Supplementary Information

Comment on "Realization of the Zn^{3+} oxidation state" by H. Fang, H. Banjade, Deepika and P. Jena, Nanoscale, 2021, 13, 14041-14048

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1. Computational Details

1.1 Geometry Optimization and Wavefunction Analysis

Geometry optimizations of $ZnBeB_{11}(CN)_{12}$ and $ZnBeB_{23}(CN)_{22}$ clusters are carried out in Gaussian16 Program (Revision C.01) using the TPSSh functional with the def2-SVP basis set developed by Alhrichs and co-workers.[1-5] Grimme's third dispersion correction (D3) is adopted for consideration of intramolecular weak interactions and rational damping to finite values for small interatomic distances according to Becke and Johnson (BJ-damping) has been used.[6, 7] Frequency calculations are carried out under the same level of theory with that of optimization to make sure no imaginary frequency existed. Additionally, Multiwfn Program (Version 3.8)[8] is used for wavefunction analyses, including oxidation state analysis, density of states analysis, spin density calculation and spin population analysis. Oxidation state analysis is carried out using localized orbital bonding analysis (LOBA) method which proposed by Thom et al.[9] Constraint DFT (CDFT) calculations are carried out by NWChem Program (Version 7.0.0). In terms of Koopmans theorem, XPS of two clusters are simulated by Multiwfn Program. Visual Molecular Dynamics (VMD, Version 1.9.3) is taken for realizing better visualization effect.[10] More details and results are available in electronic supplementary information.

Note:

To use BJ-damping for TPSSh functional in Gaussian16 Program (Revision C.01), below input can be followed:

```
%nprocshared=28
%mem=400MW
%chk=Zn1.chk
#P opt TPSSh/def2SVP em=GD3BJ
IOp(3/174=1000000,3/175=2238200, 3/177=452900,3/178=4655000)
Guess=Read Geom=AllCheck
```

1.2 Geometric Structures

1.2.1 $ZnBeB_{11}(CN)_{12}$

1	C	-1.13014929	-2.40050950	-2.12000621
2	N	-1.23363998	-3.27512913	-2.88446642
3	C	-0.07818190	2.46502383	2.02312775
4	N	0.29727336	3.35547478	2.68229168
5	C	-1.14718474	-0.62544678	3.14753275
6	N	-1.26507990	-0.83561949	4.28828014
7	C	-3.11296478	-2.00211999	0.68653959
8	N	-3.97147796	-2.74892444	0.94368074
9	C	-3.33877544	0.20435195	-1.88944557
10	N	-4.27880093	0.25432872	-2.57456885
11	C	-1.52197374	3.01604542	-1.01113603
12	N	-1.73196163	4.11248206	-1.34917462
13	C	0.20533721	-2.95024844	1.00010634
14	N	0.62654866	-3.98135696	1.33840594
15	C	-0.09109162	0.67938454	-3.13355394
16	N	0.27594045	0.91437521	-4.21714928
17	C	2.05665237	-0.25351585	1.64466250
18	N	3.22168778	-0.33187036	1.77883321
19	C	2.38400352	1.86992553	-0.63332270
20	N	3.55569831	1.78997716	-0.60869000
21	C	2.04952066	-1.19462565	-1.15113635
22	N	3.21491146	-1.32702145	-1.21564581
23	C	-3.30704307	1.35432694	1.36762117
24	N	-4.23542066	1.82661079	1.88938620
25	B	0.66248859	-0.69217594	-0.70858731
26	B	-2.07538811	0.73631726	0.69489967
27	B	-2.09088174	0.13905238	-0.99922299
28	B	-0.43716027	1.30227359	1.10392316
29	B	-0.94626295	-0.33877529	1.65752920
30	B	-1.97595797	-1.03642966	0.35173455
31	B	-1.15078000	1.59659167	-0.56714816
32	B	-0.94644703	-1.25630937	-1.12088754
33	B	-0.25149293	-1.55824164	0.53996641
34	B	-0.44084107	0.39573242	-1.67094069
35	B	0.67245326	-0.10850550	0.98768673
36	Be	0.77143535	1.29116287	-0.43820561
37	Zn	4.08923207	-0.01037137	0.01079470

1.2.2 $ZnBeB_{23}(CN)_{22}$

1	C	-4.71052322	2.23026759	1.46618966	35	C	3.19572473	0.81731579	-2.99925393
2	N	-5.06631743	3.23231312	1.94235210	36	N	2.93274909	1.31887430	-4.01618293
3	C	-2.05098771	-2.94171150	-1.44152014	37	C	3.61945775	-1.35709179	3.10963664
4	N	-1.45304163	-3.82481598	-1.91563334	38	N	3.59096370	-1.72744787	4.21278150
5	C	-3.31103365	-0.30667146	-3.21279606	39	C	4.59830958	1.84316749	2.21850916
6	N	-3.18798082	-0.18022389	-4.36492158	40	N	4.91224398	2.67070219	2.97391677
7	C	-5.99105207	0.98015348	-1.43118784	41	C	5.84209243	1.71323088	-0.97145252
8	N	-6.86640988	1.53336518	-1.96633297	42	N	6.63049060	2.48790552	-1.33612756
9	C	-6.29520146	-0.86017741	1.47778991	43	C	5.64397678	-1.55116317	-2.06912455
10	N	-7.32297480	-0.99603172	2.00940297	44	N	6.40667868	-1.98381589	-2.83396843
11	C	-3.90498425	-3.27930840	1.46247290	45	C	4.25922870	-3.45024944	0.46153708
12	N	-3.99970371	-4.29554495	2.02931944	46	N	4.49341189	-4.57802056	0.62736821
13	C	-2.67514435	2.44893915	-1.27121139	47	C	2.35521941	2.65658000	-0.40362095
14	N	-1.96880074	3.36366502	-1.44978587	48	N	1.53675367	3.47385455	-0.55442351
15	C	-3.39255499	-0.46010980	3.27421045	49	C	2.24327954	-2.34867711	-2.16875892
16	N	-3.28287669	-0.51312219	4.43840596	50	N	1.68379323	-2.99713252	-2.95687770
17	C	-0.53274595	0.08414755	-1.10099293	51	C	1.33395924	0.80006765	2.15176757
18	N	0.62469678	0.18755834	-1.04369690	52	N	0.47915539	0.99299700	2.91794848
19	C	-1.55859659	1.91043906	1.27482923	53	C	6.46299663	-0.90306111	1.19426239
20	N	-1.00631673	2.94028890	1.25900300	54	N	7.52719060	-1.10647823	1.62008640
21	C	-5.49963887	-2.40853391	-1.49517214	55	B	2.00060854	-0.00502061	-0.57964988
22	N	-6.23537384	-3.11940132	-2.05084192	56	B	5.06125595	-0.62621644	0.64020006
23	B	-2.38371627	0.67950103	0.84215865	57	B	4.63216914	-0.97183482	-1.07403240
24	B	-4.52706885	-1.47264526	-0.76985662	58	B	3.60156518	-0.87132780	1.65615021
25	B	-4.94299636	-0.66342886	0.78479576	59	B	4.11625748	0.80566361	1.19602369
26	B	-2.75706564	-1.78123881	-0.73995196	60	B	4.75647632	0.74093431	-0.49495865
27	B	-3.41836014	-0.39676569	-1.68861088	61	B	3.91228304	-1.97210502	0.25406265
28	B	-4.80749430	0.29884162	-0.74293207	62	B	3.42167253	0.24170800	-1.59387385
29	B	-3.69100434	-1.94136139	0.75141402	63	B	3.09886697	1.31265876	-0.18250603
30	B	-4.14649175	0.96884318	0.80451178	64	B	2.90030395	-1.43190390	-1.13143591
31	B	-3.21349266	1.10392675	-0.71071753	65	B	2.40069596	0.34561391	1.14490519
32	B	-3.45383405	-0.40803869	1.75464605	66	C	0.85323375	-1.85873111	0.96722768
33	B	-1.97873119	-0.13882207	-0.68819726	67	N	-0.29775117	-1.82813290	1.14708271
34	Be	-1.83471539	-1.27263909	0.93170049	68	B	2.26983125	-1.34462382	0.55708010
					69	Zn	-0.35813154	3.82721130	-0.38183664

2. Wavefunction Analysis

2.1 Mayer Bond Order

Table S1a. Mayer bond order of $ZnBeB_{11}(CN)_{12}$

No.	1[a]	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37
1	1.974	1.468	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.003	0.007	0.017	0.000	0.006	0.012	0.004	0.433	0.011	0.005	0.004	0.000	0.000
2	1.468	1.542	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.011	0.002	0.012	0.000	0.002	0.011	0.002	0.000	0.012	0.014	0.003	0.001	0.000
3	0.001	0.000	2.022	1.403	0.000	0.000	0.001	0.000	0.000	0.000	0.002	0.000	0.000	0.000	0.002	0.000	0.001	0.000	0.003	0.000	0.003	0.000	0.000	0.000	0.000	0.013	0.004	0.559	0.019	0.000	0.000	0.000	0.008	0.000	0.000	0.002	0.000
4	0.000	0.001	1.403	1.482	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.003	0.003	0.002	0.000	0.004	0.000	0.010	0.001	0.002	0.003	0.015	0.028	0.000
5	0.000	0.000	0.000	0.001	1.973	1.469	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.015	0.007	0.004	0.427	0.014	0.004	0.006	0.014	0.000	0.004	0.000	0.000
6	0.000	0.000	0.000	0.000	1.469	1.545	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.012	0.002	0.015	0.000	0.012	0.002	0.002	0.012	0.000	0.011	0.001	0.000
7	0.000	0.000	0.001	0.000	0.000	0.000	1.962	1.464	0.000	0.000	0.001	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.012	0.012	0.007	0.007	0.423	0.006	0.009	0.001	0.008	0.006	0.000	0.000
8	0.000	0.000	0.000	0.000	0.000	0.000	1.464	1.537	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.012	0.012	0.001	0.012	0.000	0.002	0.012	0.012	0.002	0.002	0.001	0.000
9	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	1.976	1.470	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.002	0.019	0.427	0.005	0.007	0.014	0.002	0.015	0.006	0.002	0.000	0.000	0.000
10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.470	1.540	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.011	0.000	0.002	0.001	0.011	0.012	0.012	0.002	0.011	0.001	0.001	0.000
11	0.000	0.000	0.002	0.000	0.000	0.000	0.001	0.000	0.001	0.000	2.020	1.411	0.001	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.004	0.000	0.010	0.000	0.008	0.002	0.565	0.007	0.000	0.000	0.003	0.000	0.000
12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	1.411	1.487	0.000	0.001	0.000	0.000	0.001	0.001	0.001	0.000	0.001	0.001	0.001	0.000	0.003	0.004	0.004	0.012	0.002	0.000	0.000	0.002	0.001	0.011	0.003	0.027	0.001
13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	1.990	1.468	0.000	0.000	0.001	0.001	0.000	0.000	0.001	0.001	0.001	0.000	0.003	0.005	0.005	0.006	0.019	0.009	0.000	0.018	0.437	0.006	0.005	0.000	0.000
14	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.001	1.468	1.536	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.011	0.002	0.002	0.003	0.013	0.005	0.000	0.013	0.000	0.003	0.011	0.001	0.000
15	0.001	0.000	0.002	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.000	2.018	1.412	0.002	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.012	0.000	0.000	0.000	0.000	0.010	0.009	0.558	0.000	0.001	0.000
16	0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.412	1.490	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.016	0.002	0.003	0.003	0.000	0.000	0.010	0.004	0.002	0.000	0.003	0.027	0.000
17	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.001	0.000	0.002	0.000	1.920	1.240	0.000	0.000	0.000	0.002	0.001	0.000	0.023	0.000	0.001	0.000	0.037	0.000	0.001	0.005	0.000	0.001	0.562	0.000	0.039
18	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.000	0.000	0.001	1.240	1.575	0.002	0.000	0.002	0.000	0.000	0.000	0.017	0.003	0.001	0.005	0.001	0.000	0.002	0.002	0.001	0.004	0.007	0.015	0.267
19	0.001	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.000	0.000	0.002	0.000	0.000	0.002	1.827	1.265	0.000	0.002	0.001	0.000	0.017	0.000	0.000	0.000	0.000	0.011	0.049	0.000	0.000	0.000	0.010	0.409	0.052
20	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.265	1.589	0.000	0.000	0.000	0.000	0.013	0.000	0.000	0.001	0.000	0.002	0.001	0.000	0.004	0.001	0.013	0.011	0.274
21	0.000	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.002	0.000	0.000	1.915	1.237	0.000	0.000	0.557	0.000	0.000	0.000	0.006	0.000	0.001	0.043	0.000	0.000	0.023	0.000	0.037
22	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.002	0.000	0.002	0.000	1.237	1.571	0.000	0.001	0.009	0.001	0.003	0.004	0.002	0.000	0.002	0.002	0.000	0.005	0.017	0.016	0.264
23	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	1.976	1.469	0.000	0.428	0.022	0.004	0.014	0.012	0.003	0.007	0.005	0.005	0.002	0.000	0.000
24	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	1.469	1.540	0.001	0.000	0.012	0.011	0.013	0.011	0.011	0.002	0.002	0.002	0.002	0.001	0.000
25	0.003	0.011	0.000	0.003	0.004	0.002	0.003	0.002	0.002	0.002	0.004	0.003	0.003	0.011	0.000	0.016	0.023	0.017	0.017	0.013	0.557	0.009	0.000	0.001	2.075	0.011	0.041	0.000	0.015	0.047	0.000	0.122	0.135	0.342	0.396	0.246	0.013
26	0.007	0.002	0.013	0.003	0.015	0.012	0.012	0.012	0.019	0.011	0.000	0.004	0.005	0.002	0.005	0.002	0.000	0.003	0.000	0.000	0.000	0.001	0.428	0.000	0.011	1.900	0.299	0.136	0.287	0.314	0.152	0.037	0.026	0.031	0.042	0.006	0.000
27	0.017	0.012	0.004	0.002	0.007	0.002	0.012	0.012	0.427	0.000	0.010	0.004	0.005	0.002	0.012	0.003	0.001	0.001	0.000	0.000	0.000	0.003	0.022	0.012	0.041	0.299	1.870	0.030	0.022	0.270	0.155	0.295	0.022	0.156	0.002	0.009	0.001
28	0.000	0.000	0.559	0.000	0.004	0.015	0.007	0.001	0.005	0.002	0.000	0.012	0.006	0.003	0.000	0.003	0.000	0.005	0.000	0.001	0.000	0.004	0.004	0.011	0.000	0.136	0.030	1.976	0.145	0.037	0.389	0.001	0.031	0.000	0.349	0.214	0.001
29	0.006	0.002	0.019	0.004	0.427	0.000	0.007	0.012	0.007	0.001	0.008	0.002	0.019	0.013	0.000	0.000	0.037	0.001	0.000	0.000	0.006	0.002	0.014	0.013	0.015	0.287	0.022	0.145	1.845	0.342	0.012	0.019	0.262	0.000	0.123	0.014	0.003
30	0.012	0.011	0.000	0.000	0.014	0.012	0.423	0.000	0.014	0.011	0.002	0.000	0.009	0.005	0.000	0.000	0.000	0.000	0.011	0.002	0.000	0.000	0.012	0.011	0.047	0.314	0.270	0.037	0.342	2.358	0.040	0.350	0.319	0.037	0.053	0.000	0.000
31	0.004	0.002	0.000	0.010	0.004	0.002	0.006	0.002	0.002	0.012	0.565	0.000	0.000	0.000	0.000	0.010	0.001	0.002	0.049	0.001	0.001	0.002	0.003	0.011	0.000	0.152	0.155	0.389	0.012	0.040	2.032	0.018	0.007	0.349	0.000	0.217	0.002
32	0.433	0.000	0.000	0.001	0.006	0.002	0.009	0.012	0.015	0.012	0.007	0.002	0.018	0.013	0.010	0.004	0.005	0.002	0.000	0.000	0.043	0.002	0.007	0.002	0.122	0.037	0.295	0.001	0.019	0.350	0.018	1.904	0.257	0.161	0.017	0.018	0.003
33	0.011	0.012	0.008	0.002	0.014	0.012	0.001	0.012	0.006	0.002	0.000	0.001	0.437	0.000	0.009	0.002	0.000	0.001	0.000	0.004	0.000	0.000	0.005	0.002	0.135	0.026	0.022	0.031	0.262	0.319	0.007	0.257	1.772	0.025	0.136	0.008	0.001
34	0.005	0.014	0.000	0.003	0.000	0.000	0.008	0.002	0.002	0.011	0.000	0.011	0.006	0.003	0.558	0.000	0.001	0.004	0.000	0.001	0.000	0.005	0.005	0.002	0.342	0.031	0.156	0.000	0.000	0.037	0.349	0.161	0.025	1.936	0.000	0.193	0.001
35	0.004	0.003	0.000	0.015	0.004	0.011	0.006	0.002	0.000	0.001	0.003	0.003	0.005	0.011	0.000	0.003	0.562	0.007	0.010	0.013	0.023	0.017	0.002	0.002	0.396	0.042	0.002	0.349	0.123	0.053	0.000	0.017	0.136	0.000	2.055	0.216	0.013
36	0.000	0.001	0.002	0.028	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.027	0.000	0.001	0.001	0.027	0.000	0.015	0.409	0.011	0.000	0.016	0.000	0.001	0.246	0.006	0.009	0.214	0.014	0.000	0.217	0.018	0.008	0.193	0.216	1.687	0.002
37	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.039	0.267	0.052	0.274	0.037	0.264	0.000	0.000	0.013	0.000	0.001	0.001	0.003	0.000	0.002	0.003	0.001	0.001	0.013	0.002	0.976

[a] Matrix element M_{ij} denotes the Mayer bond order between atom i and atom j, where atomic serial is defined in **1.2**. When $i = j$, it sums all Mayer bond order possessed by atom i.

