Supplementary Material (ESI) for Chemical Communications

The Isolable Matryoshka Nesting Doll Icosahedral Cluster $[As@Ni_{12}@As_{20}]^{3-}$ as a "Superatom": Analogy with the Jellium Cluster Al_{13}^- Generated in the Gas Phase by Laser Vaporization

R. Bruce King*[a] and Jijun Zhao*[b]

[a]Department of Chemistry and Center for Computational Chemistry, University of Georgia, Athens, Georgia, USA and [b]State Key Laboratory of Materials Modification by Laser, Electron, and Ion Beams & College of Advanced Science and Technology, Dalian University of Technology, Dalian, China

Supporting Information

Table S1. Bonding molecular orbitals of regular dodecahedral As_{20} (I_h symmetry)

Table S2. Bonding molecular orbitals of $[As@Ni_{12}@As_{20}]^{3-}$ (I_h symmetry)

Table S1. Bonding molecular orbitals of regular dodecahedral As_{20} (I_h symmetry)

281	+	7	AG.1	-0.592216	-16.115	2.000
282	+	11	T1U.1	-0.576985	-15.701	2.000
283	+	11	T1U.2	-0.576985	-15.701	2.000
284	+	11	T1U.3	-0.576985	-15.701	2.000
285	+	15	HG.1	-0.550173	-14.971	2.000
286	+	15	HG.2	-0.550173	-14.971	2.000
287	+	15	HG.3	-0.550173	-14.971	2.000
288	+	15	HG.4	-0.550173	-14.971	2.000
289	+	15	HG.5	-0.550173	-14.971	2.000
290	+	11	GU.1	-0.526001	-14.313	2.000
291	+	11	GU.3	-0.526001	-14.313	2.000
292	+	11	GU.4	-0.526001	-14.313	2.000
293	+	11	GU.2	-0.526001	-14.313	2.000
294	+	11	GG.1	-0.470432	-12.801	2.000
295	+	11	GG.2	-0.470432	-12.801	2.000
296	+	11	GG.3	-0.470432	-12.801	2.000
297	+	11	GG.4	-0.470432	-12.801	2.000
298	+	11	T2U.1	-0.463842	-12.622	2.000
299	+	11	T2U.3	-0.463842	-12.622	2.000
300	+	11	T2U.2	-0.463842	-12.622	2.000
301	+	16	HG.1	-0.283424	-7.712	2.000
302	+	16	HG.5	-0.283424	-7.712	2.000
303	+	16	HG.2	-0.283424	-7.712	2.000
304	+	16	HG.3	-0.283424	-7.712	2.000
305	+	16	HG.4	-0.283424	-7.712	2.000
306	+	12	T2U.1	-0.270769	-7.368	2.000
307	+	12	T2U.2	-0.270769	-7.368	2.000
308	+	12	T2U.3	-0.270769	-7.368	2.000
309	+	9	HU.1	-0.266235	-7.245	2.000
310	+	9	HU.4	-0.266235	-7.245	2.000
311	+	9	HU.5	-0.266235	-7.245	2.000
312	+	9	HU.2	-0.266235	-7.245	2.000
313	+	9	HU.3	-0.266235	-7.245	2.000
314	+	8	AG.1	-0.254177	-6.917	2.000
315	+	12	T1U.1	-0.238380	-6.487	2.000
316	+	12	T1U.2	-0.238380	-6.487	2.000
317	+	12	T1U.3	-0.238380	-6.487	2.000
318	+	12	GG.1	-0.227590	-6.193	2.000
319	+	12	GG.4	-0.227590	-6.193	2.000
320	+	12	GG.2	-0.227590	-6.193	2.000
321	+	12	GG.3	-0.227590	-6.193	2.000
322	+	17	HG.1	-0.209652	-5.705	2.000
323	+	17	HG.2	-0.209652	-5.705	2.000
324	+	17	HG.5	-0.209652	-5.705	2.000

