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CHEMISORPTION AND THE PROPERTIES
OF METAL CLUSTERS

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Abstract

In an earlier paper¹ we reported model studies of the chemisorption of atomic hydrogen on the (0001) surface of metallic beryllium. Four distinct sites for chemisorption were considered and the surface was modeled by clusters as large as Be₁₀. In the present paper, this work has been extended in two directions. First, two distinct Be₁₃ clusters have been studied in an analogous manner. Second, the predicted chemisorption characteristics have been correlated with several properties of the isolated metal clusters. Metal cluster properties investigated include the ionization potential, cohesive energy, and singlet-triplet separation. The various sites for chemisorption are compared and electronic structure considerations discussed.

¹ C. W. Bauschlicher, D. H. Liskow, C. F. Bender, and H. F. Schaefer, J. Chem. Phys. 62, 4815 (1975).

Introduction

The critical importance of catalysis in meeting the world's near-term energy needs has created a tremendous surge of interest¹ in surface chemistry.² Until recently, theory has played only a limited role³ in the development of surface chemistry. However during the past five years, quantitative molecular orbital theories have been used to provide considerable insight⁴⁻²⁰ into the properties of small metal clusters and the nature of the chemisorptive bond. Although most of these theoretical studies have employed semi-empirical methods, ab initio techniques have been used in several cases.^{7,9,10,17-19} Among the more important questions addressed theoretically have been (a) the convergence of metal cluster properties to the analogous properties of the infinite metal surface; (b) the nature of and number of surface atoms participating in the chemisorptive bond; and (c) the energetics and structures of various plausible sites (on the surface) for chemisorption.

In our previous work,¹⁸ the chemisorption of atomic hydrogen on the (0001) surface² of Be metal was studied. The surface was modeled by metal clusters Be_n ($n = 1-10$) and four different sites for chemisorption considered. The choice of the $\text{Be}_n\text{-H}$ system was discussed in detail in the earlier paper, where we pointed out that the single-configuration Hartree-Fock approximation is particularly appropriate for this system. Although the H-(Be surface) system has not been investigated experimentally (the toxicity of beryllium is one obvious inhibiting factor), such studies are feasible²¹ and should be forthcoming.

LEED experiments²² have already been reported for the (0001) surface of beryllium and show that the surface is not reconstructed--i.e., the surface atoms maintain the approximate positions given by the crystal structure of the metal. In addition the Auger electron spectra of Be surfaces have been reported recently.²³ Thus we remain optimistic that the beryllium surfaces will in the near future become the crucial link between experiment and rigorous theoretical methods.

In the present paper, our earlier work is extended in two directions. To begin, two thirteen atom Be clusters have been studied. These larger clusters allow an adequate number of surface atoms (10) to be supplemented by a modest number (3) of second-layer atoms. Since the previous study suggested that Be_{10} is nearly adequate in size to model the (0001) surface, the Be_{13} results provide a test of this hypothesis. Secondly the predicted chemisorption characteristics have been correlated with several properties of the isolated metal clusters. Metal cluster properties investigated include the ionization potential, cohesive energy (dissociation energy per atom), and the separation between the lowest singlet and triplet electronic states of each cluster.

Details of the Calculations

The two Be_{13} clusters chosen for investigation are shown in Figures 1 and 2. The first has C_s symmetry and is referred to as Cluster A. This cluster possesses at least 3 sites of interest:¹⁸ an eclipsed site (above atom 7), a bond midpoint (between the two equivalent atoms 4) and an open site (above the center of the triangle formed by atoms 4 (two of these) and 6). The second cluster (cluster B) also has 10 Be atoms in the first layer and 3 in the lower, but the lower layer is positioned to give the cluster no symmetry. This cluster has both an eclipsed site (above atom 11) and a directly overhead site (over atom 7) suitable for study. In the notation adopted earlier,¹⁸ both clusters A and B are labeled $\text{Be}(10,3)$, indicating the presence of 10 surface atoms and 3 second-layer atoms.