Table S1b. Mayer bond order of $ZnBeB_{23}(CN)_{22}$ (Part I)

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
1	1.986	1.463	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.003	0.001	0.001	0.000	0.000	0.004	0.014	0.000	0.007	0.020	0.003	0.445	0.019	0.000	0.001	0.001
2	1.463	1.530	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.011	0.001	0.006	0.000	0.003	0.011	0.002	0.000	0.011	0.013	0.003	0.001
3	0.001	0.000	2.036	1.413	0.002	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.003	0.015	0.004	0.554	0.019	0.003	0.000	0.000	0.007	0.002	0.000	0.000
4	0.000	0.001	1.413	1.488	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.002	0.002	0.002	0.000	0.005	0.000	0.011	0.001	0.002	0.004	0.014	0.022
5	0.001	0.000	0.002	0.001	1.980	1.469	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.004	0.018	0.005	0.000	0.419	0.020	0.003	0.004	0.028	0.000	0.003	0.000
6	0.000	0.000	0.000	0.000	1.469	1.548	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.011	0.002	0.014	0.000	0.012	0.002	0.003	0.018	0.000	0.010	0.001
7	0.000	0.000	0.000	0.000	0.000	0.000	1.966	1.464	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.014	0.012	0.008	0.002	0.435	0.004	0.002	0.009	0.007	0.001	0.000
8	0.000	0.000	0.000	0.000	0.000	0.000	1.464	1.536	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.002	0.011	0.012	0.001	0.012	0.000	0.001	0.012	0.012	0.001	0.002	0.001
9	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	1.979	1.467	0.001	0.001	0.001	0.000	0.001	0.001	0.000	0.000	0.001	0.000	0.000	0.000	0.002	0.020	0.438	0.005	0.006	0.018	0.004	0.006	0.003	0.003	0.000	0.000
10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.467	1.540	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.003	0.012	0.000	0.002	0.002	0.010	0.012	0.013	0.002	0.011	0.001	0.001
11	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.000	2.031	1.417	0.000	0.000	0.001	0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.005	0.000	0.012	0.000	0.008	0.002	0.569	0.006	0.000	0.000	0.000	0.000
12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	1.417	1.491	0.001	0.001	0.000	0.000	0.001	0.001	0.000	0.000	0.001	0.000	0.002	0.004	0.004	0.011	0.002	0.000	0.000	0.002	0.001	0.012	0.003	0.023
13	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	1.895	1.290	0.001	0.000	0.000	0.002	0.004	0.004	0.001	0.000	0.000	0.001	0.000	0.002	0.023	0.004	0.000	0.007	0.500	0.000	0.021	0.000
14	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.001	1.290	1.624	0.000	0.001	0.000	0.000	0.002	0.000	0.000	0.000	0.011	0.001	0.002	0.005	0.003	0.004	0.002	0.005	0.002	0.003	0.018	0.002
15	0.001	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.001	0.000	2.027	1.408	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.006	0.003	0.000	0.002	0.000	0.022	0.007	0.560	0.003	0.000
16	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.001	1.408	1.486	0.001	0.001	0.000	0.000	0.000	0.000	0.016	0.002	0.006	0.003	0.000	0.000	0.012	0.004	0.002	0.000	0.003	0.021
17	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.004	0.001	0.000	0.000	0.001	0.001	1.917	1.208	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.006	0.000	0.000	0.000	0.025	0.010	0.575	0.020
18	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.002	0.000	0.000	0.001	1.208	1.813	0.000	0.000	0.000	0.000	0.017	0.002	0.002	0.007	0.002	0.000	0.003	0.002	0.002	0.003	0.008	0.010
19	0.003	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.004	0.002	0.000	0.000	0.000	0.000	1.931	1.262	0.000	0.000	0.535	0.000	0.000	0.003	0.000	0.007	0.000	0.013	0.014	0.011	0.017	0.000
20	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.000	0.000	0.000	0.000	0.000	1.262	1.596	0.000	0.001	0.000	0.001	0.003	0.002	0.003	0.003	0.002	0.008	0.010	0.003	0.010	0.003
21	0.001	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.972	1.468	0.000	0.430	0.019	0.000	0.011	0.018	0.002	0.005	0.005	0.006	0.002	0.000
22	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	1.468	1.540	0.002	0.000	0.012	0.011	0.012	0.011	0.012	0.002	0.002	0.002	0.002	0.001
23	0.000	0.011	0.003	0.002	0.004	0.003	0.004	0.002	0.002	0.003	0.005	0.002	0.000	0.011	0.000	0.016	0.001	0.017	0.535	0.000	0.000	0.002	1.918	0.013	0.042	0.000	0.000	0.019	0.000	0.156	0.200	0.334	0.320	0.187
24	0.004	0.001	0.015	0.002	0.018	0.011	0.014	0.011	0.020	0.012	0.000	0.004	0.001	0.001	0.005	0.002	0.000	0.002	0.000	0.001	0.430	0.000	0.013	1.852	0.294	0.140	0.309	0.276	0.112	0.034	0.034	0.013	0.065	0.004
25	0.014	0.006	0.004	0.002	0.005	0.002	0.012	0.012	0.438	0.000	0.012	0.004	0.000	0.002	0.006	0.006	0.000	0.002	0.000	0.003	0.019	0.012	0.042	0.294	2.029	0.040	0.054	0.315	0.157	0.328	0.053	0.162	0.008	0.012
26	0.000	0.000	0.554	0.000	0.000	0.014	0.008	0.001	0.005	0.002	0.000	0.011	0.002	0.005	0.003	0.003	0.001	0.007	0.003	0.002	0.000	0.011	0.000	0.140	0.040	1.976	0.122	0.027	0.386	0.003	0.042	0.000	0.394	0.182
27	0.007	0.003	0.019	0.005	0.419	0.000	0.002	0.012	0.006	0.002	0.008	0.002	0.023	0.003	0.000	0.000	0.006	0.002	0.000	0.003	0.011	0.012	0.000	0.309	0.054	0.122	1.783	0.331	0.031	0.037	0.256	0.006	0.086	0.001
28	0.020	0.011	0.003	0.000	0.020	0.012	0.435	0.000	0.018	0.010	0.002	0.000	0.004	0.004	0.002	0.000	0.000	0.000	0.007	0.003	0.018	0.011	0.019	0.276	0.315	0.027	0.331	2.206	0.062	0.296	0.259	0.008	0.019	0.000
29	0.003	0.002	0.000	0.011	0.003	0.002	0.004	0.001	0.004	0.012	0.569	0.000	0.000	0.002	0.000	0.012	0.000	0.003	0.000	0.002	0.002	0.012	0.000	0.112	0.157	0.386	0.031	0.062	2.007	0.024	0.006	0.394	0.000	0.178
30	0.445	0.000	0.000	0.001	0.004	0.003	0.002	0.012	0.006	0.013	0.006	0.002	0.007	0.005	0.022	0.004	0.000	0.002	0.013	0.008	0.005	0.002	0.156	0.034	0.328	0.003	0.037	0.296	0.024	1.892	0.239	0.178	0.025	0.007
31	0.019	0.011	0.007	0.002	0.028	0.018	0.009	0.012	0.003	0.002	0.000	0.001	0.500	0.002	0.007	0.002	0.025	0.002	0.014	0.010	0.005	0.002	0.200	0.034	0.053	0.042	0.256	0.259	0.006	0.239	1.974	0.003	0.174	0.008
32	0.000	0.013	0.002	0.004	0.000	0.000	0.007	0.001	0.003	0.011	0.000	0.012	0.000	0.003	0.560	0.000	0.010	0.003	0.011	0.003	0.006	0.002	0.334	0.013	0.162	0.000	0.006	0.008	0.394	0.178	0.003	2.061	0.000	0.251
33	0.001	0.003	0.000	0.014	0.003	0.010	0.001	0.002	0.000	0.001	0.000	0.003	0.021	0.018	0.003	0.003	0.575	0.008	0.017	0.010	0.002	0.002	0.320	0.065	0.008	0.394	0.086	0.019	0.000	0.025	0.174	0.000	2.083	0.254
34	0.001	0.001	0.000	0.022	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.023	0.000	0.002	0.000	0.021	0.020	0.010	0.000	0.003	0.000	0.001	0.187	0.004	0.012	0.182	0.001	0.000	0.178	0.007	0.008	0.251	0.254	1.607
35	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
36	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
37	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
38	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
39	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
40	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
41	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
42	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
43	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
44	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
45	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
46	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
47	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.001	0.004	0.001	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
48	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
49	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001
50	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002
51	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.001	0.000	0.000	0.005	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.003
52	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.015	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.039
53	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
54	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
55	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.467	0.001	0.001	0.000	0.000	0.003	0.000	0.000	0.003	0.001	0.000	0.000	0.000	0.004	0.000	0.000	0.000
56	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000
57	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000
58	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.002
59	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.001	0.001
60	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
61	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000
62	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.010	0.002	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001
63	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.009	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.001
64	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.008	0.018	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.004	0.001
65	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.009	0.034	0.002	0.003	0.000	0.000	0.003	0.001	0.001	0.002	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000
66	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.002	0.001	0.002	0.000	0.000	0.003	0.002	0.010	0.021
67	0.000	0.000	0.004	0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.002	0.000	0.000	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.010	0.005	0.000	0.000	0.046	0.016	0.339
68	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.007	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.005	0.000	0.000	0.003	0.003	0.000
69	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.027	0.267	0.000	0.000	0.001	0.002	0.030	0.268	0.000	0.000	0.005	0.000	0.000	0.001	0.001	0.002	0.000	0.000	0.004	0.003	0.001	0.000

Table S1c. Mayer bond order of $ZnBeB_{23}(CN)_{22}$ (Part II)

No.	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.004	0.001	0.000
4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000
5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000
10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000
12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.027
14	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.267
15	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000
16	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
17	0.001	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.001	0.001	0.000	0.000	0.001	0.000	0.001	0.000	0.003	0.000	0.001	0.001	0.000	0.000	0.010	0.009	0.008	0.009	0.000	0.000	0.007	0.001
18	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.000	0.002	0.000	0.001	0.000	0.000	0.000	0.467	0.001	0.000	0.000	0.000	0.000	0.000	0.002	0.001	0.018	0.034	0.005	0.000	0.000	0.002
19	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.003	0.015	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.001	0.000	0.000	0.030
20	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.268
21	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
22	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
23	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.003	0.000	0.000	0.003	0.001	0.000	0.000	0.000	0.001	0.001	0.001	0.000	0.000	0.003	0.000	0.000	0.001	0.005
24	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000
25	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000
26	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.002	0.000	0.000	0.001
27	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001
28	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.010	0.000	0.002
29	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.005	0.005	0.000
30	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000
31	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.000	0.000	0.004
32	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.001	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.002	0.046	0.003	0.003
33	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000	0.000	0.002	0.004	0.000	0.010	0.016	0.003	0.001
34	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.003	0.039	0.000	0.000	0.000	0.000	0.000	0.002	0.001	0.000	0.000	0.001	0.001	0.001	0.000	0.021	0.339	0.000	0.000
35	1.986	1.466	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.001	0.000	0.001	0.000	0.023	0.000	0.011	0.000	0.009	0.019	0.005	0.412	0.021	0.000	0.003	0.001	0.000	0.006	0.000
36	1.466	1.545	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.016	0.002	0.010	0.000	0.002	0.012	0.002	0.000	0.016	0.009	0.003	0.000	0.000	0.003	0.000
37	0.001	0.000	1.979	1.465	0.001	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.003	0.007	0.004	0.419	0.013	0.006	0.021	0.000	0.006	0.006	0.010	0.000	0.000	0.013	0.000
38	0.000	0.001	1.465	1.540	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.010	0.002	0.000	0.013	0.002	0.014	0.001	0.003	0.002	0.010	0.000	0.000	0.013	0.000
39	0.001	0.000	0.001	0.000	1.981	1.468	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.000	0.000	0.004	0.008	0.005	0.006	0.417	0.021	0.006	0.006	0.023	0.000	0.008	0.001	0.000	0.005	0.000
40	0.000	0.000	0.000	0.000	1.468	1.545	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.002	0.012	0.002	0.011	0.000	0.013	0.002	0.002	0.017	0.001	0.011	0.000	0.000	0.002	0.000
41	0.000	0.000	0.001	0.000	0.000	0.000	1.980	1.468	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.004	0.011	0.019	0.005	0.016	0.421	0.006	0.005	0.013	0.003	0.003	0.001	0.000	0.000	0.000
42	0.000	0.000	0.000	0.000	0.000	0.000	1.468	1.541	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.011	0.012	0.002	0.014	0.000	0.001	0.012	0.011	0.002	0.002	0.000	0.001	0.001	0.000
43	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	1.982	1.466	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.003	0.015	0.432	0.005	0.007	0.015	0.017	0.008	0.005	0.000	0.000	0.001	0.000	0.005	0.000
44	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.466	1.539	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.013	0.000	0.002	0.002	0.012	0.012	0.011	0.002	0.011	0.002	0.000	0.000	0.002	0.000
45	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	1.971	1.468	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.008	0.013	0.013	0.008	0.005	0.405	0.005	0.000	0.009	0.005	0.000	0.000	0.024	0.000
46	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.468	1.543	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.013	0.013	0.012	0.001	0.001	0.000	0.001	0.001	0.012	0.002	0.001	0.000	0.011	0.000
47	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.001	1.919	1.306	0.001	0.000	0.001	0.001	0.001	0.000	0.052	0.000	0.000	0.006	0.004	0.000	0.002	0.006	0.455	0.008	0.030	0.001	0.000	0.003	0.027
48	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	1.306	1.664	0.000	0.000	0.000	0.000	0.000	0.000	0.017	0.001	0.002	0.002	0.005	0.006	0.000	0.005	0.002	0.004	0.008	0.000	0.000	0.004	0.290
49	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.000	1.981	1.461	0.001	0.000	0.001	0.000	0.022	0.001	0.011	0.006	0.000	0.005	0.013	0.008	0.008	0.420	0.004	0.001	0.001	0.009	0.000

