

Supplementary information for

On the Existence of Designer Magnetic Superatoms

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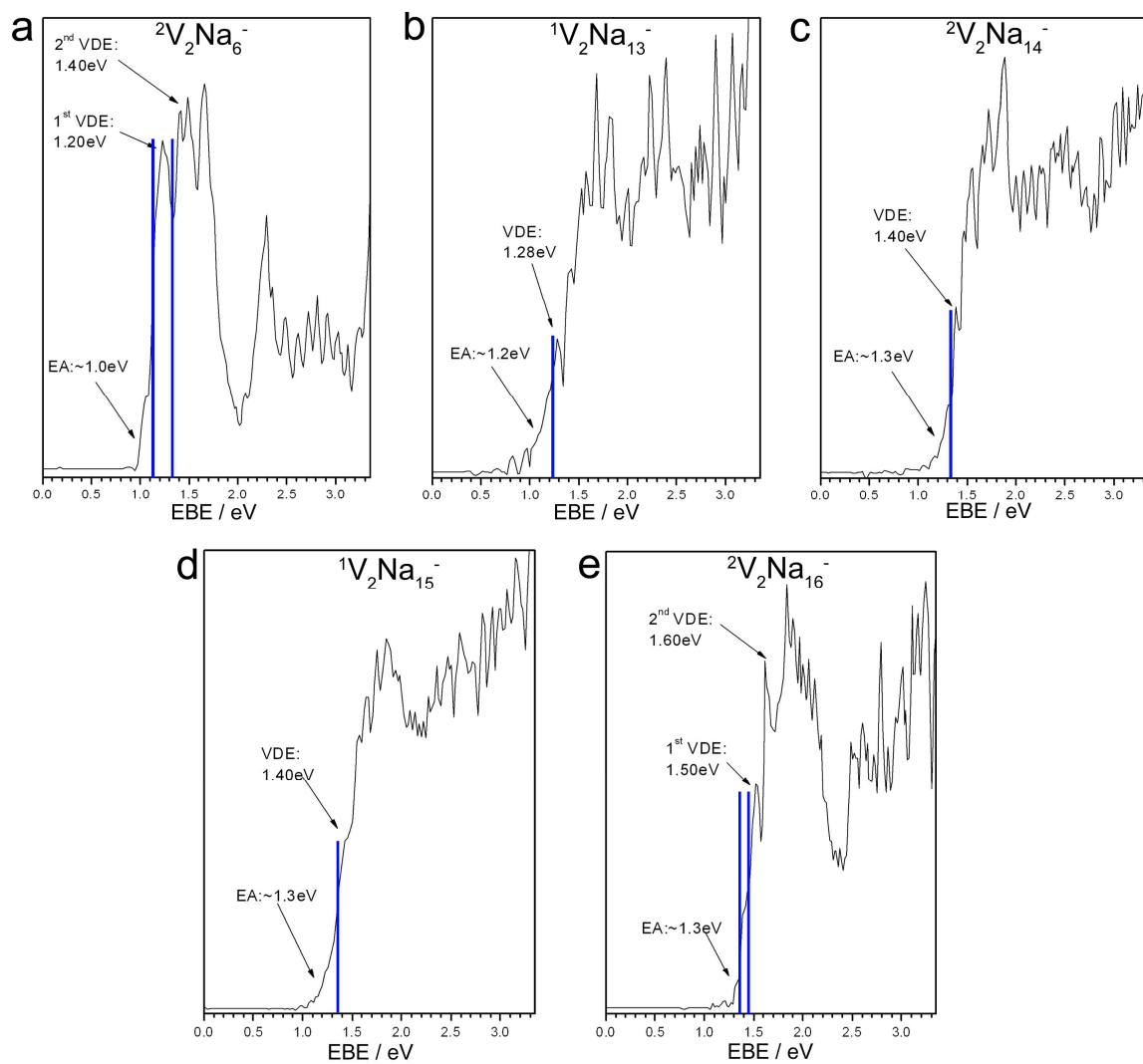


Figure S1. Photoelectron spectra at 355 nm for $V_2Na_x^-$ clusters ($n = 6, 13-16$). The theoretical detachment energies (VDE) are marked with blue lines.