As in the earlier work, the structure of the present two Be_{13} clusters is based on the known²⁴ crystal structure of Be metal: $a = 2.2866 \text{ \AA}$, $c = 3.5833 \text{ \AA}$. a is the nearest neighbor distance within a layer, while c implies a nearest neighbor distance between adjacent layers of $2.2255 \text{ \AA}$. As before, only sites on the face of highest symmetry (0001) were considered.

One of the most important technical conclusions of the earlier paper was that for clusters as large as Be_5 , self-consistent-field (SCF) wave functions using a minimum basis set yield predictions which are qualitatively very similar to those obtained with a much larger basis set. In the interim, calculations involving the large

basis set (which is of near-Hartree-Fock quality²⁵) have been completed²⁶ for clusters as large as Be_{10} . Fortunately these more extensive calculations on the large clusters are in good qualitative agreement with the analogous minimum basis set predictions. Thus we can be reasonably confident in $\text{Be}_n\text{-H}$ predictions made at the minimum basis level of SCF theory.

Actually, one refinement was made in the minimum basis set used earlier. Specifically the Slater function orbital exponent $\zeta(2s) = \zeta(2p) = 1.00$ was optimized for Be_{13} cluster A. Following Hehre, Stewart, and Pople,²⁷ each Slater function was expanded as a linear combination of three gaussians. For Be_{13} cluster A, this optimized STO-3G basis set yields a total energy 0.0630 hartrees lower than the previously adopted minimum basis, which had $\zeta(2s) = 0.956$ and $\zeta(2p) = 0.890$.

To obtain ionization potentials and singlet-triplet splittings, numerous additional calculations on the earlier studied smaller clusters were required. Spatially unrestricted¹⁸ single configuration wave functions were calculated for the various Be_n^+ , Be_n , and $\text{Be}_n\text{-H}$ systems. Our previous experience suggested that this provides somewhat more realistic results than those obtained requiring each molecular orbital to transform according to a pre-determined irreducible representation. For the $\text{Be}_{13}\text{-H}$ systems, of course, there is little conflict since at most a single plane of symmetry exists. All calculations are of the spin-restricted type; that is, each wave function is of pure singlet, doublet (positive ions Be_n^+), or triplet character.

Results and Discussion of Cluster Properties

The results for the chemisorption of hydrogen on Be_{13} clusters are summarized in Table I. Perhaps the most striking result is the similarity between the two eclipsed sites, with chemisorptive bond energies 57.2 kcal/mole (cluster A) and 58.3 kcal/mole (cluster B). This is particularly encouraging, since the repositioning of one atom (not directly involved in the bonding) should not effect the adsorption energy as the finite cluster becomes a realistic model for the surface. Hence, on this basis, our 13 atom clusters appear to be reasonable models for the study of chemisorption.

In Table II are given the predicted ionization potential, singlet-triplet separation, cohesive energy, and chemisorbed bond energy for each cluster studied to date. Our goal is to try to use these data to understand why certain clusters serve as better models for chemisorption studies than others.

In general, the ionization potential becomes smaller as a function of n in Be_n . As $n \rightarrow \infty$ the predicted cluster ionization potential should approach that of the (0001) surface of Be. The latter quantity in turn should be comparable to the beryllium metal work function, for which the two most reliable measurements are 3.92 eV²⁸ and 3.22 eV²⁹. Thus it is clear that the cluster ionization potentials approach the infinite surface result from above. Further, it is generally true that the chemisorptive bond energies show an increase with cluster size. Hence, we may conclude that a decrease

in ionization potential is usually associated with an increase in the strength with which the H atom is bound.

Similarly, the cluster cohesive energies are seen to increase with cluster size. The largest cohesive energy, 14.2 kcal/mole, occurs for Be₁₃ cluster A. Hence an increase in cohesive energy is often associated with increasing chemisorptive bond energy. In general, the singlet-triplet separation is small, of the order of 1 eV, which is not surprising in light of the low-lying but unoccupied 2p orbital of the Be atom. The triplet electronic state usually lies the lower but this situation is reversed in seven cases. Unfortunately we have been unable to find a simple correlation between singlet-triplet separation and chemisorption.