No.	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69
50	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.461	1.546	0.000	0.000	0.000	0.000	0.015	0.001	0.009	0.002	0.000	0.002	0.013	0.013	0.004	0.000	0.004	0.000	0.000	0.012	0.000
51	0.001	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.000	1.964	1.413	0.001	0.000	0.014	0.000	0.000	0.016	0.017	0.002	0.005	0.001	0.000	0.002	0.473	0.000	0.000	0.000	0.001
52	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000	0.000	1.413	1.533	0.000	0.000	0.009	0.002	0.000	0.010	0.005	0.001	0.003	0.003	0.007	0.004	0.000	0.001	0.001	0.010	0.001
53	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.001	0.000	1.975	1.467	0.000	0.416	0.020	0.009	0.019	0.007	0.011	0.004	0.005	0.003	0.000	0.000	0.000	0.006	0.000
54	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.467	1.540	0.002	0.000	0.013	0.012	0.011	0.012	0.011	0.002	0.002	0.001	0.002	0.000	0.000	0.001	0.000
55	0.023	0.016	0.003	0.002	0.004	0.002	0.004	0.002	0.003	0.001	0.005	0.002	0.052	0.017	0.022	0.015	0.014	0.009	0.000	0.002	2.137	0.000	0.063	0.024	0.034	0.040	0.027	0.226	0.258	0.253	0.239	0.042	0.018	0.231	0.001
56	0.000	0.002	0.007	0.010	0.008	0.012	0.011	0.011	0.015	0.013	0.008	0.013	0.000	0.001	0.001	0.001	0.000	0.002	0.416	0.000	0.000	2.201	0.253	0.296	0.261	0.284	0.292	0.048	0.057	0.051	0.073	0.000	0.000	0.049	0.000
57	0.011	0.010	0.004	0.002	0.005	0.002	0.019	0.012	0.432	0.000	0.013	0.013	0.000	0.002	0.011	0.009	0.000	0.000	0.020	0.013	0.063	0.253	2.116	0.029	0.022	0.240	0.261	0.268	0.053	0.297	0.000	0.000	0.002	0.049	0.000
58	0.000	0.000	0.419	0.000	0.006	0.011	0.005	0.002	0.005	0.002	0.013	0.012	0.006	0.002	0.006	0.002	0.016	0.010	0.009	0.012	0.024	0.296	0.029	2.015	0.244	0.031	0.286	0.000	0.031	0.036	0.273	0.000	0.002	0.221	0.000
59	0.009	0.002	0.013	0.013	0.417	0.000	0.016	0.014	0.007	0.002	0.008	0.001	0.004	0.005	0.000	0.000	0.017	0.005	0.019	0.011	0.034	0.261	0.022	0.244	1.958	0.258	0.017	0.030	0.231	0.000	0.256	0.004	0.004	0.027	0.001
60	0.019	0.012	0.006	0.002	0.021	0.013	0.421	0.000	0.015	0.012	0.005	0.001	0.000	0.006	0.005	0.002	0.002	0.001	0.007	0.012	0.040	0.284	0.240	0.031	0.258	2.033	0.023	0.274	0.240	0.035	0.043	0.000	0.000	0.000	0.002
61	0.005	0.002	0.021	0.014	0.006	0.002	0.006	0.001	0.017	0.012	0.405	0.000	0.002	0.000	0.013	0.013	0.005	0.003	0.011	0.011	0.027	0.292	0.261	0.286	0.017	0.023	2.031	0.025	0.000	0.278	0.015	0.003	0.002	0.249	0.000
62	0.412	0.000	0.000	0.001	0.006	0.002	0.005	0.012	0.008	0.011	0.005	0.001	0.006	0.005	0.008	0.013	0.001	0.003	0.004	0.002	0.226	0.048	0.268	0.000	0.030	0.274	0.025	1.963	0.257	0.255	0.021	0.009	0.005	0.024	0.001
63	0.021	0.016	0.006	0.003	0.023	0.017	0.013	0.011	0.005	0.002	0.000	0.001	0.455	0.002	0.008	0.004	0.000	0.007	0.005	0.002	0.258	0.057	0.053	0.031	0.231	0.240	0.000	0.257	2.057	0.009	0.280	0.008	0.004	0.011	0.001
64	0.000	0.009	0.006	0.002	0.000	0.001	0.003	0.002	0.000	0.011	0.009	0.012	0.008	0.004	0.420	0.000	0.002	0.004	0.003	0.001	0.253	0.051	0.297	0.036	0.000	0.035	0.278	0.255	0.009	2.024	0.026	0.001	0.001	0.249	0.000
65	0.003	0.003	0.010	0.010	0.008	0.011	0.003	0.002	0.000	0.002	0.005	0.002	0.030	0.008	0.004	0.004	0.473	0.000	0.000	0.002	0.239	0.073	0.000	0.273	0.256	0.043	0.015	0.021	0.280	0.026	2.170	0.031	0.015	0.261	0.000
66	0.001	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.001	0.000	0.000	0.001	0.001	0.000	0.001	0.000	0.000	0.001	0.000	0.000	0.042	0.000	0.000	0.000	0.004	0.000	0.003	0.009	0.008	0.001	0.031	1.979	1.344	0.479	0.000
67	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000	0.018	0.000	0.002	0.002	0.004	0.000	0.002	0.005	0.004	0.001	0.015	1.344	1.829	0.000	0.000
68	0.006	0.003	0.013	0.013	0.005	0.002	0.000	0.001	0.005	0.002	0.024	0.011	0.003	0.004	0.009	0.012	0.000	0.010	0.006	0.001	0.231	0.049	0.049	0.221	0.027	0.000	0.249	0.024	0.011	0.249	0.261	0.479	0.000	2.004	0.000
69	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.027	0.290	0.000	0.000	0.001	0.001	0.000	0.000	0.001	0.000	0.000	0.000	0.001	0.002	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.941

2.2 Localized Orbital Bonding Analysis

Localized orbital bonding analysis (LOBA),[9] which proposed by Thom et al. is suitable for evaluating oxidation state of metal atoms in transition metal complexes and has been proved to be reliable in most cases. Herein, we firstly combined Pipek-Mezey localization method and Hirshfeld population to realized LOBA.[11-13] To prove LOBA method is not sensitive to different localization and population methods, we further perform extra analyses with below listed methods for calculating orbital composition and localization methods.

a). Pipek-Mezey method & Mulliken population for localization (used in article)

b). Pipek-Mezey method & Lowdin population for localization

c). Pipek-Mezey method & Becke population for localization

d). Foster-Boys method for localization

e). Hirsfeld method for orbital composition (used in article)

f). Mulliken method for occupied LMO and SCPA method for unoccupied LMO

g). Becke method for orbital composition

Table S2a. Oxidation states of atoms in $ZnBeB_{11}(CN)_{12}$ with threshold ranges from 20% to 90% calculated by Pipek-Mezey localization method and Mulliken population

Threshold / %	20	30	40	50	60	70	80	90
Atom 1 (C)	2	-4	-4	2	4	4	4	4
Atom 2 (N)	-2	-3	-3	-2	3	3	3	3
Atom 3 (C)	2	-4	-4	2	4	4	4	4
Atom 4 (N)	-2	-3	-3	-2	3	3	3	3
Atom 5 (C)	2	-4	-4	2	4	4	4	4
Atom 6 (N)	-2	-3	-3	-2	3	3	3	3
Atom 7 (C)	2	-4	-4	2	4	4	4	4
Atom 8 (N)	-2	-3	-3	-2	3	3	3	3
Atom 9 (C)	2	-4	-4	2	4	4	4	4
Atom 10 (N)	-3	-3	-3	-3	3	3	3	3
Atom 11 (C)	2	-4	-4	2	4	4	4	4
Atom 12 (N)	-2	-3	-3	-2	3	3	3	3
Atom 13 (C)	2	-4	-4	2	4	4	4	4
Atom 14 (N)	-3	-3	-3	-3	3	3	3	3
Atom 15 (C)	2	-4	-4	2	4	4	4	4
Atom 16 (N)	-2	-3	-3	-2	3	3	3	3
Atom 17 (C)	2	-4	0	2	2	4	4	4
Atom 18 (N)	-3	-3	-3	-3	3	3	3	5
Atom 19 (C)	3	-4	1	3	4	4	4	4
Atom 20 (N)	-3	-3	-3	-3	3	3	3	5
Atom 21 (C)	2	-4	0	2	2	4	4	4
Atom 22 (N)	-3	-3	-3	-3	3	3	3	5
Atom 23 (C)	2	-4	-4	2	4	4	4	4
Atom 24 (N)	-2	-3	-3	-2	3	3	3	3
Atom 25 (B)	3	1	3	3	3	3	3	3

Atom 26 (B)	3	1	3	3	3	3	3	3
Atom 27 (B)	3	1	3	3	3	3	3	3
Atom 28 (B)	3	0	3	3	3	3	3	3
Atom 29 (B)	3	1	3	3	3	3	3	3
Atom 30 (B)	3	1	3	3	3	3	3	3
Atom 31 (B)	3	1	3	3	3	3	3	3
Atom 32 (B)	3	1	3	3	3	3	3	3
Atom 33 (B)	3	1	3	3	3	3	3	3
Atom 34 (B)	3	0	3	3	3	3	3	3
Atom 35 (B)	3	1	3	3	3	3	3	3
Atom 36 (Be)	2	2	2	2	2	2	2	2
Atom 37 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2b. Oxidation states of atoms in $ZnBeB_{23}(CN)_{22}$ with threshold ranges from 20% to 90% calculated by Pipek-Mezey localization method and Mulliken population

Threshold / %	20	30	40	50	60	70	80	90	Threshold / %	20	30	40	50	60	70	80	90
Atom 1 (C)	-4	-4	-4	2	4	4	4	4	Atom35 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3	Atom36 (N)	-3	-3	-3	-3	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4	Atom37 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3	Atom38 (N)	-3	-3	-3	-3	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4	Atom39 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3	Atom40 (N)	-3	-3	-3	-3	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4	Atom41 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3	Atom42 (N)	-3	-3	-3	-3	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4	Atom43 (C)	-4	-4	-4	2	4	4	4	4
Atom10 (N)	-3	-3	-3	-2	3	3	3	3	Atom44 (N)	-3	-3	-3	-3	3	3	3	3
Atom11 (C)	-4	-4	-4	2	4	4	4	4	Atom45 (C)	-4	-4	-4	2	4	4	4	4
Atom12 (N)	-3	-3	-3	-2	3	3	3	3	Atom46 (N)	-3	-3	-3	-3	3	3	3	3
Atom13 (C)	-4	-4	0	2	2	4	4	4	Atom47 (C)	-4	-4	0	2	2	4	4	4
Atom14 (N)	-3	-3	-3	-3	3	3	3	5	Atom48 (N)	-3	-3	-3	-3	3	3	5	5
Atom15 (C)	-4	-4	-4	2	4	4	4	4	Atom49 (C)	-4	-4	-4	2	4	4	4	4
Atom16 (N)	-3	-3	-2	-2	3	3	3	3	Atom50 (N)	-3	-3	-3	-3	3	3	3	3
Atom17 (C)	-4	-4	2	2	3	4	4	4	Atom51 (C)	-4	-4	-4	2	4	4	4	4
Atom18 (N)	-3	-3	-3	-3	3	5	5	5	Atom52 (N)	-3	-3	-3	-3	3	3	3	3
Atom19 (C)	-4	-4	0	2	2	4	4	4	Atom53 (C)	-4	-4	-4	2	4	4	4	4
Atom20 (N)	-3	-3	-3	-3	3	3	3	5	Atom54 (N)	-3	-3	-3	-3	3	3	3	3
Atom21 (C)	-4	-4	-4	2	4	4	4	4	Atom55 (B)	-5	3	3	3	3	3	3	3
Atom22 (N)	-3	-3	-3	-3	3	3	3	3	Atom56 (B)	-5	1	3	3	3	3	3	3
Atom23 (B)	-5	0	3	3	3	3	3	3	Atom57 (B)	-5	1	3	3	3	3	3	3
Atom24 (B)	-1	1	3	3	3	3	3	3	Atom58 (B)	-3	1	3	3	3	3	3	3
Atom25 (B)	-1	1	3	3	3	3	3	3	Atom59 (B)	-3	1	3	3	3	3	3	3
Atom26 (B)	-5	0	3	3	3	3	3	3	Atom60 (B)	1	1	3	3	3	3	3	3
Atom27 (B)	-1	1	3	3	3	3	3	3	Atom61 (B)	-5	1	3	3	3	3	3	3
Atom28 (B)	-3	1	3	3	3	3	3	3	Atom62 (B)	-5	1	3	3	3	3	3	3
Atom29 (B)	-4	0	3	3	3	3	3	3	Atom63 (B)	-3	3	3	3	3	3	3	3
Atom30 (B)	0	1	3	3	3	3	3	3	Atom64 (B)	-3	1	3	3	3	3	3	3
Atom31 (B)	-4	3	3	3	3	3	3	3	Atom65 (B)	-2	1	3	3	3	3	3	3
Atom32 (B)	-4	0	3	3	3	3	3	3	Atom66 (C)	-4	-4	2	2	2	4	4	4
Atom33 (B)	-5	1	3	3	3	3	3	3	Atom67 (N)	-5	-3	-1	-1	5	5	5	5
Atom34 (Be)	2	2	2	2	2	2	2	2	Atom68 (B)	-5	3	3	3	3	3	3	3
									Atom69 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2c. Oxidation states of atoms in $ZnBeB_{11}(CN)_{12}$ with threshold ranges from 20% to 90% calculated by Pipek-Mezey method & Lowdin population for localization

Threshold / %	**20**	**30**	**40**	**50**	**60**	**70**	**80**	**90**
Atom 1 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3
Atom 3 (C)	-4	-4	-3	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4
Atom 10 (N)	-3	-3	-3	-3	3	3	3	3
Atom 11 (C)	-4	-4	-4	2	4	4	4	4
Atom 12 (N)	-3	-3	-3	-2	3	3	3	3
Atom 13 (C)	-4	-4	-4	2	4	4	4	4
Atom 14 (N)	-3	-3	-3	-3	3	3	3	3
Atom 15 (C)	-4	-4	-4	2	4	4	4	4
Atom 16 (N)	-3	-3	-3	-2	3	3	3	3
Atom 17 (C)	-4	-4	0	2	2	4	4	4
Atom 18 (N)	-3	-3	-3	-3	3	3	3	5
Atom 19 (C)	-4	-4	0	2	2	2	4	4
Atom 20 (N)	-3	-3	-3	-3	3	3	3	5
Atom 21 (C)	-4	-4	0	2	2	4	4	4
Atom 22 (N)	-3	-3	-3	-3	3	3	3	5
Atom 23 (C)	-4	-4	-4	2	4	4	4	4
Atom 24 (N)	-3	-3	-3	-2	3	3	3	3
Atom 25 (B)	-5	0	3	3	3	3	3	3
Atom 26 (B)	-5	1	3	3	3	3	3	3
Atom 27 (B)	-5	1	3	3	3	3	3	3
Atom 28 (B)	-4	-1	3	3	3	3	3	3
Atom 29 (B)	-3	1	3	3	3	3	3	3
Atom 30 (B)	-4	1	3	3	3	3	3	3
Atom 31 (B)	-5	-1	3	3	3	3	3	3
Atom 32 (B)	-4	1	3	3	3	3	3	3
Atom 33 (B)	-4	1	3	3	3	3	3	3
Atom 34 (B)	-5	0	3	3	3	3	3	3
Atom 35 (B)	-5	0	3	3	3	3	3	3
Atom 36 (Be)	0	2	2	2	2	2	2	2
Atom 37 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2d. Oxidation states of atoms in $ZnBeB_{23}(CN)_{22}$ with threshold ranges from 20% to 90% calculated by Pipek-Mezey method & Lowdin population for localization