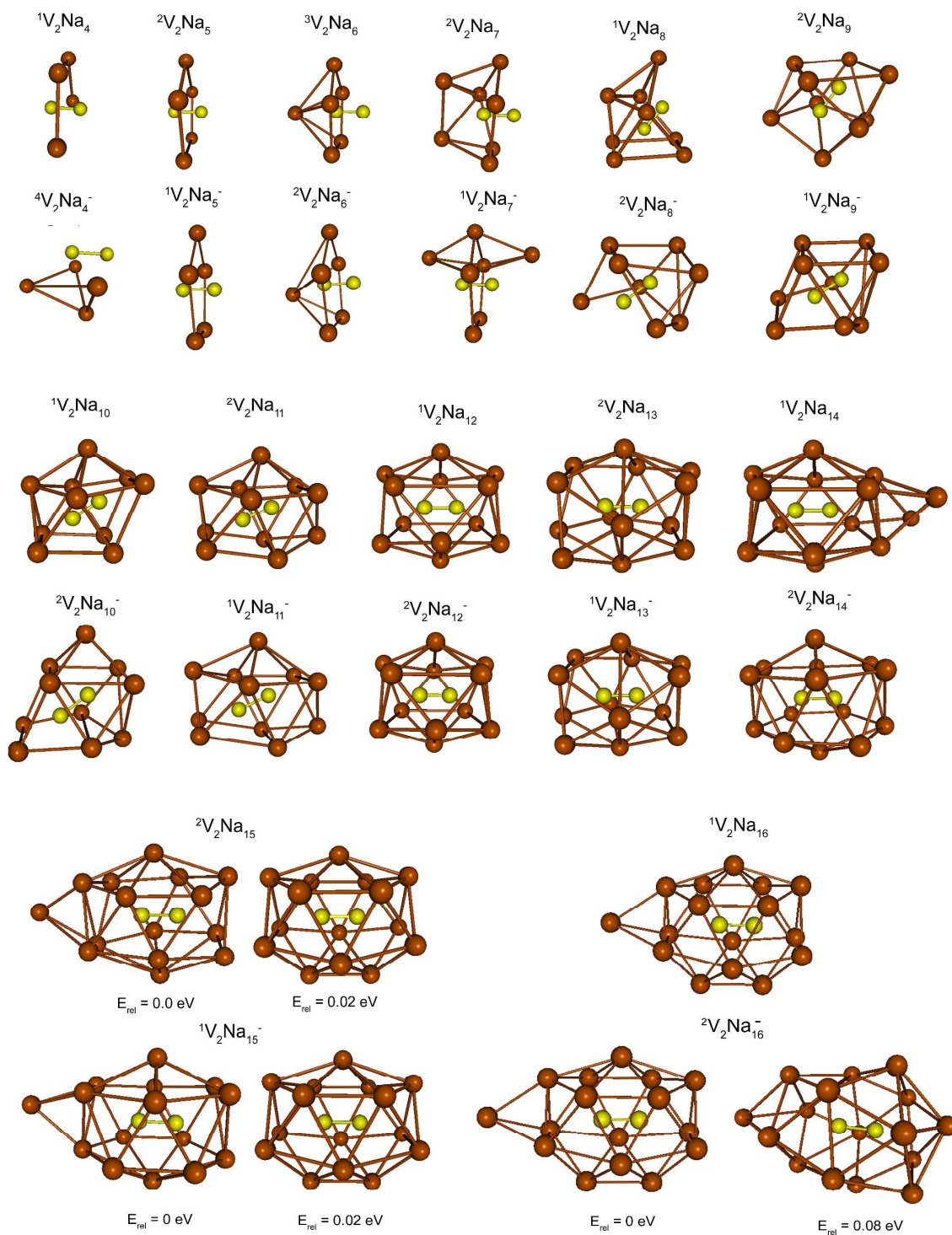


Figure S2. Ground-state geometries of neutral and anionic V_2Na_x ($n=4-16$) clusters The superscripts indicate spin multiplicity. Brown and yellow circles represent sodium and vanadium atoms, respectively.