325	+	17	HG.3	-0.209652	-5.705	2.000
326	+	17	HG.4	-0.209652	-5.705	2.000
327	+	12	GU.1	-0.189784	-5.164	2.000
328	+	12	GU.2	-0.189784	-5.164	2.000
329	+	12	GU.3	-0.189784	-5.164	2.000
330	+	12	GU.4	-0.189784	-5.164	2.000
331	+	13	T1U.1	-0.139560	-3.798	0.000
332	+	13	T1U.2	-0.139560	-3.798	0.000
333	+	13	T1U.3	-0.139560	-3.798	0.000
334	+	18	HG.1	-0.121714	-3.312	0.000
335	+	18	HG.2	-0.121714	-3.312	0.000
336	+	18	HG.3	-0.121714	-3.312	0.000
337	+	18	HG.4	-0.121714	-3.312	0.000
338	+	18	HG.5	-0.121714	-3.312	0.000
339	+	13	GU.1	-0.113385	-3.085	0.000
340	+	13	GU.2	-0.113385	-3.085	0.000
341	+	13	GU.3	-0.113385	-3.085	0.000
342	+	13	GU.4	-0.113385	-3.085	0.000
343	+	13	GG.1	-0.107567	-2.927	0.000
344	+	13	GG.4	-0.107567	-2.927	0.000
345	+	13	GG.2	-0.107567	-2.927	0.000
346	+	13	GG.3	-0.107567	-2.927	0.000
347	+	13	T2U.1	-0.104395	-2.841	0.000
348	+	13	T2U.2	-0.104395	-2.841	0.000
349	+	13	T2U.3	-0.104395	-2.841	0.000
350	+	5	T1G.1	-0.103972	-2.829	0.000
351	+	5	T1G.2	-0.103972	-2.829	0.000
352	+	5	T1G.3	-0.103972	-2.829	0.000
353	+	10	HU.1	-0.050920	-1.386	0.000
354	+	10	HU.4	-0.050920	-1.386	0.000
355	+	10	HU.5	-0.050920	-1.386	0.000
356	+	10	HU.2	-0.050920	-1.386	0.000
357	+	10	HU.3	-0.050920	-1.386	0.000
358	+	5	T2G.1	-0.026431	-0.719	0.000
359	+	5	T2G.2	-0.026431	-0.719	0.000
360	+	5	T2G.3	-0.026431	-0.719	0.000
361	+	14	T2U.1	0.062171	1.692	0.000
362	+	14	T2U.2	0.062171	1.692	0.000
363	+	14	T2U.3	0.062171	1.692	0.000
364	+	9	AG.1	0.075162	2.045	0.000
365	+	19	HG.1	0.090629	2.466	0.000
366	+	19	HG.5	0.090629	2.466	0.000
367	+	19	HG.2	0.090629	2.466	0.000
368	+	19	HG.3	0.090629	2.466	0.000

Table S2. Bonding molecular orbitals of $[As@Ni_{12}@As_{20}]^{3-}$ (I_h symmetry)

403	+	15	AG.1	-0.327085	-8.900	2.000
404	+	20	T1U.1	-0.300467	-8.176	2.000
405	+	20	T1U.3	-0.300467	-8.176	2.000
406	+	20	T1U.2	-0.300467	-8.176	2.000
407	+	23	HG.1	-0.264877	-7.208	2.000
408	+	23	HG.2	-0.264877	-7.208	2.000
409	+	23	HG.3	-0.264877	-7.208	2.000
410	+	23	HG.4	-0.264877	-7.208	2.000
411	+	23	HG.5	-0.264877	-7.208	2.000
412	+	16	AG.1	-0.254350	-6.921	2.000
413	+	13	GU.1	-0.235062	-6.396	2.000
414	+	13	GU.2	-0.235062	-6.396	2.000
415	+	13	GU.3	-0.235062	-6.396	2.000
416	+	13	GU.4	-0.235062	-6.396	2.000
417	+	13	GG.1	-0.179752	-4.891	2.000
418	+	13	GG.2	-0.179752	-4.891	2.000
419	+	13	GG.3	-0.179752	-4.891	2.000
420	+	13	GG.4	-0.179752	-4.891	2.000
421	+	16	T2U.1	-0.176898	-4.814	2.000
422	+	16	T2U.2	-0.176898	-4.814	2.000
423	+	16	T2U.3	-0.176898	-4.814	2.000
424	+	21	T1U.1	-0.047508	-1.293	2.000
425	+	21	T1U.3	-0.047508	-1.293	2.000
426	+	21	T1U.2	-0.047508	-1.293	2.000
427	+	24	HG.1	-0.022716	-0.618	2.000
428	+	24	HG.2	-0.022716	-0.618	2.000
429	+	24	HG.3	-0.022716	-0.618	2.000
430	+	24	HG.4	-0.022716	-0.618	2.000
431	+	24	HG.5	-0.022716	-0.618	2.000
432	+	17	AG.1	-0.014547	-0.396	2.000
433	+	11	HU.1	0.000945	0.026	2.000
434	+	11	HU.4	0.000945	0.026	2.000
435	+	11	HU.2	0.000945	0.026	2.000
436	+	11	HU.3	0.000945	0.026	2.000
437	+	11	HU.5	0.000945	0.026	2.000
438	+	17	T2U.1	0.009444	0.257	2.000
439	+	17	T2U.2	0.009444	0.257	2.000
440	+	17	T2U.3	0.009444	0.257	2.000
441	+	22	T1U.1	0.029891	0.813	2.000
442	+	22	T1U.3	0.029891	0.813	2.000
443	+	22	T1U.2	0.029891	0.813	2.000
444	+	25	HG.1	0.035878	0.976	2.000
445	+	25	HG.2	0.035878	0.976	2.000
446	+	25	HG.3	0.035878	0.976	2.000