Threshold / %	20	30	40	50	60	70	80	90	Threshold / %	20	30	40	50	60	70	80	90
Atom 1 (C)	-4	-4	-4	2	4	4	4	4	Atom35 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3	Atom36 (N)	-3	-3	-3	-3	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4	Atom37 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3	Atom38 (N)	-3	-3	-3	-3	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4	Atom39 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3	Atom40 (N)	-3	-3	-3	-3	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4	Atom41 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3	Atom42 (N)	-3	-3	-3	-3	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4	Atom43 (C)	-4	-4	-4	2	4	4	4	4
Atom10 (N)	-3	-3	-3	-2	3	3	3	3	Atom44 (N)	-3	-3	-3	-3	3	3	3	3
Atom11 (C)	-4	-4	-4	2	4	4	4	4	Atom45 (C)	-4	-4	-4	2	4	4	4	4
Atom12 (N)	-3	-3	-3	-2	3	3	3	3	Atom46 (N)	-3	-3	-3	-3	3	3	3	3
Atom13 (C)	-4	-4	0	2	2	4	4	4	Atom47 (C)	-4	-4	0	2	2	4	4	4
Atom14 (N)	-3	-3	-3	-3	3	3	5	5	Atom48 (N)	-3	-3	-3	-3	3	3	5	5
Atom15 (C)	-4	-4	-4	2	4	4	4	4	Atom49 (C)	-4	-4	-4	2	4	4	4	4
Atom16 (N)	-3	-3	-2	-2	3	3	3	3	Atom50 (N)	-3	-3	-3	-3	3	3	3	3
Atom17 (C)	-4	-4	0	2	2	4	4	4	Atom51 (C)	-4	-4	-4	2	4	4	4	4
Atom18 (N)	-3	-3	-3	-3	3	5	5	5	Atom52 (N)	-3	-3	-3	-3	3	3	3	3
Atom19 (C)	-4	-4	0	2	4	4	4	4	Atom53 (C)	-4	-4	-4	2	4	4	4	4
Atom20 (N)	-3	-3	-3	-3	3	3	4	5	Atom54 (N)	-3	-3	-3	-3	3	3	3	3
Atom21 (C)	-4	-4	-4	2	4	4	4	4	Atom55 (B)	-5	3	3	3	3	3	3	3
Atom22 (N)	-3	-3	-3	-3	3	3	3	3	Atom56 (B)	-5	1	3	3	3	3	3	3
Atom23 (B)	-5	0	3	3	3	3	3	3	Atom57 (B)	-5	1	3	3	3	3	3	3
Atom24 (B)	-5	1	3	3	3	3	3	3	Atom58 (B)	-5	1	3	3	3	3	3	3
Atom25 (B)	-5	1	3	3	3	3	3	3	Atom59 (B)	-5	1	3	3	3	3	3	3
Atom26 (B)	-5	0	3	3	3	3	3	3	Atom60 (B)	-4	1	3	3	3	3	3	3
Atom27 (B)	-3	1	3	3	3	3	3	3	Atom61 (B)	-2	1	3	3	3	3	3	3
Atom28 (B)	-4	1	3	3	3	3	3	3	Atom62 (B)	-4	1	3	3	3	3	3	3
Atom29 (B)	-4	0	3	3	3	3	3	3	Atom63 (B)	-5	1	3	3	3	3	3	3
Atom30 (B)	-3	1	3	3	3	3	3	3	Atom64 (B)	-5	1	3	3	3	3	3	3
Atom31 (B)	-5	3	3	3	3	3	3	3	Atom65 (B)	-3	1	3	3	3	3	3	3
Atom32 (B)	-4	0	3	3	3	3	3	3	Atom66 (C)	-4	-4	0	2	2	4	4	4
Atom33 (B)	-5	1	3	3	3	3	3	3	Atom67 (N)	-3	-3	-3	-3	3	3	5	5
Atom34 (Be)	2	2	2	2	2	2	2	2	Atom68 (B)	-5	-1	3	3	3	3	3	3
									Atom69 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2e. Oxidation states of atoms in $ZnBeB_{11}(CN)_{12}$ with threshold ranges from 20% to 90% calculated by c). Pipek-Mezey method & Becke population for localization

Threshold / %	**20**	**30**	**40**	**50**	**60**	**70**	**80**	**90**
Atom 1 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4
Atom 10 (N)	-3	-3	-3	-3	3	3	3	3
Atom 11 (C)	-4	-4	-4	2	4	4	4	4
Atom 12 (N)	-3	-3	-3	-2	3	3	3	3
Atom 13 (C)	-4	-4	-4	2	4	4	4	4
Atom 14 (N)	-3	-3	-3	-3	3	3	3	3
Atom 15 (C)	-4	-4	-4	2	4	4	4	4
Atom 16 (N)	-3	-3	-3	-2	3	3	3	3
Atom 17 (C)	-4	-4	0	2	2	4	4	4
Atom 18 (N)	-3	-3	-3	-3	3	3	3	5
Atom 19 (C)	-4	-4	0	2	2	2	4	4
Atom 20 (N)	-3	-3	-3	-3	3	3	3	5
Atom 21 (C)	-4	-4	0	2	2	4	4	4
Atom 22 (N)	-3	-3	-3	-3	3	3	3	5
Atom 23 (C)	-4	-4	-4	2	4	4	4	4
Atom 24 (N)	-3	-3	-3	-2	3	3	3	3
Atom 25 (B)	-5	0	3	3	3	3	3	3
Atom 26 (B)	-5	1	3	3	3	3	3	3
Atom 27 (B)	-5	1	3	3	3	3	3	3
Atom 28 (B)	-4	0	3	3	3	3	3	3
Atom 29 (B)	-3	1	3	3	3	3	3	3
Atom 30 (B)	-4	1	3	3	3	3	3	3
Atom 31 (B)	-5	-1	3	3	3	3	3	3
Atom 32 (B)	-4	1	3	3	3	3	3	3
Atom 33 (B)	-4	1	3	3	3	3	3	3
Atom 34 (B)	-5	0	3	3	3	3	3	3
Atom 35 (B)	-5	0	3	3	3	3	3	3
Atom 36 (Be)	2	2	2	2	2	2	2	2
Atom 37 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2f. Oxidation states of atoms in $ZnBeB_{23}(CN)_{22}$ with threshold ranges from 20% to 90% calculated by c). Pipek-Mezey method & Becke population for localization

Threshold / %	20	30	40	50	60	70	80	90	Threshold / %	20	30	40	50	60	70	80	90
Atom 1 (C)	-4	-4	-4	2	4	4	4	4	Atom35 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3	Atom36 (N)	-3	-3	-3	-3	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4	Atom37 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3	Atom38 (N)	-3	-3	-3	-3	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4	Atom39 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3	Atom40 (N)	-3	-3	-3	-3	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4	Atom41 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3	Atom42 (N)	-3	-3	-3	-3	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4	Atom43 (C)	-4	-4	-4	2	4	4	4	4
Atom10 (N)	-3	-3	-3	-2	3	3	3	3	Atom44 (N)	-3	-3	-3	-3	3	3	3	3
Atom11 (C)	-4	-4	-4	2	4	4	4	4	Atom45 (C)	-4	-4	-4	2	4	4	4	4
Atom12 (N)	-3	-3	-3	-2	3	3	3	3	Atom46 (N)	-3	-3	-3	-3	3	3	3	3
Atom13 (C)	-4	-4	0	2	2	4	4	4	Atom47 (C)	-4	-4	0	2	2	4	4	4
Atom14 (N)	-3	-3	-3	-3	3	3	3	5	Atom48 (N)	-3	-3	-3	-3	3	3	5	5
Atom15 (C)	-4	-4	-4	2	4	4	4	4	Atom49 (C)	-4	-4	-4	2	4	4	4	4
Atom16 (N)	-3	-3	-2	-2	3	3	3	3	Atom50 (N)	-3	-3	-3	-3	3	3	3	3
Atom17 (C)	-4	-4	0	2	2	4	4	4	Atom51 (C)	-4	-4	-4	2	4	4	4	4
Atom18 (N)	-3	-3	-3	-3	3	5	5	5	Atom52 (N)	-3	-3	-3	-3	3	3	3	3
Atom19 (C)	-4	-4	0	2	2	4	4	4	Atom53 (C)	-4	-4	-4	2	4	4	4	4
Atom20 (N)	-3	-3	-3	-3	3	3	3	5	Atom54 (N)	-3	-3	-3	-3	3	3	3	3
Atom21 (C)	-4	-4	-4	2	4	4	4	4	Atom55 (B)	-5	3	3	3	3	3	3	3
Atom22 (N)	-3	-3	-3	-3	3	3	3	3	Atom56 (B)	-5	1	3	3	3	3	3	3
Atom23 (B)	-5	0	3	3	3	3	3	3	Atom57 (B)	-5	1	3	3	3	3	3	3
Atom24 (B)	-5	1	3	3	3	3	3	3	Atom58 (B)	-5	1	3	3	3	3	3	3
Atom25 (B)	-5	1	3	3	3	3	3	3	Atom59 (B)	-5	1	3	3	3	3	3	3
Atom26 (B)	-5	0	3	3	3	3	3	3	Atom60 (B)	-4	1	3	3	3	3	3	3
Atom27 (B)	-3	1	3	3	3	3	3	3	Atom61 (B)	-3	1	3	3	3	3	3	3
Atom28 (B)	-4	1	3	3	3	3	3	3	Atom62 (B)	-5	1	3	3	3	3	3	3
Atom29 (B)	-4	-1	3	3	3	3	3	3	Atom63 (B)	-5	0	3	3	3	3	3	3
Atom30 (B)	-3	1	3	3	3	3	3	3	Atom64 (B)	-5	1	3	3	3	3	3	3
Atom31 (B)	-5	2	3	3	3	3	3	3	Atom65 (B)	-2	1	3	3	3	3	3	3
Atom32 (B)	-4	-1	3	3	3	3	3	3	Atom66 (C)	-4	-4	0	2	2	4	4	4
Atom33 (B)	-5	0	3	3	3	3	3	3	Atom67 (N)	-3	-3	-3	-3	3	3	5	5
Atom34 (Be)	2	2	2	2	2	2	2	2	Atom68 (B)	-5	0	3	3	3	3	3	3
									Atom69 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2g. Oxidation states of atoms in $ZnBeB_{11}(CN)_{12}$ with threshold ranges from 20% to 90% calculated by Foster-Boys method for localization

Threshold / %	**20**	**30**	**40**	**50**	**60**	**70**	**80**	**90**
Atom 1 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4
Atom 10 (N)	-3	-3	-3	-3	3	3	3	3
Atom 11 (C)	-4	-4	-4	2	4	4	4	4
Atom 12 (N)	-3	-3	-3	-3	3	3	3	3
Atom 13 (C)	-4	-4	-4	2	4	4	4	4
Atom 14 (N)	-3	-3	-3	-3	3	3	3	3
Atom 15 (C)	-4	-4	-4	2	4	4	4	4
Atom 16 (N)	-3	-3	-3	-2	3	3	3	3
Atom 17 (C)	-4	-4	2	2	4	4	4	4
Atom 18 (N)	-3	-3	-3	-3	3	3	3	5
Atom 19 (C)	-4	-4	2	2	2	2	4	4
Atom 20 (N)	-3	-3	-3	-3	3	3	3	5
Atom 21 (C)	-4	-4	2	2	4	4	4	4
Atom 22 (N)	-3	-3	-3	-3	3	3	3	5
Atom 23 (C)	-4	-4	-4	2	4	4	4	4
Atom 24 (N)	-3	-3	-3	-3	3	3	3	3
Atom 25 (B)	-5	-1	3	3	3	3	3	3
Atom 26 (B)	-5	1	3	3	3	3	3	3
Atom 27 (B)	-5	1	3	3	3	3	3	3
Atom 28 (B)	-4	0	3	3	3	3	3	3
Atom 29 (B)	-3	1	3	3	3	3	3	3
Atom 30 (B)	-4	1	3	3	3	3	3	3
Atom 31 (B)	-5	-1	3	3	3	3	3	3
Atom 32 (B)	-4	1	3	3	3	3	3	3
Atom 33 (B)	-4	1	3	3	3	3	3	3
Atom 34 (B)	-5	0	3	3	3	3	3	3
Atom 35 (B)	-5	-2	3	3	3	3	3	3
Atom 36 (Be)	0	2	2	2	2	2	2	2
Atom 37 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2h. Oxidation states of atoms in $ZnBeB_{23}(CN)_{22}$ with threshold ranges from 20% to 90% calculated by Foster-Boys method for localization

Threshold / %	20	30	40	50	60	70	80	90	Threshold / %	20	30	40	50	60	70	80	90
Atom 1 (C)	-4	-4	-4	2	4	4	4	4	Atom35 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-3	3	3	3	3	Atom36 (N)	-3	-3	-3	-3	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4	Atom37 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3	Atom38 (N)	-3	-3	-3	-3	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4	Atom39 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-3	3	3	3	3	Atom40 (N)	-3	-3	-3	-3	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4	Atom41 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3	Atom42 (N)	-3	-3	-3	-3	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4	Atom43 (C)	-4	-4	-4	2	4	4	4	4
Atom10 (N)	-3	-3	-3	-3	3	3	3	3	Atom44 (N)	-3	-3	-3	-3	3	3	3	3
Atom11 (C)	-4	-4	-4	2	4	4	4	4	Atom45 (C)	-4	-4	-4	2	4	4	4	4
Atom12 (N)	-3	-3	-3	-2	3	3	3	3	Atom46 (N)	-3	-3	-3	-3	3	3	3	3
Atom13 (C)	-4	-4	2	2	4	4	4	4	Atom47 (C)	-4	-4	2	2	2	4	4	4
Atom14 (N)	-3	-3	-3	-3	3	3	5	5	Atom48 (N)	-3	-3	-3	-3	3	3	5	5
Atom15 (C)	-4	-4	-4	2	4	4	4	4	Atom49 (C)	-4	-4	-4	2	4	4	4	4
Atom16 (N)	-3	-3	-2	-2	3	3	3	3	Atom50 (N)	-3	-3	-3	-3	3	3	3	3
Atom17 (C)	-4	-4	2	2	2	4	4	4	Atom51 (C)	-4	-4	-4	2	4	4	4	4
Atom18 (N)	-3	-3	-3	-3	3	5	5	5	Atom52 (N)	-3	-3	-3	-3	3	3	3	3
Atom19 (C)	-4	-4	2	2	4	4	4	4	Atom53 (C)	-4	-4	-4	2	4	4	4	4
Atom20 (N)	-3	-3	-3	-3	3	3	5	5	Atom54 (N)	-3	-3	-3	-3	3	3	3	3
Atom21 (C)	-4	-4	-4	2	4	4	4	4	Atom55 (B)	-5	3	3	3	3	3	3	3
Atom22 (N)	-3	-3	-3	-3	3	3	3	3	Atom56 (B)	-5	1	3	3	3	3	3	3
Atom23 (B)	-5	-2	3	3	3	3	3	3	Atom57 (B)	-5	1	3	3	3	3	3	3
Atom24 (B)	-5	1	3	3	3	3	3	3	Atom58 (B)	-5	1	3	3	3	3	3	3
Atom25 (B)	-5	1	3	3	3	3	3	3	Atom59 (B)	-5	1	3	3	3	3	3	3
Atom26 (B)	-5	0	3	3	3	3	3	3	Atom60 (B)	-4	1	3	3	3	3	3	3
Atom27 (B)	-3	1	3	3	3	3	3	3	Atom61 (B)	-5	1	3	3	3	3	3	3
Atom28 (B)	-4	1	3	3	3	3	3	3	Atom62 (B)	-5	1	3	3	3	3	3	3
Atom29 (B)	-4	0	3	3	3	3	3	3	Atom63 (B)	-5	-2	3	3	3	3	3	3
Atom30 (B)	-4	1	3	3	3	3	3	3	Atom64 (B)	-5	1	3	3	3	3	3	3
Atom31 (B)	-5	0	3	3	3	3	3	3	Atom65 (B)	-1	1	3	3	3	3	3	3
Atom32 (B)	-4	-1	3	3	3	3	3	3	Atom66 (C)	-4	-4	2	2	2	4	4	4
Atom33 (B)	-5	1	3	3	3	3	3	3	Atom67 (N)	-3	-3	-3	-3	3	3	5	5
Atom34 (Be)	2	2	2	2	2	2	2	2	Atom68 (B)	-5	-2	3	3	3	3	3	3
									Atom69 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2i. Oxidation states of atoms in $ZnBeB_{11}(CN)_{12}$ with threshold ranges from 20% to 90% calculated by Mulliken method for occupied LMO and SCPA method for unoccupied LMO

Threshold / %	**20**	**30**	**40**	**50**	**60**	**70**	**80**	**90**
Atom 1 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4
Atom 10 (N)	-3	-3	-3	-3	3	3	3	3
Atom 11 (C)	-4	-4	-4	2	4	4	4	4
Atom 12 (N)	-3	-3	-3	-2	3	3	3	3
Atom 13 (C)	-4	-4	-4	2	4	4	4	4
Atom 14 (N)	-3	-3	-3	-3	3	3	3	3
Atom 15 (C)	-4	-4	-4	2	4	4	4	4
Atom 16 (N)	-3	-3	-3	-2	3	3	3	3
Atom 17 (C)	-4	-4	0	2	2	4	4	4
Atom 18 (N)	-3	-3	-3	-3	3	3	3	5
Atom 19 (C)	-5	-4	1	3	3	4	4	4
Atom 20 (N)	-3	-3	-3	-3	3	3	3	5
Atom 21 (C)	-4	-4	0	2	2	4	4	4
Atom 22 (N)	-3	-3	-3	-3	3	3	3	5
Atom 23 (C)	-4	-4	-4	2	4	4	4	4
Atom 24 (N)	-3	-3	-3	-2	3	3	3	3
Atom 25 (B)	-5	1	3	3	3	3	3	3
Atom 26 (B)	-3	1	3	3	3	3	3	3
Atom 27 (B)	-3	1	3	3	3	3	3	3
Atom 28 (B)	-4	0	3	3	3	3	3	3
Atom 29 (B)	-1	1	3	3	3	3	3	3
Atom 30 (B)	-2	1	3	3	3	3	3	3
Atom 31 (B)	-5	1	3	3	3	3	3	3
Atom 32 (B)	-1	1	3	3	3	3	3	3
Atom 33 (B)	-3	1	3	3	3	3	3	3
Atom 34 (B)	-4	0	3	3	3	3	3	3
Atom 35 (B)	-5	1	3	3	3	3	3	3
Atom 36 (Be)	2	2	2	2	2	2	2	2
Atom 37 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2j. Oxidation states of atoms in $ZnBeB_{23}(CN)_{22}$ with threshold ranges from 20% to 90% calculated by Mulliken method for occupied LMO and SCPA method for unoccupied LMO