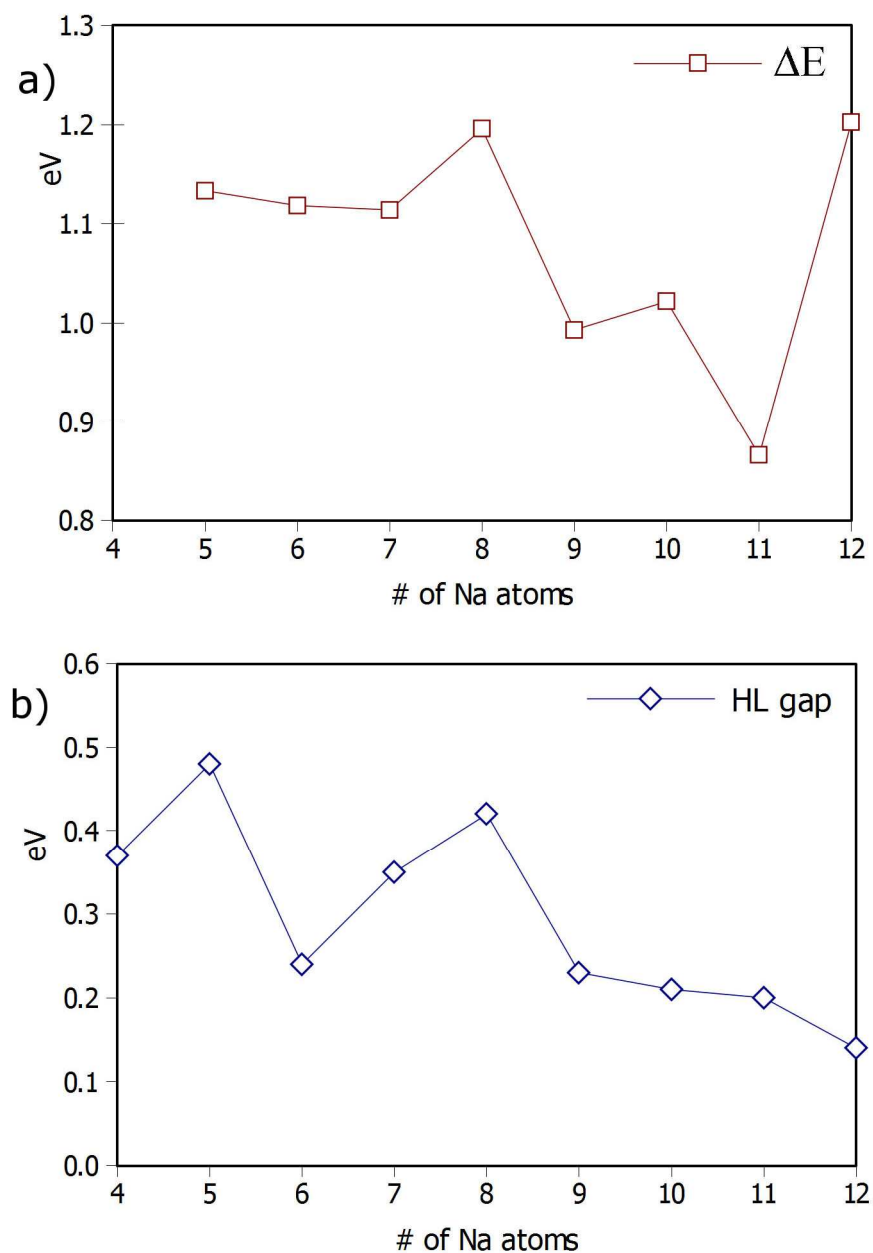


Figure S3. Variation in the energy gain (ΔE) and HOMO-LUMO gap (HL gap) of anionic VNa_n^- clusters with the number of Na atoms.

ADFT optimized neutral and anionic $V_xNa_y^{0/-}$ geometries. Total energies are given in atomic units [h], and the superscripts indicate the spin multiplicity.

6VNa_6				5VNa_7			
Total Energy: -1916.148831				Total Energy: -2078.308861			
V	0.0000	0.0000	0.0000	V	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.1340	Na	0.0000	0.0000	3.0498
Na	2.3785	0.0000	-2.0413	Na	3.0126	0.0000	0.5196
Na	2.5170	1.4663	1.1560	Na	-2.2025	-2.0542	0.5357
Na	-0.2262	-2.3678	-2.0413	Na	-1.9714	-0.0441	-2.3798
Na	-1.6957	-2.3685	1.1572	Na	1.4670	1.2474	-2.4168
Na	2.0044	-2.2051	0.9211	Na	1.1402	-2.8845	1.2062
				Na	0.8597	-2.3328	-2.0429
6VNa_8				7VNa_9			
Total Energy: -2240.478290				Total Energy: -2402.633932			
V	2.6954	-1.4971	4.8267	V	2.0431	1.5564	1.6823
Na	0.0000	0.0000	0.0000	Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	9.6530	Na	0.0000	0.0000	3.5600
Na	7.0379	0.0000	1.4033	Na	3.4972	0.0000	-0.6787
Na	3.7306	-5.9762	1.4112	Na	1.8014	3.1231	-0.9437
Na	3.7236	-5.9790	8.2443	Na	5.0643	2.0857	1.7459
Na	7.0496	-0.0149	8.2389	Na	-0.5768	3.1272	1.9520
Na	2.3618	4.2220	4.8306	Na	2.6721	2.0938	4.6353
Na	-2.3379	-4.2322	4.8258	Na	2.6332	4.6500	2.1605
				Na	3.2977	-1.0470	2.7208
${}^6VNa_{10}$				${}^5VNa_{11}$			
Total Energy: -2564.785549				Total Energy: -2726.936319			
V	1.5744	-2.4240	2.4681	V	0.0000	0.0000	0.0000
Na	0.0000	0.0000	0.0000	Na	0.0000	0.0000	3.0603
Na	0.0000	0.0000	3.5088	Na	2.5610	0.0000	-1.6731
Na	3.1822	0.0000	1.4802	Na	-0.5612	2.0025	-2.3148
Na	3.1184	-1.3362	4.8908	Na	1.3245	2.7048	0.7324
Na	1.8899	-2.9081	-0.5487	Na	1.4771	-2.6906	0.7830
Na	-1.2930	-2.9088	1.4795	Na	-0.3852	-2.0074	-2.2980
Na	1.2905	-5.4495	2.0204	Na	-2.1215	-2.0196	0.9274
Na	4.4558	-3.3912	2.0215	Na	-2.2559	1.9897	0.8056
Na	-0.0463	-3.3911	4.8916	Na	-3.9495	3.3064	-2.1152
Na	3.1486	-4.8464	4.9347	Na	3.2241	0.0772	1.7529
				Na	-3.2386	-0.1392	-1.7639