447	+	25	HG.4	0.035878	0.976	2.000
448	+	25	HG.5	0.035878	0.976	2.000
449	+	14	GU.1	0.043412	1.181	2.000
450	+	14	GU.3	0.043412	1.181	2.000
451	+	14	GU.2	0.043412	1.181	2.000
452	+	14	GU.4	0.043412	1.181	2.000
453	+	14	GG.1	0.045727	1.244	2.000
454	+	14	GG.2	0.045727	1.244	2.000
455	+	14	GG.3	0.045727	1.244	2.000
456	+	14	GG.4	0.045727	1.244	2.000
457	+	18	T2U.1	0.049796	1.355	2.000
458	+	18	T2U.2	0.049796	1.355	2.000
459	+	18	T2U.3	0.049796	1.355	2.000
460	+	15	GG.1	0.052679	1.433	2.000
461	+	15	GG.2	0.052679	1.433	2.000
462	+	15	GG.3	0.052679	1.433	2.000
463	+	15	GG.4	0.052679	1.433	2.000
464	+	26	HG.1	0.074546	2.028	2.000
465	+	26	HG.2	0.074546	2.028	2.000
466	+	26	HG.3	0.074546	2.028	2.000
467	+	26	HG.4	0.074546	2.028	2.000
468	+	26	HG.5	0.074546	2.028	2.000
469	+	12	HU.1	0.082416	2.243	2.000
470	+	12	HU.4	0.082416	2.243	2.000
471	+	12	HU.2	0.082416	2.243	2.000
472	+	12	HU.3	0.082416	2.243	2.000
473	+	12	HU.5	0.082416	2.243	2.000
474	+	15	GU.1	0.086333	2.349	2.000
475	+	15	GU.4	0.086333	2.349	2.000
476	+	15	GU.2	0.086333	2.349	2.000
477	+	15	GU.3	0.086333	2.349	2.000
478	+	27	HG.1	0.088900	2.419	2.000
479	+	27	HG.2	0.088900	2.419	2.000
480	+	27	HG.3	0.088900	2.419	2.000
481	+	27	HG.4	0.088900	2.419	2.000
482	+	27	HG.5	0.088900	2.419	2.000
483	+	7	T1G.1	0.097029	2.640	2.000
484	+	7	T1G.2	0.097029	2.640	2.000
485	+	7	T1G.3	0.097029	2.640	2.000
486	+	5	T2G.1	0.099113	2.697	2.000
487	+	5	T2G.2	0.099113	2.697	2.000
488	+	5	T2G.3	0.099113	2.697	2.000
489	+	23	T1U.1	0.100012	2.721	2.000
490	+	23	T1U.3	0.100012	2.721	2.000

491	+	23	T1U.2	0.100012	2.721	2.000
492	+	16	GU.1	0.111758	3.041	2.000
493	+	16	GU.2	0.111758	3.041	2.000
494	+	16	GU.4	0.111758	3.041	2.000
495	+	16	GU.3	0.111758	3.041	2.000
496	+	19	T2U.1	0.116231	3.163	2.000
497	+	19	T2U.2	0.116231	3.163	2.000
498	+	19	T2U.3	0.116231	3.163	2.000
499	+	28	HG.1	0.118089	3.213	2.000
500	+	28	HG.2	0.118089	3.213	2.000
501	+	28	HG.3	0.118089	3.213	2.000
502	+	28	HG.4	0.118089	3.213	2.000
503	+	28	HG.5	0.118089	3.213	2.000
504	+	16	GG.1	0.138311	3.764	2.000
505	+	16	GG.2	0.138311	3.764	2.000
506	+	16	GG.3	0.138311	3.764	2.000
507	+	16	GG.4	0.138311	3.764	2.000
508	+	18	AG.1	0.141082	3.839	2.000
509	+	13	HU.1	0.144218	3.924	2.000
510	+	13	HU.2	0.144218	3.924	2.000
511	+	13	HU.3	0.144218	3.924	2.000
512	+	13	HU.4	0.144218	3.924	2.000
513	+	13	HU.5	0.144218	3.924	2.000
514	+	24	T1U.1	0.145880	3.970	2.000
515	+	24	T1U.3	0.145880	3.970	2.000
516	+	24	T1U.2	0.145880	3.970	2.000
517	+	29	HG.1	0.199563	5.430	0.020
518	+	29	HG.5	0.199563	5.430	0.020
519	+	29	HG.2	0.199563	5.430	0.020
520	+	29	HG.3	0.199563	5.430	0.020
521	+	29	HG.4	0.199563	5.430	0.020
522	+	25	T1U.1	0.211887	5.766	0.000
523	+	25	T1U.3	0.211887	5.766	0.000
524	+	25	T1U.2	0.211887	5.766	0.000
525	+	17	GU.1	0.213597	5.812	0.000
526	+	17	GU.2	0.213597	5.812	0.000
527	+	17	GU.3	0.213597	5.812	0.000
528	+	17	GU.4	0.213597	5.812	0.000
529	+	8	T1G.1	0.223074	6.070	0.000
530	+	8	T1G.2	0.223074	6.070	0.000
531	+	8	T1G.3	0.223074	6.070	0.000