Threshold / %	20	30	40	50	60	70	80	90	Threshold / %	20	30	40	50	60	70	80	90
Atom 1 (C)	-4	-4	-4	2	4	4	4	4	Atom35 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3	Atom36 (N)	-3	-3	-3	-3	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4	Atom37 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3	Atom38 (N)	-3	-3	-3	-3	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4	Atom39 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3	Atom40 (N)	-3	-3	-3	-3	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4	Atom41 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3	Atom42 (N)	-3	-3	-3	-3	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4	Atom43 (C)	-4	-4	-4	2	4	4	4	4
Atom10 (N)	-3	-3	-3	-2	3	3	3	3	Atom44 (N)	-3	-3	-3	-3	3	3	3	3
Atom11 (C)	-4	-4	-4	2	4	4	4	4	Atom45 (C)	-4	-4	-4	2	4	4	4	4
Atom12 (N)	-3	-3	-3	-2	3	3	3	3	Atom46 (N)	-3	-3	-3	-3	3	3	3	3
Atom13 (C)	-4	-4	0	2	2	4	4	4	Atom47 (C)	-4	-4	0	2	2	4	4	4
Atom14 (N)	-3	-3	-3	-3	3	3	3	5	Atom48 (N)	-3	-3	-3	-3	3	3	5	5
Atom15 (C)	-4	-4	-4	2	4	4	4	4	Atom49 (C)	-4	-4	-4	2	4	4	4	4
Atom16 (N)	-3	-3	-2	-2	3	3	3	3	Atom50 (N)	-3	-3	-3	-3	3	3	3	3
Atom17 (C)	-4	-4	2	2	3	4	4	4	Atom51 (C)	-4	-4	-4	2	4	4	4	4
Atom18 (N)	-3	-3	-3	-3	3	5	5	5	Atom52 (N)	-3	-3	-3	-3	3	3	3	3
Atom19 (C)	-4	-4	0	2	2	4	4	4	Atom53 (C)	-4	-4	-4	2	4	4	4	4
Atom20 (N)	-3	-3	-3	-3	3	3	3	5	Atom54 (N)	-3	-3	-3	-3	3	3	3	3
Atom21 (C)	-4	-4	-4	2	4	4	4	4	Atom55 (B)	-5	3	3	3	3	3	3	3
Atom22 (N)	-3	-3	-3	-3	3	3	3	3	Atom56 (B)	-5	1	3	3	3	3	3	3
Atom23 (B)	-5	0	3	3	3	3	3	3	Atom57 (B)	-5	1	3	3	3	3	3	3
Atom24 (B)	-1	1	3	3	3	3	3	3	Atom58 (B)	-3	1	3	3	3	3	3	3
Atom25 (B)	-1	1	3	3	3	3	3	3	Atom59 (B)	-3	1	3	3	3	3	3	3
Atom26 (B)	-5	0	3	3	3	3	3	3	Atom60 (B)	1	1	3	3	3	3	3	3
Atom27 (B)	-1	1	3	3	3	3	3	3	Atom61 (B)	-5	1	3	3	3	3	3	3
Atom28 (B)	-3	1	3	3	3	3	3	3	Atom62 (B)	-5	1	3	3	3	3	3	3
Atom29 (B)	-4	0	3	3	3	3	3	3	Atom63 (B)	-3	3	3	3	3	3	3	3
Atom30 (B)	0	1	3	3	3	3	3	3	Atom64 (B)	-3	1	3	3	3	3	3	3
Atom31 (B)	-4	3	3	3	3	3	3	3	Atom65 (B)	-2	1	3	3	3	3	3	3
Atom32 (B)	-4	0	3	3	3	3	3	3	Atom66 (C)	-4	-4	2	2	2	4	4	4
Atom33 (B)	-5	1	3	3	3	3	3	3	Atom67 (N)	-5	-3	-1	-1	5	5	5	5
Atom34 (Be)	2	2	2	2	2	2	2	2	Atom68 (B)	-5	3	3	3	3	3	3	3
									Atom69 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2k. Oxidation states of atoms in $ZnBeB_{11}(CN)_{12}$ with threshold ranges from 20% to 90% calculated by Becke method for orbital composition

Threshold / %	**20**	**30**	**40**	**50**	**60**	**70**	**80**	**90**
Atom 1 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4
Atom 10 (N)	-3	-3	-3	-3	3	3	3	3
Atom 11 (C)	-4	-4	-4	2	4	4	4	4
Atom 12 (N)	-3	-3	-3	-2	3	3	3	3
Atom 13 (C)	-4	-4	-4	2	4	4	4	4
Atom 14 (N)	-3	-3	-3	-3	3	3	3	3
Atom 15 (C)	-4	-4	-4	2	4	4	4	4
Atom 16 (N)	-3	-3	-3	-2	3	3	3	3
Atom 17 (C)	-4	-4	0	2	2	4	4	4
Atom 18 (N)	-3	-3	-3	-3	3	3	3	5
Atom 19 (C)	-5	-4	1	3	3	4	4	4
Atom 20 (N)	-3	-3	-3	-3	3	3	3	5
Atom 21 (C)	-4	-4	0	2	2	4	4	4
Atom 22 (N)	-3	-3	-3	-3	3	3	3	5
Atom 23 (C)	-4	-4	-4	2	4	4	4	4
Atom 24 (N)	-3	-3	-3	-2	3	3	3	3
Atom 25 (B)	-5	1	3	3	3	3	3	3
Atom 26 (B)	-3	1	3	3	3	3	3	3
Atom 27 (B)	-3	1	3	3	3	3	3	3
Atom 28 (B)	-4	0	3	3	3	3	3	3
Atom 29 (B)	-1	1	3	3	3	3	3	3
Atom 30 (B)	-2	1	3	3	3	3	3	3
Atom 31 (B)	-5	1	3	3	3	3	3	3
Atom 32 (B)	-1	1	3	3	3	3	3	3
Atom 33 (B)	-3	1	3	3	3	3	3	3
Atom 34 (B)	-4	0	3	3	3	3	3	3
Atom 35 (B)	-5	1	3	3	3	3	3	3
Atom 36 (Be)	2	2	2	2	2	2	2	2
Atom 37 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

Table S2l. Oxidation states of atoms in $ZnBeB_{23}(CN)_{22}$ with threshold ranges from 20% to 90% calculated by Becke method for orbital composition

Threshold / %	20	30	40	50	60	70	80	90	Threshold / %	20	30	40	50	60	70	80	90
Atom 1 (C)	-4	-4	-4	2	4	4	4	4	Atom35 (C)	-4	-4	-4	2	4	4	4	4
Atom 2 (N)	-3	-3	-3	-2	3	3	3	3	Atom36 (N)	-3	-3	-3	-3	3	3	3	3
Atom 3 (C)	-4	-4	-4	2	4	4	4	4	Atom37 (C)	-4	-4	-4	2	4	4	4	4
Atom 4 (N)	-3	-3	-3	-2	3	3	3	3	Atom38 (N)	-3	-3	-3	-3	3	3	3	3
Atom 5 (C)	-4	-4	-4	2	4	4	4	4	Atom39 (C)	-4	-4	-4	2	4	4	4	4
Atom 6 (N)	-3	-3	-3	-2	3	3	3	3	Atom40 (N)	-3	-3	-3	-3	3	3	3	3
Atom 7 (C)	-4	-4	-4	2	4	4	4	4	Atom41 (C)	-4	-4	-4	2	4	4	4	4
Atom 8 (N)	-3	-3	-3	-2	3	3	3	3	Atom42 (N)	-3	-3	-3	-3	3	3	3	3
Atom 9 (C)	-4	-4	-4	2	4	4	4	4	Atom43 (C)	-4	-4	-4	2	4	4	4	4
Atom10 (N)	-3	-3	-3	-2	3	3	3	3	Atom44 (N)	-3	-3	-3	-3	3	3	3	3
Atom11 (C)	-4	-4	-4	2	4	4	4	4	Atom45 (C)	-4	-4	-4	2	4	4	4	4
Atom12 (N)	-3	-3	-3	-2	3	3	3	3	Atom46 (N)	-3	-3	-3	-3	3	3	3	3
Atom13 (C)	-4	-4	0	2	2	4	4	4	Atom47 (C)	-4	-4	0	2	2	4	4	4
Atom14 (N)	-3	-3	-3	-3	3	3	3	5	Atom48 (N)	-3	-3	-3	-3	3	3	5	5
Atom15 (C)	-4	-4	-4	2	4	4	4	4	Atom49 (C)	-4	-4	-4	2	4	4	4	4
Atom16 (N)	-3	-3	-2	-2	3	3	3	3	Atom50 (N)	-3	-3	-3	-3	3	3	3	3
Atom17 (C)	-4	-4	2	2	3	4	4	4	Atom51 (C)	-4	-4	-4	2	4	4	4	4
Atom18 (N)	-3	-3	-3	-3	3	5	5	5	Atom52 (N)	-3	-3	-3	-3	3	3	3	3
Atom19 (C)	-4	-4	0	2	2	4	4	4	Atom53 (C)	-4	-4	-4	2	4	4	4	4
Atom20 (N)	-3	-3	-3	-3	3	3	3	5	Atom54 (N)	-3	-3	-3	-3	3	3	3	3
Atom21 (C)	-4	-4	-4	2	4	4	4	4	Atom55 (B)	-5	3	3	3	3	3	3	3
Atom22 (N)	-3	-3	-3	-3	3	3	3	3	Atom56 (B)	-5	1	3	3	3	3	3	3
Atom23 (B)	-5	0	3	3	3	3	3	3	Atom57 (B)	-5	1	3	3	3	3	3	3
Atom24 (B)	-1	1	3	3	3	3	3	3	Atom58 (B)	-3	1	3	3	3	3	3	3
Atom25 (B)	-1	1	3	3	3	3	3	3	Atom59 (B)	-3	1	3	3	3	3	3	3
Atom26 (B)	-5	0	3	3	3	3	3	3	Atom60 (B)	1	1	3	3	3	3	3	3
Atom27 (B)	-1	1	3	3	3	3	3	3	Atom61 (B)	-5	1	3	3	3	3	3	3
Atom28 (B)	-3	1	3	3	3	3	3	3	Atom62 (B)	-5	1	3	3	3	3	3	3
Atom29 (B)	-4	0	3	3	3	3	3	3	Atom63 (B)	-3	3	3	3	3	3	3	3
Atom30 (B)	0	1	3	3	3	3	3	3	Atom64 (B)	-3	1	3	3	3	3	3	3
Atom31 (B)	-4	3	3	3	3	3	3	3	Atom65 (B)	-2	1	3	3	3	3	3	3
Atom32 (B)	-4	0	3	3	3	3	3	3	Atom66 (C)	-4	-4	2	2	2	4	4	4
Atom33 (B)	-5	1	3	3	3	3	3	3	Atom67 (N)	-5	-3	-1	-1	5	5	5	5
Atom34 (Be)	2	2	2	2	2	2	2	2	Atom68 (B)	-5	3	3	3	3	3	3	3
									Atom69 (Zn)	*2*	*2*	*2*	*2*	*2*	*2*	*2*	*2*

2.3 Spin Population Calculation

Spin population of atoms in the two clusters is calculated based on Hirshfeld method in fuzzy atomic space.[14] Summing up population numbers of $ZnBeB_{11}(CN)_{12}$ is 0.99999739; Summing up population numbers of $ZnBeB_{23}(CN)_{22}$ is 1.00000034.

Table S3a. Spin population numbers of atoms in $ZnBeB_{11}(CN)_{12}$.

Atom No.	Population	Percentage in the sum / %
1(C)	-0.00381091	-0.381092
2(N)	0.06726689	6.726706
3(C)	-0.01137886	-1.137889
4(N)	0.13442169	13.442204
5(C)	-0.00346344	-0.346345
6(N)	0.05916124	5.916139
7(C)	-0.00106026	-0.106026
8(N)	0.07297396	7.297415
9(C)	0.00168301	0.168302
10(N)	0.01360409	1.360412
11(C)	0.00135799	0.135799
12(N)	0.04253076	4.253087
13(C)	-0.00013998	-0.013998
14(N)	0.00592646	0.592648
15(C)	-0.00492935	-0.492936
16(N)	0.08509824	8.509846
17(C)	-0.00080067	-0.080067
18(N)	-0.00070639	-0.070639
19(C)	-0.00080271	-0.080271
20(N)	0.00964187	0.964190
21(C)	-0.00030065	-0.030065
22(N)	0.01917194	1.917199
23(C)	0.00245538	0.245539
24(N)	0.03134561	3.134569
25(B)	0.05175818	5.175831
26(B)	0.00987435	0.987437
27(B)	-0.00000836	-0.000836
28(B)	0.11176852	11.176882
29(B)	0.04034242	4.034252
30(B)	0.04166255	4.166266
31(B)	0.01699502	1.699506
32(B)	0.04803256	4.803269
33(B)	0.00287181	0.287182
34(B)	0.06028110	6.028126
35(B)	0.00127915	0.127915
36(Be)	0.09284098	9.284123
37(Zn)	*0.00305320*	*0.305321*

Table S3b. Spin population numbers of atoms in $ZnBeB_{23}(CN)_{22}$.

Atom No.	Population	Percentage in the sum / %	Atom No.	Population	Percentage in the sum / %
1(C)	-0.00378937	-0.378936	35(C)	-0.00050529	-0.050529
2(N)	0.03604578	3.604577	36(N)	0.00449206	0.449205
3(C)	-0.00011909	-0.011909	37(C)	0.00013401	0.013401
4(N)	0.06079844	6.079842	38(N)	0.01051140	1.051139
5(C)	-0.00308855	-0.308854	39(C)	0.00006544	0.006544
6(N)	0.04910678	4.910676	40(N)	0.00006323	0.006323
7(C)	-0.00250503	-0.250503	41(C)	0.00011543	0.011543
8(N)	0.05176358	5.176357	42(N)	0.00846953	0.846953
9(C)	0.00351014	0.351014	43(C)	0.00036321	0.036321
10(N)	0.03290391	3.290389	44(N)	0.00201523	0.201523
11(C)	0.00415114	0.415114	45(C)	0.00030885	0.030885
12(N)	0.06470121	6.470119	46(N)	0.00218067	0.218067
13(C)	-0.00062171	-0.062171	47(C)	0.00021597	0.021597
14(N)	0.00158932	0.158932	48(N)	-0.00001910	-0.001910
15(C)	-0.00589945	-0.589945	49(C)	-0.00003288	-0.003288
16(N)	0.14971477	14.971472	50(N)	0.00037909	0.037909
17(C)	-0.00422571	-0.422571	51(C)	-0.00021170	-0.021170
18(N)	0.02734336	2.734335	52(N)	0.00063204	0.063204
19(C)	-0.00043722	-0.043722	53(C)	0.00173762	0.173762
20(N)	-0.00157839	-0.157839	54(N)	0.01439608	1.439608
21(C)	0.00174631	0.174631	55(B)	0.00448912	0.448912
22(N)	0.01132812	1.132812	56(B)	0.00500654	0.500654
23(B)	-0.00058891	-0.058891	57(B)	0.00012102	0.012102
24(B)	-0.00045253	-0.045253	58(B)	0.00695917	0.695917
25(B)	0.01011027	1.011027	59(B)	-0.00006526	-0.006526
26(B)	0.03515251	3.515250	60(B)	0.00463688	0.463688
27(B)	0.03534165	3.534164	61(B)	0.00036625	0.036625
28(B)	0.03175344	3.175343	62(B)	0.00625580	0.625580
29(B)	0.02545566	2.545565	63(B)	0.00087376	0.087376
30(B)	0.03236424	3.236423	64(B)	0.00083154	0.083154
31(B)	0.00336323	0.336322	65(B)	0.00198491	0.198491
32(B)	0.11146481	11.146478	66(C)	0.00863017	0.863017
33(B)	0.06980406	6.980404	67(N)	0.00101877	0.101877
34(Be)	0.08065860	8.065857	68(B)	0.00673025	0.673025
			69(Zn)	*-0.001486*	*-0.001417*

2.4 Extended Transition State - Natural Orbitals for Chemical Valence

2.4.1 Pair and NOCV Orbital Information

$ZnBeB_{11}(CN)_{12}$: **Table S1a** and **S1b**. There are totally 530 NOCV pairs and 1060 NOCV orbitals. NOCV orbitals with absolute eigenvalues smaller than 10^{-3} are not shown. All energies are given in kcal·mol^{-1}. Sum of pair energies: Alpha = - 68.97 kcal·mol^{-1}; Beta = - 83.96 kcal·mol^{-1}; Total = - 152.93 kcal·mol^{-1}.