$^2\text{VNa}_{12}$

Total Energy: -2889.093198

V	1.1382	-2.6343	1.6918
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.4028
Na	3.1325	0.0000	1.4952
Na	2.7057	-2.0822	-1.1882
Na	-0.5751	-3.2008	-1.0841
Na	-2.2295	-2.0560	1.7572
Na	-0.4393	-3.1721	4.5626
Na	2.8475	-2.0559	4.4598
Na	-0.8644	-5.2566	1.8761
Na	2.2754	-5.2563	-0.0283
Na	2.2617	-5.2598	3.3804
Na	4.4992	-3.2005	1.6182

$^7\text{VNa}_6^-$

Total Energy: -1916.183313

V	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.1940
Na	2.5256	0.0000	-1.9600
Na	2.4962	1.5744	1.2194
Na	0.0787	-2.5518	-1.9366
Na	-1.4605	-2.5612	1.2501
Na	2.1039	-2.0161	1.0232

$^5\text{VNa}_6^-$ (isomer)

Total Energy: -1916.182570

V	-0.3760	2.5595	1.9813
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.9634
Na	2.7457	0.0000	1.9999
Na	2.1298	2.9450	3.8192
Na	-2.8265	0.5901	1.9923
Na	2.1447	2.9148	0.1144

$^6\text{VNa}_7^-$

Total Energy: -2078.344275

V	2.1839	1.3873	1.9120
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.7022
Na	3.3254	0.0000	-0.8286
Na	2.5972	-1.7395	2.0692
Na	-0.5591	3.0207	1.9241
Na	1.6740	3.0510	-0.7747
Na	4.8702	2.6435	0.9569

$^7\text{VNa}_8^-$

Total Energy: 2240.508236

V	1.4397	-0.8285	2.5551
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	5.1112
Na	3.7174	0.0000	0.6861
Na	1.9341	-3.2101	0.7239
Na	1.8788	-3.2175	4.4151
Na	3.7538	-0.0622	4.3813
Na	1.3787	2.2394	2.5680
Na	-1.2369	-2.3131	2.5508

$^6\text{VNa}_9^-$

Total Energy: 2402.664756

V	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.1624
Na	2.9140	0.0000	1.1449
Na	-2.3675	-1.8221	0.9858
Na	-2.5586	1.6994	0.3130
Na	2.0127	-0.7318	-2.2861
Na	-0.1594	2.1282	-2.2863
Na	0.9975	-2.9023	0.3498
Na	0.7134	2.8261	1.1542
Na	-1.4984	-1.1521	-2.5381

${}^5\text{VNa}_{10}^-$

Total Energy: 2564.822330

V	1.9524	1.5579	1.7997
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.7135
Na	3.2402	0.0000	-1.3132
Na	2.8225	-1.4390	1.7659
Na	0.6501	3.1191	4.9119
Na	-0.5683	3.3034	1.6169
Na	2.7786	4.4708	2.6270
Na	4.9425	1.8583	1.1214
Na	3.4474	1.0507	4.4309
Na	2.2236	3.2319	-0.8350

