.0335	0.6748	0.0000

Wiberg bond index, Totals by atom:

	Atom	1
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1.	As	3.2237
2.	Ni	1.4542
3.	Ni	1.4553
4.	Ni	1.4535
5.	Ni	1.4541
6.	Ni	1.4558
7.	Ni	1.4540
8.	Ni	1.4541
9.	Ni	1.4558
10.	Ni	1.4540
11.	Ni	1.4553
12.	Ni	1.4535
13.	Ni	1.4542
14.	As	3.1615
15.	As	3.1612
16.	As	3.1618
17.	As	3.1616
18.	As	3.1618
19.	As	3.1617
20.	As	3.1612
21.	As	3.1619
22.	As	3.1618
23.	As	3.1617
24.	As	3.1617
25.	As	3.1612
26.	As	3.1619
27.	As	3.1618
28.	As	3.1617
29.	As	3.1612
30.	As	3.1618

31.	As	3.1616
32.	As	3.1618
33.	As	3.1615