$ZnBeB_{23}(CN)_{22}$: **Table S1c** and **S1d**. There are totally 978 NOCV pairs and 1956 NOCV orbitals. Sum of pair energies: Alpha = - 74.57 kcal·mol^{-1}; Beta = - 85.24 kcal·mol^{-1}; Total = - 159.81 kcal·mol^{-1}.

Table S4a. Alpha NOCV orbitals of $ZnBeB_{11}(CN)_{12}$

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
1	*-23.71*	*1*	*0.32963*	*-256.31*	*530*	*-0.32963*	*-184.39*
2	*-9.62*	*2*	*0.19488*	*-207.06*	*529*	*-0.19488*	*-157.71*
3	*-9.76*	*3*	*0.18820*	*-206.40*	*528*	*-0.18820*	*-154.55*
4	*-2.64*	*4*	*0.10447*	*-177.64*	*527*	*-0.10447*	*-152.41*
5	*-3.41*	*5*	*0.10319*	*-171.89*	*526*	*-0.10319*	*-138.87*
6	-2.51	6	0.09603	-179.95	525	-0.09603	-153.83
7	-2.33	7	0.08736	-189.16	524	-0.08736	-162.48
8	-1.92	8	0.07632	-171.20	523	-0.07632	-146.01
9	-1.73	9	0.07132	-162.80	522	-0.07132	-138.50
10	-1.17	10	0.06954	-159.79	521	-0.06954	-142.98
11	-1.08	11	0.05470	-155.07	520	-0.05470	-135.30
12	-0.87	12	0.04748	-140.88	519	-0.04748	-122.56
13	-0.86	13	0.04407	-103.29	518	-0.04407	-83.87
14	-0.78	14	0.04076	-107.55	517	-0.04076	-88.45
15	-0.77	15	0.03745	-75.95	516	-0.03745	-55.26
16	-0.67	16	0.03619	-104.99	515	-0.03619	-86.34
17	-0.39	17	0.03096	-107.30	514	-0.03096	-94.79
18	-0.32	18	0.02891	-98.56	513	-0.02891	-87.38
19	-0.27	19	0.02566	-99.76	512	-0.02566	-89.33
20	-0.19	20	0.02477	-117.98	511	-0.02477	-110.37
21	-0.17	21	0.02256	-103.73	510	-0.02256	-96.33
22	-0.16	22	0.02240	-112.37	509	-0.02240	-105.41
23	-0.19	23	0.02135	-87.78	508	-0.02135	-78.85
24	-0.15	24	0.02027	-97.38	507	-0.02027	-90.23
25	-0.15	25	0.01901	-87.02	506	-0.01901	-79.38
26	-0.18	26	0.01886	-60.00	505	-0.01886	-50.67
27	-0.17	27	0.01766	-42.72	504	-0.01766	-33.31
28	-0.11	28	0.01642	-70.85	503	-0.01642	-64.15
29	-0.12	29	0.01581	-49.93	502	-0.01581	-42.12
30	-0.11	30	0.01519	-32.20	501	-0.01519	-25.16
31	-0.10	31	0.01491	-56.50	500	-0.01491	-49.99
32	-0.10	32	0.01447	-48.68	499	-0.01447	-42.07
33	-0.10	33	0.01431	-40.59	498	-0.01431	-33.82
34	-0.10	34	0.01423	-19.59	497	-0.01423	-12.48
35	-0.09	35	0.01400	-34.57	496	-0.01400	-27.94
36	-0.09	36	0.01365	-21.05	495	-0.01365	-14.27
37	-0.09	37	0.01341	-19.59	494	-0.01341	-12.85
38	-0.08	38	0.01312	-37.95	493	-0.01312	-32.08
39	-0.08	39	0.01302	-47.65	492	-0.01302	-41.85
40	-0.08	40	0.01260	-11.80	491	-0.01260	-5.31
41	-0.11	41	0.01216	-102.17	490	-0.01216	-93.39

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
42	-0.07	42	0.01154	-25.13	489	-0.01154	-19.32
43	-0.09	43	0.01101	-62.26	488	-0.01101	-54.14
44	-0.07	44	0.01067	-7.58	487	-0.01067	-0.91
45	-0.07	45	0.01057	-30.62	486	-0.01057	-23.68
46	-0.06	46	0.01036	2.21	485	-0.01036	8.29
47	-0.09	47	0.01009	-21.16	484	-0.01009	-12.01
48	-0.06	48	0.00991	18.46	483	-0.00991	24.22
49	-0.06	49	0.00958	13.34	482	-0.00958	19.18
50	-0.09	50	0.00946	-20.26	481	-0.00946	-11.27
51	-0.05	51	0.00931	-17.88	480	-0.00931	-12.40
52	-0.06	52	0.00914	-8.06	479	-0.00914	-1.92
53	-0.05	53	0.00907	11.55	478	-0.00907	17.12
54	-0.05	54	0.00876	-5.10	477	-0.00876	0.27
55	-0.05	55	0.00843	7.84	476	-0.00843	13.19
56	-0.04	56	0.00790	-47.85	475	-0.00790	-43.11
57	-0.04	57	0.00782	-42.4	474	-0.00782	-37.27
58	-0.03	58	0.00744	16.02	473	-0.00744	20.51
59	-0.03	59	0.00721	-63.67	472	-0.00721	-59.37
60	-0.03	60	0.00692	-32.09	471	-0.00692	-28.08
61	-0.03	61	0.00661	-41.18	470	-0.00661	-37.17
62	-0.02	62	0.00625	-4.38	469	-0.00625	-0.67
63	-0.02	63	0.00588	-38.71	468	-0.00588	-35.13
64	-0.02	64	0.00563	-68.18	467	-0.00563	-64.65
65	-0.02	65	0.00528	-67.26	466	-0.00528	-63.78
66	-0.02	66	0.00481	-86.42	465	-0.00481	-83.02
67	-0.01	67	0.00413	-102.05	464	-0.00413	-98.94
68	-0.01	68	0.00372	-112.08	463	-0.00372	-108.91
69	-0.13	69	0.00272	-8104.65	462	-0.00272	-8056.65
70	-0.01	70	0.00265	-271.97	461	-0.00265	-268.91
71	-0.01	71	0.00243	-25.69	460	-0.00243	-23.08
72	-0.01	72	0.00242	-85.24	459	-0.00242	-82.40
73	-0.01	73	0.00219	-20.10	458	-0.00219	-17.57
74	-0.01	74	0.00212	-16.66	457	-0.00212	-14.30
75	0.00	75	0.00206	-38.28	456	-0.00206	-35.98
76	0.00	76	0.00196	-30.84	455	-0.00196	-28.77
77	0.00	77	0.00182	-97.30	454	-0.00182	-95.22
78	0.00	78	0.00175	-89.38	453	-0.00175	-87.36
79	0.00	79	0.00171	-73.97	452	-0.00171	-71.91
80	-0.03	80	0.00166	-4346.64	451	-0.00166	-4329.16
81	-0.03	81	0.00165	-4313.30	450	-0.00165	-4296.18
82	-0.01	82	0.00133	-2990.86	449	-0.00133	-2981.20
83	-0.01	83	0.00106	-1726.66	448	-0.00106	-1720.52

Table S4b. Beta NOCV orbitals of $ZnBeB_{11}(CN)_{12}$

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
266	*-25.40*	*531*	*0.60014*	*-238.52*	*1060*	*-0.60014*	*-196.19*
267	*-15.43*	*532*	*0.26495*	*-251.09*	*1059*	*-0.26495*	*-192.85*
268	*-9.93*	*533*	*0.19200*	*-207.92*	*1058*	*-0.19200*	*-156.22*
269	*-9.12*	*534*	*0.18002*	*-213.88*	*1057*	*-0.18002*	*-163.23*
270	*-2.81*	*535*	*0.10314*	*-178.23*	*1056*	*-0.10314*	*-150.94*
271	*-3.19*	*536*	*0.10169*	*-174.43*	*1055*	*-0.10169*	*-143.03*
272	-2.34	537	0.09020	-184.90	1054	-0.09020	-158.93
273	-2.17	538	0.08504	-183.43	1053	-0.08504	-157.89
274	-1.84	539	0.07341	-158.69	1052	-0.07341	-133.56
275	-1.42	540	0.06790	-170.45	1051	-0.06790	-149.59
276	-1.30	541	0.05710	-153.98	1050	-0.05710	-131.17
277	-0.87	542	0.05018	-159.40	1049	-0.05018	-141.98
278	-0.86	543	0.04716	-143.43	1048	-0.04716	-125.30
279	-0.76	544	0.04060	-95.02	1047	-0.04060	-76.23
280	-0.68	545	0.03794	-110.14	1046	-0.03794	-92.13
281	-0.71	546	0.03646	-74.45	1045	-0.03646	-55.06
282	-0.27	547	0.03149	-132.67	1044	-0.03149	-124.16
283	-0.33	548	0.02919	-113.17	1043	-0.02919	-101.92
284	-0.30	549	0.02814	-102.79	1042	-0.02814	-92.19
285	-0.21	550	0.02551	-113.09	1041	-0.02551	-105.02
286	-0.17	551	0.02477	-121.59	1040	-0.02477	-114.55
287	-0.19	552	0.02453	-115.64	1039	-0.02453	-107.98
288	-0.18	553	0.02364	-103.19	1038	-0.02364	-95.73
289	-0.16	554	0.02068	-92.55	1037	-0.02068	-84.70
290	-0.16	555	0.02049	-98.45	1036	-0.02049	-90.85
291	-0.13	556	0.02033	-106.64	1035	-0.02033	-100.01
292	-0.12	557	0.01904	-87.09	1034	-0.01904	-80.69
293	-0.13	558	0.01892	-90.73	1033	-0.01892	-83.70
294	-0.13	559	0.01806	-71.59	1032	-0.01806	-64.35
295	-0.13	560	0.01778	-79.61	1031	-0.01778	-72.28
296	-0.13	561	0.01620	-56.41	1030	-0.01620	-48.48
297	-0.09	562	0.01601	-81.18	1029	-0.01601	-75.45
298	-0.09	563	0.01554	-73.73	1028	-0.01554	-67.69
299	-0.09	564	0.01495	-54.00	1027	-0.01495	-47.72
300	-0.09	565	0.01442	-79.76	1026	-0.01442	-73.22
301	-0.09	566	0.01399	-28.79	1025	-0.01399	-22.11
302	-0.09	567	0.01385	-44.38	1024	-0.01385	-37.97
303	-0.09	568	0.01363	-24.66	1023	-0.01363	-17.85
304	-0.09	569	0.01342	-15.89	1022	-0.01342	-9.45
305	-0.08	570	0.01287	-49.96	1021	-0.01287	-43.99
306	-0.09	571	0.01284	-3.29	1020	-0.01284	3.47
307	-0.08	572	0.01277	-10.59	1019	-0.01277	-4.05
308	-0.08	573	0.01227	-11.05	1018	-0.01227	-4.73
309	-0.11	574	0.01173	-150.12	1017	-0.01173	-140.61
310	-0.06	575	0.01092	-25.65	1016	-0.01092	-19.88
311	-0.09	576	0.01062	-29.61	1015	-0.01062	-21.42
312	-0.07	577	0.01034	-62.81	1014	-0.01034	-55.64
313	-0.10	578	0.01012	-20.14	1013	-0.01012	-10.38
314	-0.07	579	0.00975	-11.03	1012	-0.00975	-3.38
315	-0.05	580	0.00922	-14.33	1011	-0.00922	-8.39
316	-0.05	581	0.00907	4.61	1010	-0.00907	10.13
317	-0.05	582	0.00900	17.07	1009	-0.00900	23.00

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
318	-0.05	583	0.00868	5.60	1008	-0.00868	11.79
319	-0.04	584	0.00841	-25.45	1007	-0.00841	-20.63
320	-0.04	585	0.00832	11.74	1006	-0.00832	17.11
321	-0.04	586	0.00791	-58.31	1005	-0.00791	-53.74
322	-0.03	587	0.00738	-38.08	1004	-0.00738	-33.79
323	-0.03	588	0.00673	-86.25	1003	-0.00673	-82.31
324	-0.03	589	0.00648	-67.60	1002	-0.00648	-63.56
325	-0.02	590	0.00617	-47.73	1001	-0.00617	-43.77
326	-0.02	591	0.00589	-27.89	1000	-0.00589	-24.43
327	-0.02	592	0.00569	-43.14	999	-0.00569	-39.47
328	-0.02	593	0.00503	-59.32	998	-0.00503	-56.33
329	-0.01	594	0.00483	-59.66	997	-0.00483	-56.58
330	-0.01	595	0.00435	-90.18	996	-0.00435	-87.18
331	-0.01	596	0.00336	-143.65	995	-0.00336	-140.85
332	-0.01	597	0.00313	-94.21	994	-0.00313	-91.83
333	-0.14	598	0.00273	-8326.22	993	-0.00273	-8276.71
334	-0.01	599	0.00246	-67.78	992	-0.00246	-65.29
335	-0.01	600	0.00238	-55.22	991	-0.00238	-52.79
336	0.00	601	0.00219	-88.90	990	-0.00219	-86.70
337	0.00	602	0.00209	-79.04	989	-0.00209	-76.79
338	0.00	603	0.00208	-71.11	988	-0.00208	-68.89
339	0.00	604	0.00203	-61.47	987	-0.00203	-59.25
340	0.00	605	0.00196	-43.88	986	-0.00196	-41.84
341	0.00	606	0.00187	-89.51	985	-0.00187	-87.41
342	0.00	607	0.00185	-87.42	984	-0.00185	-85.37
343	0.00	608	0.00182	-116.41	983	-0.00182	-114.19
344	-0.03	609	0.00167	-4396.11	982	-0.00167	-4378.50
345	-0.03	610	0.00165	-4230.38	981	-0.00165	-4213.63
346	-0.01	611	0.00139	-3073.79	980	-0.00139	-3063.60
347	-0.01	612	0.00106	-1749.74	979	-0.00106	-1743.57
348	-0.01	613	0.00106	-1667.44	978	-0.00106	-1661.35