${}^4\text{VNa}_{11}^-$

Total Energy: -2726.974178

V	3.1101	-0.5303	2.9823
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.4329
Na	3.4260	0.0000	-0.1254
Na	5.8416	-1.8009	1.9024
Na	1.6409	-2.7742	1.5816
Na	4.2289	-3.7795	4.0103
Na	2.8014	1.5846	5.2313
Na	2.1231	-1.8642	5.6995
Na	5.5026	-0.7647	5.3043
Na	5.3192	1.6138	2.6119
Na	1.8792	2.4001	1.8127

${}^3\text{VNa}_{12}^-$

Total Energy: 2889.138394

V	1.1382	-2.6343	1.6918
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.4028
Na	3.1325	0.0000	1.4952
Na	2.7057	-2.0822	-1.1882
Na	-0.5751	-3.2008	-1.0841
Na	-2.2295	-2.0560	1.7572
Na	-0.4393	-3.1721	4.5626
Na	2.8475	-2.0559	4.4598
Na	-0.8644	-5.2566	1.8761
Na	2.2754	-5.2563	-0.0283
Na	2.2617	-5.2598	3.3804
Na	4.4992	-3.2005	1.6182

${}^1\text{V}_2\text{Na}_4$

Total Energy: 2535.156778

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7523
Na	3.0883	0.0000	0.8416
Na	1.1586	2.8618	0.9493
Na	-2.3280	2.0904	0.9358
Na	1.0451	-2.9461	0.7756

${}^2\text{V}_2\text{Na}_5$

Total Energy: 2697.323918

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7545
Na	3.1041	0.0000	0.9276
Na	-2.6290	-1.6552	0.8219
Na	0.9356	2.9636	0.8818
Na	0.7735	-3.0067	0.8750
Na	-2.4710	1.9025	0.8167

${}^3\text{V}_2\text{Na}_6$

Total Energy: 2859.491640

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7626
Na	3.0054	0.0000	-0.0610
Na	-2.3794	1.8637	0.0579
Na	0.9959	2.8651	0.0926
Na	-0.0388	0.4704	-2.8487
Na	0.9330	-2.8894	0.0646
Na	-2.5044	-1.6921	-0.1126

2V_2Na_7

Total Energy: 3021.660716

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7484
Na	1.8437	0.0000	-2.3515
Na	0.3899	2.9512	-0.0928
Na	1.4192	-2.6433	0.3033
Na	-2.0476	-2.1950	0.3386
Na	-2.6722	1.4099	0.8081
Na	2.9448	0.6668	0.8291
Na	-1.7943	0.3908	-2.3537

1V_2Na_8

Total Energy: 3183.829822

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7413
Na	2.9929	0.0000	1.2670
Na	0.8479	-2.8858	0.5622
Na	0.8774	2.8622	1.2764
Na	-2.5241	1.6464	0.5334
Na	-1.6573	-1.1452	-2.1609
Na	-2.4118	-1.7826	1.4527
Na	-1.6645	1.1468	3.8888
Na	0.5001	-1.9286	3.9161

2V_2Na_9

Total Energy: 3345.984445

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7387
Na	2.9993	0.0000	0.5938
Na	1.9303	0.4821	3.9898
Na	0.8973	2.8653	1.3531
Na	0.9470	1.8249	-2.1201
Na	0.8311	-2.8665	0.7713
Na	-1.7524	-1.0142	-2.2050
Na	-2.5245	-1.6401	1.2091
Na	-2.3895	1.7983	0.2117

$^1V_2Na_{10}$

Total Energy: 3508.144546

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7412
Na	3.0461	0.0000	0.8886
Na	1.8436	0.9396	3.9957
Na	0.7957	2.8671	0.8604
Na	1.8761	0.8953	-2.2365
Na	-1.9582	-0.7033	-2.2365
Na	1.0833	-2.5736	-0.8860
Na	-2.0970	-2.2073	0.8877
Na	-2.6356	1.3862	0.8788
Na	1.0941	-2.5236	2.7624
Na	-1.9763	-0.6654	3.9851

$^2V_2Na_{11}$

Total Energy: 3670.303039

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7549
Na	3.0503	0.0000	1.1205
Na	1.6561	-1.1405	4.0710
Na	0.8863	-2.8465	0.9033
Na	2.0311	-0.7169	-2.1661
Na	-1.1349	-2.2919	-1.8951
Na	-1.9160	0.6217	4.0715
Na	-2.7995	-1.0247	0.9010
Na	-1.8475	2.4222	1.1262
Na	1.2987	2.6273	-0.4855
Na	1.1969	2.4074	3.2496
Na	-1.8085	1.1811	-2.1574