Table S4c. Alpha NOCV orbitals of $ZnBeB_{23}(CN)_{22}$

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
1	*-23.16*	*1*	*0.30001*	*-286.87*	*978*	*-0.30001*	*-209.67*
2	*-10.79*	*2*	*0.19492*	*-230.17*	*977*	*-0.19492*	*-174.84*
3	*-9.10*	*3*	*0.18190*	*-220.86*	*976*	*-0.18190*	*-170.83*
4	*-4.61*	*4*	*0.14436*	*-210.52*	*975*	*-0.14436*	*-178.58*
5	*-4.04*	*5*	*0.13040*	*-218.72*	*974*	*-0.13040*	*-187.74*
6	*-3.43*	*6*	*0.12183*	*-210.97*	*973*	*-0.12183*	*-182.86*
7	*-2.22*	*7*	*0.10148*	*-193.31*	*972*	*-0.10148*	*-171.39*
8	-2.46	8	0.08210	-156.42	971	-0.08210	-126.49
9	-2.09	9	0.07967	-166.43	970	-0.07967	-140.16
10	-1.07	10	0.05786	-186.26	969	-0.05786	-167.83
11	-1.10	11	0.05403	-172.33	968	-0.05403	-151.92
12	-0.81	12	0.04952	-178.43	967	-0.04952	-162.10
13	-0.78	13	0.04633	-168.50	966	-0.04633	-151.61
14	-0.68	14	0.04444	-158.66	965	-0.04444	-143.39
15	-0.48	15	0.04169	-163.04	964	-0.04169	-151.61
16	-0.62	16	0.03839	-150.81	963	-0.03839	-134.69
17	-0.34	17	0.03613	-152.10	962	-0.03613	-142.67
18	-0.41	18	0.03502	-145.05	961	-0.03502	-133.44
19	-0.44	19	0.03325	-128.48	960	-0.03325	-115.29
20	-0.42	20	0.03006	-104.38	959	-0.03006	-90.31
21	-0.27	21	0.02662	-128.39	958	-0.02662	-118.13
22	-0.21	22	0.02428	-103.83	957	-0.02428	-95.13
23	-0.24	23	0.02404	-114.55	956	-0.02404	-104.53
24	-0.19	24	0.02360	-120.54	955	-0.02360	-112.46
25	-0.18	25	0.02284	-126.57	954	-0.02284	-118.67
26	-0.15	26	0.02111	-130.05	953	-0.02111	-122.90
27	-0.18	27	0.02074	-113.21	952	-0.02074	-104.38
28	-0.15	28	0.02012	-117.72	951	-0.02012	-110.44
29	-0.13	29	0.01996	-129.22	950	-0.01996	-122.83
30	-0.12	30	0.01928	-128.14	949	-0.01928	-122.04
31	-0.12	31	0.01828	-120.66	948	-0.01828	-114.34
32	-0.11	32	0.01797	-122.02	947	-0.01797	-116.16
33	-0.10	33	0.01739	-118.69	946	-0.01739	-113.19
34	-0.09	34	0.01673	-126.66	945	-0.01673	-121.17
35	-0.10	35	0.01662	-110.58	944	-0.01662	-104.75
36	-0.08	36	0.01610	-124.69	943	-0.01610	-119.63
37	-0.10	37	0.01540	-106.96	942	-0.01540	-100.38
38	-0.08	38	0.01502	-117.58	941	-0.01502	-112.58
39	-0.07	39	0.01436	-115.29	940	-0.01436	-110.33
40	-0.07	40	0.01368	-109.27	939	-0.01368	-104.30
41	-0.08	41	0.01319	-90.39	938	-0.01319	-84.38
42	-0.07	42	0.01299	-108.99	937	-0.01299	-103.90
43	-0.07	43	0.01285	-97.72	936	-0.01285	-92.16
44	-0.06	44	0.01260	-91.45	935	-0.01260	-86.55
45	-0.06	45	0.01251	-85.42	934	-0.01251	-80.39
46	-0.06	46	0.01223	-87.25	933	-0.01223	-82.39
47	-0.06	47	0.01208	-89.14	932	-0.01208	-84.00
48	-0.06	48	0.01204	-78.01	931	-0.01204	-73.06
49	-0.05	49	0.01181	-92.81	930	-0.01181	-88.49
50	-0.06	50	0.01152	-75.65	929	-0.01152	-70.78
51	-0.05	51	0.01142	-94.91	928	-0.01142	-90.41
52	-0.06	52	0.01128	-44.23	927	-0.01128	-39.00

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
53	-0.06	53	0.01112	-71.54	926	-0.01112	-66.25
54	-0.06	54	0.01095	-62.73	925	-0.01095	-57.56
55	-0.05	55	0.01072	-76.06	924	-0.01072	-71.26
56	-0.05	56	0.01052	-70.57	923	-0.01052	-66.15
57	-0.04	57	0.01032	-85.20	922	-0.01032	-81.72
58	-0.05	58	0.01021	-71.25	921	-0.01021	-66.79
59	-0.04	59	0.01010	-63.44	920	-0.01010	-59.12
60	-0.04	60	0.00995	-55.51	919	-0.00995	-51.00
61	-0.05	61	0.00981	-54.95	918	-0.00981	-50.10
62	-0.05	62	0.00960	-41.79	917	-0.00960	-37.05
63	-0.04	63	0.00947	-52.98	916	-0.00947	-48.61
64	-0.04	64	0.00935	-43.92	915	-0.00935	-39.40
65	-0.04	65	0.00924	-78.19	914	-0.00924	-73.69
66	-0.05	66	0.00912	-78.24	913	-0.00912	-72.26
67	-0.04	67	0.00909	-68.25	912	-0.00909	-64.07
68	-0.04	68	0.00891	-73.86	911	-0.00891	-69.71
69	-0.05	69	0.00872	-52.39	910	-0.00872	-46.64
70	-0.04	70	0.00862	-42.94	909	-0.00862	-37.74
71	-0.04	71	0.00848	-49.45	908	-0.00848	-44.36
72	-0.03	72	0.00830	-48.49	907	-0.00830	-44.56
73	-0.04	73	0.00824	-47.57	906	-0.00824	-42.31
74	-0.05	74	0.00811	-67.50	905	-0.00811	-61.86
75	-0.05	75	0.00798	-49.21	904	-0.00798	-43.15
76	-0.04	76	0.00764	-37.62	903	-0.00764	-32.95
77	-0.03	77	0.00755	-32.70	902	-0.00755	-28.48
78	-0.03	78	0.00738	-32.92	901	-0.00738	-28.86
79	-0.03	79	0.00729	-31.53	900	-0.00729	-26.92
80	-0.03	80	0.00726	-31.82	899	-0.00726	-27.39
81	-0.03	81	0.00706	-21.31	898	-0.00706	-16.83
82	-0.03	82	0.00679	-38.65	897	-0.00679	-34.23
83	-0.03	83	0.00672	-39.42	896	-0.00672	-35.37
84	-0.03	84	0.00663	-22.72	895	-0.00663	-18.51
85	-0.03	85	0.00652	-5.27	894	-0.00652	-1.33
86	-0.03	86	0.00643	-25.76	893	-0.00643	-21.70
87	-0.02	87	0.00632	-24.39	892	-0.00632	-20.50
88	-0.02	88	0.00624	-21.99	891	-0.00624	-18.27
89	-0.02	89	0.00612	-32.26	890	-0.00612	-28.45
90	-0.02	90	0.00603	-39.61	889	-0.00603	-36.07
91	-0.02	91	0.00597	-69.05	888	-0.00597	-65.49
92	-0.02	92	0.00594	-25.21	887	-0.00594	-21.65
93	-0.02	93	0.00589	-37.21	886	-0.00589	-33.60
94	-0.02	94	0.00562	-44.84	885	-0.00562	-41.64
95	-0.02	95	0.00555	-41.22	884	-0.00555	-38.00
96	-0.02	96	0.00548	-28.25	883	-0.00548	-24.99
97	-0.02	97	0.00544	-8.91	882	-0.00544	-5.62
98	-0.02	98	0.00516	-59.65	881	-0.00516	-56.45
99	-0.02	99	0.00507	-86.89	880	-0.00507	-83.79
100	-0.02	100	0.00494	-85.04	879	-0.00494	-81.66
101	-0.01	101	0.00489	-41.72	878	-0.00489	-38.86
102	-0.01	102	0.00487	-75.50	877	-0.00487	-72.78
103	-0.01	103	0.00477	-44.00	876	-0.00477	-41.06
104	-0.01	104	0.00460	-36.27	875	-0.00460	-33.77
105	-0.01	105	0.00443	-93.14	874	-0.00443	-90.42

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
106	-0.01	106	0.00427	-89.89	873	-0.00427	-87.22
107	-0.01	107	0.00419	-105.45	872	-0.00419	-102.81
108	-0.01	108	0.00393	-73.64	871	-0.00393	-70.90
109	-0.01	109	0.00388	-111.60	870	-0.00388	-108.81
110	-0.01	110	0.00377	-115.30	869	-0.00377	-112.62
111	-0.01	111	0.00366	-67.55	868	-0.00366	-65.24
112	-0.01	112	0.00358	-204.47	867	-0.00358	-201.14
113	-0.01	113	0.00350	-59.89	866	-0.00350	-57.65
114	-0.01	114	0.00328	-111.91	865	-0.00328	-109.45
115	-0.01	115	0.00310	-63.91	864	-0.00310	-61.81
116	-0.01	116	0.00301	-143.26	863	-0.00301	-141.04
117	-0.01	117	0.00289	-115.76	862	-0.00289	-113.47
118	-0.02	118	0.00275	-938.55	861	-0.00275	-931.60
119	-0.08	119	0.00258	-5044.98	860	-0.00258	-5015.96
120	-0.01	120	0.00237	-41.67	859	-0.00237	-39.22
121	-0.01	121	0.00222	-475.59	858	-0.00222	-471.85
122	-0.01	122	0.00215	-595.44	857	-0.00215	-591.47
123	0.00	123	0.00198	-191.45	856	-0.00198	-189.55
124	-0.01	124	0.00197	-562.71	855	-0.00197	-558.77
125	-0.01	125	0.00191	-1199.10	854	-0.00191	-1192.80
126	-0.02	126	0.00183	-2133.24	853	-0.00183	-2123.21
127	-0.01	127	0.00173	-708.08	852	-0.00173	-703.83
128	0.00	128	0.00161	-89.69	851	-0.00161	-87.96
129	0.00	129	0.00160	-387.98	850	-0.00160	-385.32
130	0.00	130	0.00156	-161.00	849	-0.00156	-159.03
131	0.00	131	0.00153	-317.30	848	-0.00153	-314.67
132	0.00	132	0.00150	-162.56	847	-0.00150	-160.51
133	0.00	133	0.00149	-57.21	846	-0.00149	-55.54
134	0.00	134	0.00148	-183.93	845	-0.00148	-181.63
135	-0.01	135	0.00148	-2239.69	844	-0.00148	-2231.43
136	-0.01	136	0.00142	-1082.69	843	-0.00142	-1078.13
137	0.00	137	0.00135	-135.98	842	-0.00135	-134.42
138	0.00	138	0.00134	-159.44	841	-0.00134	-157.82
139	-0.01	139	0.00129	-919.82	840	-0.00129	-915.69
140	-0.01	140	0.00128	-1033.86	839	-0.00128	-1029.42
141	0.00	141	0.00124	-295.59	838	-0.00124	-293.60
142	0.00	142	0.00122	-82.86	837	-0.00122	-81.53
143	-0.01	143	0.00111	-2307.68	836	-0.00111	-2300.22
144	0.00	144	0.00104	-106.38	835	-0.00104	-105.23
145	0.00	145	0.00103	-66.79	834	-0.00103	-65.63

Table S4d. Beta NOCV orbitals of $ZnBeB_{23}(CN)_{22}$

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
490	*-13.36*	*979*	*0.51712*	*-238.13*	*1956*	*-0.51712*	*-212.30*
491	*-22.44*	*980*	*0.29173*	*-289.28*	*1955*	*-0.29173*	*-212.34*
492	*-10.64*	*981*	*0.19268*	*-231.90*	*1954*	*-0.19268*	*-176.66*
493	*-8.76*	*982*	*0.17904*	*-218.36*	*1953*	*-0.17904*	*-169.46*
494	*-4.59*	*983*	*0.14450*	*-210.92*	*1952*	*-0.14450*	*-179.18*
495	*-4.07*	*984*	*0.12938*	*-220.04*	*1951*	*-0.12938*	*-188.57*
496	*-3.38*	*985*	*0.11909*	*-212.80*	*1950*	*-0.11909*	*-184.41*
497	-2.35	986	0.09333	-180.16	1949	-0.09333	-154.96
498	-2.37	987	0.08086	-159.51	1948	-0.08086	-130.15
499	-1.38	988	0.06324	-180.24	1947	-0.06324	-158.49
500	-1.07	989	0.05544	-177.75	1946	-0.05544	-158.53
501	-1.06	990	0.05283	-173.98	1945	-0.05283	-153.84
502	-0.79	991	0.04930	-182.18	1944	-0.04930	-166.17
503	-0.68	992	0.04441	-160.80	1943	-0.04441	-145.54
504	-0.40	993	0.04361	-167.30	1942	-0.04361	-158.03
505	-0.61	994	0.04083	-162.99	1941	-0.04083	-148.06
506	-0.42	995	0.03561	-142.97	1940	-0.03561	-131.21
507	-0.49	996	0.03474	-148.95	1939	-0.03474	-134.87
508	-0.44	997	0.03332	-123.92	1938	-0.03332	-110.66
509	-0.36	998	0.03059	-138.49	1937	-0.03059	-126.88
510	-0.34	999	0.02894	-112.02	1936	-0.02894	-100.21
511	-0.26	1000	0.02535	-126.74	1935	-0.02535	-116.63
512	-0.19	1001	0.02423	-122.54	1934	-0.02423	-114.81
513	-0.20	1002	0.02359	-122.95	1933	-0.02359	-114.38
514	-0.18	1003	0.02287	-119.93	1932	-0.02287	-111.89
515	-0.15	1004	0.02191	-133.54	1931	-0.02191	-126.82
516	-0.14	1005	0.02145	-133.47	1930	-0.02145	-126.85
517	-0.18	1006	0.02067	-116.27	1929	-0.02067	-107.67
518	-0.15	1007	0.02010	-124.10	1928	-0.02010	-116.71
519	-0.12	1008	0.01964	-130.27	1927	-0.01964	-124.07
520	-0.13	1009	0.01872	-117.06	1926	-0.01872	-110.30
521	-0.10	1010	0.01811	-131.55	1925	-0.01811	-126.28
522	-0.11	1011	0.01785	-107.67	1924	-0.01785	-101.23
523	-0.10	1012	0.01722	-125.55	1923	-0.01722	-119.81
524	-0.08	1013	0.01694	-126.73	1922	-0.01694	-121.80
525	-0.08	1014	0.01662	-119.84	1921	-0.01662	-114.85
526	-0.09	1015	0.01617	-121.67	1920	-0.01617	-116.40
527	-0.07	1016	0.01535	-120.97	1919	-0.01535	-116.15
528	-0.08	1017	0.01510	-115.88	1918	-0.01510	-110.84
529	-0.07	1018	0.01476	-113.94	1917	-0.01476	-108.96
530	-0.07	1019	0.01424	-109.66	1916	-0.01424	-104.41
531	-0.08	1020	0.01380	-96.36	1915	-0.01380	-90.91
532	-0.06	1021	0.01338	-109.29	1914	-0.01338	-104.74
533	-0.06	1022	0.01299	-104.50	1913	-0.01299	-100.02
534	-0.07	1023	0.01279	-98.25	1912	-0.01279	-93.11
535	-0.06	1024	0.01261	-90.14	1911	-0.01261	-85.52
536	-0.07	1025	0.01248	-109.41	1910	-0.01248	-104.16
537	-0.07	1026	0.01233	-81.01	1909	-0.01233	-75.30
538	-0.06	1027	0.01221	-88.02	1908	-0.01221	-83.27
539	-0.05	1028	0.01185	-108.00	1907	-0.01185	-103.46
540	-0.05	1029	0.01141	-83.50	1906	-0.01141	-79.08
541	-0.05	1030	0.01136	-88.00	1905	-0.01136	-83.40

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
542	-0.04	1031	0.01092	-80.84	1904	-0.01093	-76.77
543	-0.05	1032	0.01089	-92.30	1903	-0.01089	-87.67
544	-0.05	1033	0.01080	-46.95	1902	-0.01080	-42.24
545	-0.05	1034	0.01065	-78.47	1901	-0.01065	-73.66
546	-0.05	1035	0.01056	-64.93	1900	-0.01056	-60.34
547	-0.05	1036	0.01032	-46.66	1899	-0.01032	-42.18
548	-0.04	1037	0.01019	-67.17	1898	-0.01019	-62.79
549	-0.04	1038	0.01016	-62.26	1897	-0.01016	-57.85
550	-0.04	1039	0.00996	-69.50	1896	-0.00996	-64.98
551	-0.05	1040	0.00990	-51.49	1895	-0.00990	-45.97
552	-0.04	1041	0.00970	-51.06	1894	-0.00970	-46.48
553	-0.04	1042	0.00948	-53.98	1893	-0.00948	-49.75
554	-0.04	1043	0.00922	-91.33	1892	-0.00922	-87.27
555	-0.04	1044	0.00916	-66.97	1891	-0.00916	-62.69
556	-0.04	1045	0.00900	-60.87	1890	-0.00900	-56.37
557	-0.04	1046	0.00897	-67.33	1889	-0.00897	-62.44
558	-0.04	1047	0.00882	-81.53	1888	-0.00882	-77.27
559	-0.05	1048	0.00857	-59.53	1887	-0.00857	-53.97
560	-0.05	1049	0.00847	-56.15	1886	-0.00847	-49.67
561	-0.05	1050	0.00831	-50.60	1885	-0.00831	-45.00
562	-0.04	1051	0.00813	-62.61	1884	-0.00813	-58.29
563	-0.04	1052	0.00802	-67.10	1883	-0.00802	-61.83
564	-0.05	1053	0.00788	-15.58	1882	-0.00788	-9.13
565	-0.03	1054	0.00764	-40.47	1881	-0.00764	-35.98
566	-0.03	1055	0.00751	-26.44	1880	-0.00751	-22.00
567	-0.03	1056	0.00723	-19.07	1879	-0.00723	-14.52
568	-0.03	1057	0.00718	-26.75	1878	-0.00718	-22.79
569	-0.03	1058	0.00710	-45.14	1877	-0.00710	-40.85
570	-0.03	1059	0.00693	-35.52	1876	-0.00693	-31.37
571	-0.03	1060	0.00675	-19.11	1875	-0.00675	-15.17
572	-0.03	1061	0.00657	-28.16	1874	-0.00657	-23.80
573	-0.02	1062	0.00645	-25.74	1873	-0.00645	-22.07
574	-0.03	1063	0.00641	-29.46	1872	-0.00641	-25.27
575	-0.02	1064	0.00631	-34.38	1871	-0.00631	-30.53
576	-0.03	1065	0.00622	-40.83	1870	-0.00622	-36.77
577	-0.02	1066	0.00620	-45.15	1869	-0.00620	-41.54
578	-0.02	1067	0.00606	-65.33	1868	-0.00606	-61.59
579	-0.02	1068	0.00604	-23.25	1867	-0.00604	-19.59
580	-0.02	1069	0.00601	-37.68	1866	-0.00601	-33.91
581	-0.02	1070	0.00570	-56.73	1865	-0.00570	-53.55
582	-0.02	1071	0.00567	-56.25	1864	-0.00567	-52.82
583	-0.02	1072	0.00558	-43.14	1863	-0.00558	-39.89
584	-0.02	1073	0.00545	-23.10	1862	-0.00545	-19.86
585	-0.02	1074	0.00540	-30.56	1861	-0.00540	-27.26
586	-0.02	1075	0.00520	-59.50	1860	-0.00520	-56.25
587	-0.01	1076	0.00511	-59.23	1859	-0.00511	-56.37
588	-0.01	1077	0.00504	-80.05	1858	-0.00504	-77.13
589	-0.02	1078	0.00483	-59.58	1857	-0.00483	-56.48
590	-0.01	1079	0.00474	-46.71	1856	-0.00474	-44.17
591	-0.01	1080	0.00465	-74.08	1855	-0.00465	-71.19
592	-0.01	1081	0.00459	-104.13	1854	-0.00459	-101.03
593	-0.01	1082	0.00437	-73.10	1853	-0.00437	-70.44
594	-0.01	1083	0.00425	-64.04	1852	-0.00425	-61.48

Pair No.	Energy	Orb. No.	Eigenvalue	Energy	Orb. No.	Eigenvalue	Energy
595	-0.01	1084	0.00417	-77.43	1851	-0.00417	-74.97
596	-0.01	1085	0.00391	-187.33	1850	-0.00391	-183.91
597	-0.01	1086	0.00386	-67.49	1849	-0.00386	-65.12
598	-0.01	1087	0.00380	-108.85	1848	-0.00380	-106.14
599	-0.01	1088	0.00364	-68.77	1847	-0.00364	-66.57
600	-0.01	1089	0.00348	-59.28	1846	-0.00348	-57.09
601	-0.01	1090	0.00318	-112.42	1845	-0.00318	-110.21
602	-0.01	1091	0.00305	-106.55	1844	-0.00305	-104.29
603	-0.01	1092	0.00298	-127.59	1843	-0.00298	-125.51
604	-0.01	1093	0.00288	-332.84	1842	-0.00288	-329.51
605	-0.03	1094	0.00273	-1799.07	1841	-0.00273	-1787.17
606	-0.06	1095	0.00260	-4084.72	1840	-0.00260	-4060.82
607	-0.01	1096	0.00230	-228.18	1839	-0.00230	-225.62
608	-0.01	1097	0.00223	-172.03	1838	-0.00223	-169.19
609	-0.01	1098	0.00216	-605.09	1837	-0.00216	-600.94
610	-0.01	1099	0.00197	-515.56	1836	-0.00197	-511.92
611	-0.01	1100	0.00195	-436.53	1835	-0.00195	-433.52
612	-0.02	1101	0.00189	-2023.41	1834	-0.00189	-2013.60
613	0.00	1102	0.00182	-327.23	1833	-0.00182	-324.73
614	-0.01	1103	0.00179	-1413.35	1832	-0.00179	-1406.35
615	0.00	1104	0.00165	-402.92	1831	-0.00165	-400.17
616	0.00	1105	0.00161	-186.70	1830	-0.00161	-184.75
617	0.00	1106	0.00160	-391.05	1829	-0.00160	-388.28
618	0.00	1107	0.00155	-361.21	1828	-0.00155	-358.61
619	0.00	1108	0.00153	-96.26	1827	-0.00153	-94.52
620	0.00	1109	0.00150	-321.67	1826	-0.00150	-319.04
621	0.00	1110	0.00149	-101.17	1825	-0.00149	-99.55
622	-0.01	1111	0.00148	-1442.35	1824	-0.00148	-1435.35
623	-0.01	1112	0.00148	-1073.23	1823	-0.00148	-1069.40
624	0.00	1113	0.00141	-662.65	1822	-0.00141	-659.47
625	0.00	1114	0.00135	-130.57	1821	-0.00135	-129.01
626	0.00	1115	0.00133	-104.93	1820	-0.00133	-103.45
627	-0.01	1116	0.00129	-1244.90	1819	-0.00129	-1239.70
628	0.00	1117	0.00128	-773.80	1818	-0.00128	-770.26
629	0.00	1118	0.00124	-287.78	1817	-0.00124	-285.90
630	0.00	1119	0.00123	-81.79	1816	-0.00123	-80.48
631	0.00	1120	0.00112	-1029.70	1815	-0.00112	-1025.50
632	0.00	1121	0.00109	-1326.95	1814	-0.00109	-1322.53
633	0.00	1122	0.00103	-170.86	1813	-0.00103	-169.55

2.4.2 NOCV Orbital Isosurfaces

Isosurfaces of NOCV orbitals with eigenvalues larger than 0.1 are shown in **Figure S1** and **S2**.

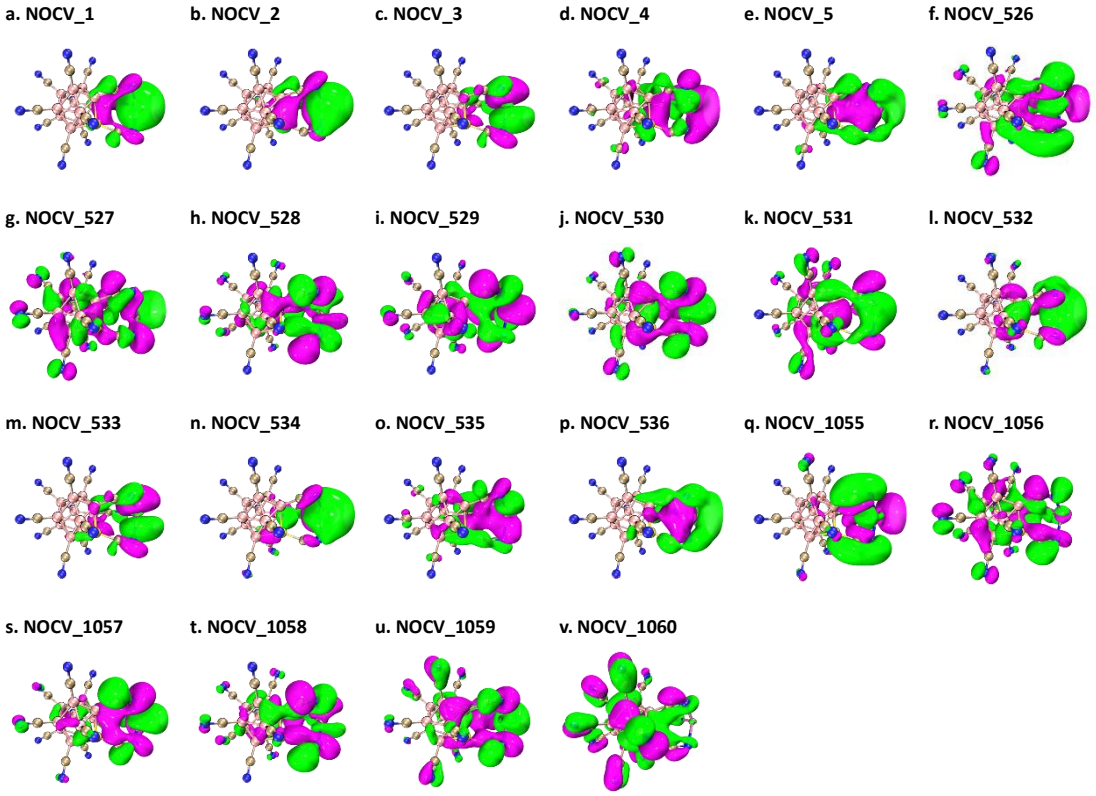

Figure S1. Key NOCV orbitals of $ZnBeB_{11}(CN)_{12}$.

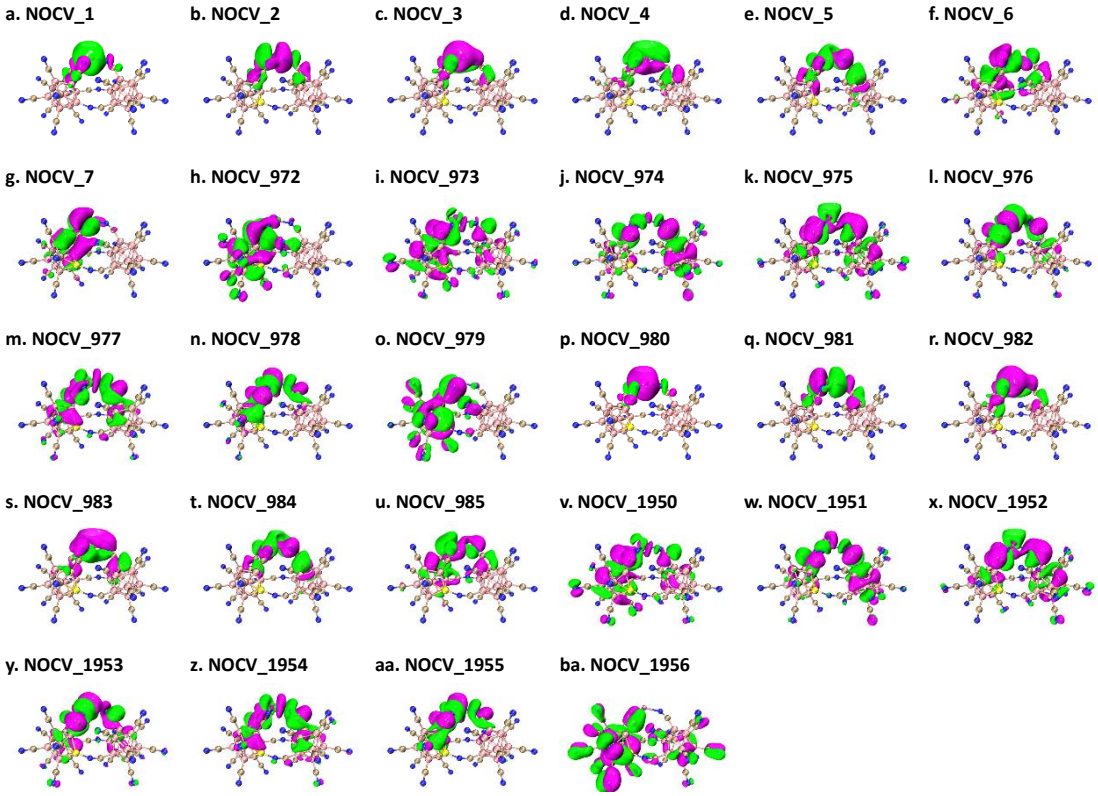

Figure S2. Key NOCV orbitals of $ZnBeB_{23}(CN)_{22}$.

3. Other Information

3.1 Isosurfaces of Molecular Orbitals (Figure S3)

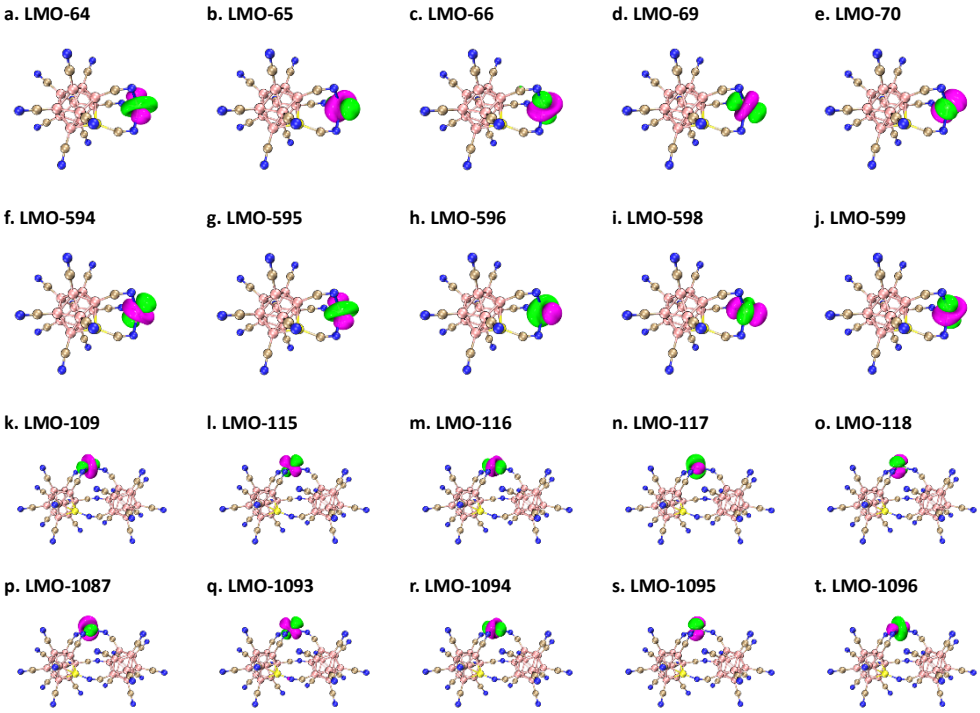

Figure S3. Isosurfaces of d-angular localized molecular orbitals. Every five orbitals in each line are α and β spin for $ZnBeB_{11}(CN)_{12}$ and $ZnBeB_{23}(CN)_{22}$, respectively.

3.2 Simulated XPS (Figure S4)

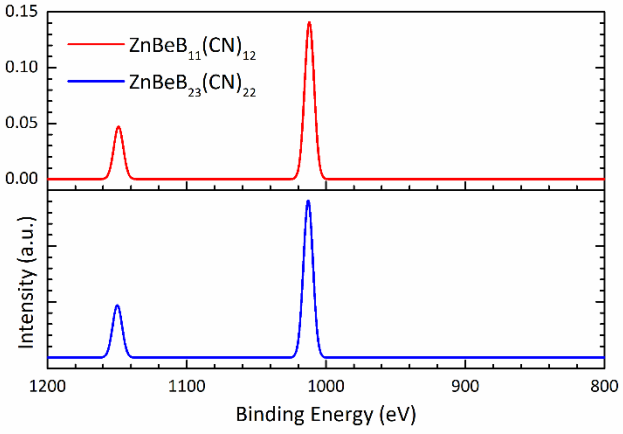

Figure S4. Simulated XPS curves for $ZnBeB_{11}(CN)_{12}$ and $ZnBeB_{23}(CN)_{22}$.

3.3 UV-Vis-NIR Spectrum (Figure S5)

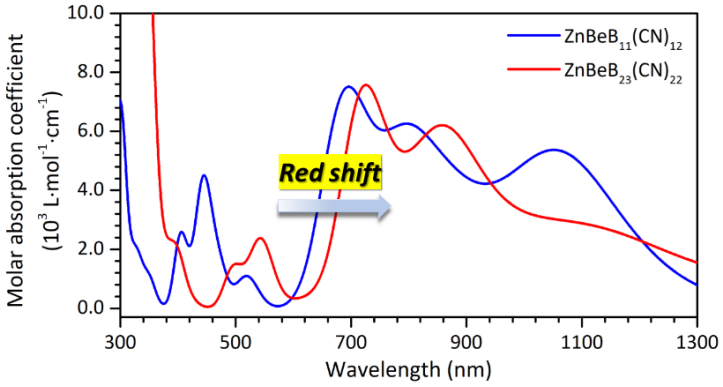

Figure S5. Simulated UV-Vis-NIR absorption spectra for $ZnBeB_{11}(CN)_{12}$ and $ZnBeB_{23}(CN)_{22}$.

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