 $^1V_2Na_{12}$

Total Energy: 3832.469133

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7548
Na	3.0338	0.0000	0.8855
Na	1.6054	2.3043	3.1187
Na	1.6759	-1.1774	4.0184
Na	1.0351	-2.8498	0.8866
Na	-1.6107	-2.2995	3.1334
Na	-1.6795	1.1750	4.0211
Na	-1.0418	2.8520	0.8762
Na	-1.6749	1.1826	-2.2674
Na	1.6881	-1.1673	-2.2516
Na	-3.0348	-0.0006	0.8758
Na	-1.6097	-2.2960	-1.3804
Na	1.6156	2.2961	-1.3603

 $^2V_2Na_{13}$

Total Energy: 3994.618427

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7986
Na	3.0208	0.0000	0.8939
Na	0.4047	-2.9844	0.9315
Na	2.3860	-1.8055	3.6560
Na	1.6733	1.6008	3.8574
Na	1.6598	-1.5808	-2.0824
Na	0.3689	2.9871	0.8825
Na	2.3508	1.8416	-1.8348
Na	-1.9137	1.6497	3.5971
Na	-2.7284	-1.5131	1.6322
Na	-2.7412	1.4827	0.1842
Na	-0.8742	1.6532	-2.5441
Na	-1.908946	-1.6742	-1.7831
Na	-0.848638	-1.6702	4.3460

 $^1V_2Na_{14}$

Total Energy: 4156.776125

V	1.8676	0.0000	2.5236
V	1.1090	1.5963	2.5263
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	5.0550
Na	-1.9546	1.4277	2.5181
Na	3.0591	1.4728	0.0110
Na	2.9182	-2.2284	0.5632
Na	5.0035	-0.1419	2.5197
Na	2.4196	-5.1726	2.5238
Na	2.9405	-2.2334	4.4608
Na	3.1346	3.9038	2.5387
Na	0.1364	3.6189	0.4897
Na	0.1267	3.6083	4.5709
Na	0.0066	-2.5268	2.5317
Na	3.0564	1.4665	5.0427
Na	5.5401	-3.6845	2.4959

$^2\text{V}_2\text{Na}_{15}$

Total Energy: 4318.929414

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.8395
Na	3.1045	0.0000	0.9026
Na	-1.5539	-2.6873	0.9649
Na	-1.5521	2.6895	0.9120
Na	1.6006	-2.8009	-0.7086
Na	1.6234	-2.7848	2.5999
Na	-1.0510	-1.7991	-2.5364
Na	-3.2300	-0.0096	-0.6915
Na	-3.2267	0.0146	2.6190
Na	-1.0491	1.7379	-2.5692
Na	1.6045	2.7932	-0.7836
Na	1.6222	2.7956	2.5255
Na	2.0173	-0.0289	-2.5768
Na	-0.9972	-1.7338	4.4374
Na	-0.9944	1.8001	4.4023
Na	2.0623	0.0300	4.4009

 $^2\text{V}_2\text{Na}_{15}$ (isomer)

Total Energy: 4318.928702

V	2.0880	1.4260	2.2330
V	1.6987	2.6632	3.4790
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	4.1461
Na	5.0297	0.0000	1.4690
Na	2.2220	1.9472	6.5769
Na	4.8043	2.3002	4.2219
Na	3.2975	-0.5997	4.4880
Na	2.1276	-1.8121	1.6005
Na	-1.2395	2.4569	2.2261
Na	-0.6040	3.4518	5.3988
Na	3.0007	5.0918	4.9132
Na	3.9015	3.8859	1.4370
Na	0.5145	5.5260	2.6161
Na	3.1188	1.0592	-0.9002
Na	0.9045	3.4261	-0.0401
Na	3.3744	-2.2672	-1.5113

 $^1\text{V}_2\text{Na}_{16}$

Total Energy: 4481.083416

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.8034
Na	3.1179	0.0000	0.6871
Na	-3.2469	0.0181	2.3385
Na	-1.0644	-1.8412	4.1336
Na	1.6290	-2.8015	2.3344
Na	-1.0483	1.8656	4.1273
Na	1.6240	2.8058	2.2926
Na	1.6336	2.8236	-0.9842
Na	-0.9890	1.7004	-2.7751
Na	-3.2611	0.0027	-0.9431
Na	-0.9946	-1.7122	-2.7642
Na	1.6196	-2.8266	-0.9486
Na	1.9758	-0.0125	-2.7829
Na	2.1589	0.0178	4.1269
Na	-1.5524	2.7008	0.6915
Na	-1.5630	-2.7002	0.7062
Na	-0.0167	-0.0040	-5.6885

 $^4\text{V}_2\text{Na}_4^-$

Total Energy: 2535.195514

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7748
Na	2.0859	0.0000	-2.2144
Na	2.9166	-1.1318	0.9484
Na	1.9587	2.3397	0.6195
Na	0.0586	-3.0573	0.7350



Total Energy: 2697.365332

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7338
Na	3.0797	0.0000	0.8941
Na	0.9458	-2.9248	0.8934
Na	-2.4941	-1.7974	0.7992
Na	0.9490	2.9258	0.9081
Na	-2.4805	1.8205	0.8451



Total Energy: 2859.531402

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7488
Na	3.0240	0.0000	0.3926
Na	-2.4823	1.7005	0.4860
Na	0.9654	2.8557	0.6671
Na	-0.2080	1.5636	-2.5016
Na	0.9641	-2.8839	0.5249
Na	-2.4191	-1.8293	0.5748



Total Energy: 3021.701518

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7465
Na	1.8947	0.0000	-2.3083
Na	1.9141	0.3194	4.0120
Na	2.5949	-1.5465	0.9323
Na	2.2134	2.0505	0.7785
Na	-0.6234	-2.9648	0.8503
Na	-1.2369	2.7689	0.9422
Na	-3.0145	-0.3224	0.8893



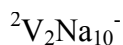
Total Energy: 3183.857578

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7631
Na	1.9877	0.0000	-2.1885
Na	1.9185	-0.7700	4.0367
Na	0.0392	2.9845	0.1492
Na	1.8349	-2.3936	0.7046
Na	-1.7239	-2.4478	0.3603
Na	-2.8599	0.9748	0.7785
Na	2.8713	1.0173	1.0811
Na	-1.8050	0.4129	-2.4218



Total Energy: 3346.017128

V	1.1944	0.0000	-1.2744
V	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.0551
Na	0.2541	-2.9964	-0.6787
Na	-0.5706	2.5725	-1.6666
Na	-2.9837	0.5939	0.2563
Na	4.2319	0.2407	-1.5184
Na	2.0403	2.1945	0.8178
Na	2.6580	-1.2903	1.1936
Na	-1.5418	-0.7194	-2.6812
Na	1.2613	0.7055	-4.2654



Total Energy: 3508.176580

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7608
Na	3.0312	0.0000	0.8488
Na	1.7638	1.1366	4.0602
Na	1.1724	2.8924	1.1266
Na	1.3789	1.7202	-2.1130
Na	-2.0497	2.2125	-0.0546
Na	-1.8365	-1.2228	-2.1043
Na	1.6912	-1.8678	-1.7449
Na	-0.2739	-3.0251	0.8446
Na	-2.9861	-0.9238	1.1230
Na	-1.2844	-1.6470	4.0610



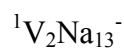
Total Energy: 3670.340223

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7782
Na	2.1268	0.0000	-2.1991
Na	1.9929	-2.2011	0.9046
Na	-0.0662	-2.7757	-1.9130
Na	-2.1191	0.0721	-2.2091
Na	-2.1201	-2.0989	0.9001
Na	1.9781	0.0091	4.1210
Na	-2.0164	0.0713	4.0988
Na	0.0532	2.8976	3.0887
Na	0.0682	2.8643	-0.6344
Na	2.7620	1.3329	1.0450
Na	-2.6833	1.4842	1.0384



Total Energy: 3832.509086

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.7695
Na	2.0555	0.0000	-2.2497
Na	-2.5233	-1.7455	0.8780
Na	-2.5241	1.7521	0.8799
Na	-2.0545	-0.0030	4.0036
Na	-0.0069	-2.8500	3.0843
Na	2.0594	-0.0165	4.0106
Na	0.0036	2.8488	3.0734
Na	2.5225	1.7379	0.8888
Na	0.0100	2.8540	-1.3015
Na	-2.0434	0.0024	-2.2561
Na	-0.0022	-2.8477	-1.3147
Na	2.5141	-1.7578	0.8790



Total Energy: 3994.663899

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.8262
Na	3.0254	0.0000	0.9268
Na	0.3989	-2.9907	0.9827
Na	2.3395	-1.7574	3.7035
Na	1.6537	1.6777	3.8940
Na	1.6620	-1.6994	-2.0449
Na	0.4273	2.9871	0.8447
Na	2.3784	1.7235	-1.8757
Na	-1.9004	1.8011	3.5660
Na	-2.7454	-1.4850	1.6184
Na	-2.7324	1.5079	0.1907
Na	-0.8630	1.5486	-2.5675
Na	-1.8979	-1.7689	-1.7651
Na	-0.9087	-1.5292	4.3804



Total Energy: 4156.823977

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.8143
Na	3.2555	0.0000	0.0465
Na	2.8339	0.3510	3.4424
Na	1.9764	-2.5926	1.7092
Na	-1.3761	-2.7431	0.9266
Na	0.0946	-1.8288	4.4052
Na	-0.0403	1.8148	4.4186
Na	-2.8044	-0.3448	3.4880
Na	1.4129	-2.4446	-1.6736
Na	1.4739	1.0577	-2.6022
Na	-1.5125	-1.0234	-2.5928
Na	-1.4272	2.4740	-1.6289
Na	-1.9528	2.5972	1.7693
Na	1.3691	2.7508	0.9018
Na	-3.2511	0.0167	0.0995

$^1\text{V}_2\text{Na}_{15}^-$

Total Energy: -4318.979049

V	1.3902	2.8562	0.9483
V	1.3477	2.8859	2.7411
Na	0.0000	0.0000	0.0000
Na	0.0000	0.0000	3.4463
Na	2.9232	0.0000	1.7268
Na	-0.3989	2.8158	5.2435
Na	-0.3116	5.6144	3.3790
Na	2.8813	4.7248	4.7945
Na	3.0722	1.2756	4.8426
Na	-1.6906	2.6977	1.7071
Na	2.5962	5.8842	1.6415
Na	4.4526	3.0370	1.7475
Na	2.8352	4.5618	-1.4818
Na	-0.3130	5.5166	-0.0601
Na	2.0631	2.8113	-4.5416
Na	-0.1769	2.7318	-1.9109
Na	3.0315	1.2610	-1.4274

$^1\text{V}_2\text{Na}_{15}^-$ (isomer)

Total Energy: -4318.978236

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.8241
Na	3.1200	0.0000	0.8893
Na	-1.5596	-2.7007	0.9310
Na	-1.5642	2.6980	0.9179
Na	1.5877	-2.7883	-0.7392
Na	1.6155	-2.7921	2.5463
Na	-1.0125	-1.7223	-2.6572
Na	-3.2211	-0.0061	-0.7092
Na	-3.2263	-0.0009	2.5836
Na	-1.0181	1.7195	-2.6540
Na	1.5954	2.7971	-0.7537
Na	1.6114	2.7885	2.5323
Na	1.9702	0.0008	-2.6614
Na	-0.9715	-1.7150	4.4850
Na	-0.9765	1.7241	4.4766
Na	2.0076	0.0054	4.4564

$^2\text{V}_2\text{Na}_{16}^-$

Total Energy: 4481.129816

V	0.0000	0.0000	0.0000
V	0.0000	0.0000	1.8179
Na	3.0868	0.0000	0.8977
Na	-3.2003	0.0082	2.5397
Na	-1.0001	-1.7067	4.4820
Na	1.5953	-2.7758	2.5594
Na	-0.9958	1.7253	4.4818
Na	1.5801	2.7760	2.5333
Na	1.5992	2.7709	-0.7588
Na	-0.9802	1.7029	-2.7052
Na	-3.2023	-0.0046	-0.7619
Na	-0.9875	-1.7320	-2.6915
Na	1.5961	-2.7831	-0.7371
Na	1.9951	-0.0167	-2.6903
Na	1.9820	0.0075	4.4766
Na	-1.5466	2.6783	0.8764
Na	-1.5457	-2.6753	0.8997
Na	0.0094	-0.0224	-5.6912

$^2\text{V}_2\text{Na}_{16}^-$ (isomer)

Total Energy: 4481.126986

V	0.0000	0.0000	0.0000
V	-1.2205	-1.1337	-0.7419
Na	0.0000	0.0000	3.3413
Na	2.9447	0.0000	-1.5188
Na	-2.1835	1.9914	-1.3645
Na	2.1404	-1.9974	1.3091
Na	-2.9977	0.2636	1.4567
Na	-0.0640	0.2200	-3.3410
Na	-4.0219	-0.6048	-2.4605
Na	-4.1566	-2.6500	0.1058
Na	-1.8232	-2.6885	-3.7221
Na	-1.1220	-2.8191	1.8867
Na	1.1554	-2.8323	-1.8476
Na	-1.7169	-4.5293	-1.0200
Na	-4.9087	-4.3070	-2.9358
Na	2.4898	1.5340	1.5253
Na	1.1320	2.8892	-1.3220
Na	-0.6498	2.8913	1.6022