The two available signs of a good model cluster Be_n for chemisorption are then (a) relatively low ionization potential and (b) relatively high cohesive energy. These guidelines can be used to rationalize some of the seemingly erratic chemisorption behavior reported in our earlier paper.¹⁸ For example, the Be₄(4,0) cluster yielded a bond midpoint adsorption energy of 70.1 kcal/mole, much greater than the other models studied. Table II shows clearly that this may be viewed as the result of the predicted negative cohesive energy (-9.8 kcal/mole) for this Be₄ cluster. That is, this particular Be₄ cluster is so unstable that it "views" the approaching H atom as a means of partially relieving its "discomfort". The same analysis can be used to rationalize the large chemisorbed bond energy associated with the Be₇(7,0) directly overhead site. In an analogous manner, the relatively small chemisorbed bond energies of the Be₄(3,1) and Be₃(3,0) clusters may be identified with their large predicted ionization potentials.

A final remark worth making is that we expect the theoretical description of chemisorption to converge much more rapidly as a function of cluster size than any of the three other properties discussed above. This expectation is based on the fact that chemisorption involves only differences between the cluster plus atom at infinite separation and the bound cluster-atom. Thus a relatively poor description of the surface may be allowable as long as it is consistent between the two appropriate end points.

Conclusions Concerning the Different Sites for Chemisorption

Given the present chemisorption predictions and those reported earlier, a qualitative discussion of the bonding by site may be attempted.

Directly overhead site. One of the most inconclusive aspects of our earlier study was the vast difference between the $\text{Be}_7(7,0)$ result (71 kcal/mole chemisorbed bond energy) and the $\text{Be}_{10}(7,3)$ result (27 kcal/mole). There we concluded that the Be_7 result might be unreliable due to relative instability (small dissociation energy with respect to 7 Be atoms) of this cluster. The present cluster B result of 31.1 kcal/mole confirms the earlier conclusions and suggests that the directly overhead site is less favorable for chemisorption than the other three sites considered. The bond distance for this site is $\sim 1.4 \text{ \AA}$ regardless of model and can be considered a converged result representative of reality.

Eclipsed site. This appears to be the most favorable site for chemisorption of hydrogen, with the bond energy approaching 60 kcal/mole, a value characteristic of transition metal surface-hydrogen bonds.³ We note, however, that larger clusters must be studied to pin this prediction down, and in addition basis set and correlation effects²⁵ should be given careful consideration. Note that the H-surface bond distances ($0.90 \text{ \AA}$ and $0.94 \text{ \AA}$) are significantly shorter ($\sim 0.2 \text{ \AA}$) than those predicted for this site from smaller clusters. However, these short distances do correlate with the chemist's intuition³⁰ that the shortest bonds are strongest.

Bond midpoint site. Note that the agreement between the $\text{Be}_{10}(10,0)$ and Be_{13} cluster A results for this site is excellent. Thus it would appear that this site is less favorable than the eclipsed site, and that a value of 45 kcal/mole may be close to the limiting value for the theoretical approach adopted here. Note that the H-surface distance r_e decreases from 1.17 Å for Be_{10} to 0.99 Å in the present Be_{13} model.

Open site. The chemisorbed bond energy reported here, 39 kcal/mole, is significantly less than the value 50 kcal/mole found for the largest cluster considered previously $\text{Be}_9(6,3)$. However, as discussed earlier,¹⁸ that result was strongly dependent on the use of C_{3v} symmetry in the computations. Here, by using clusters of inherently lower symmetry, we have sidestepped that problem. It is worth noting that the present results for both bond energy and geometry ($r_e = 0.99$ Å) are much closer to the full C_{3v} results obtained earlier. Although the open site appears less favorable than the bond midpoint, additional studies are required to confirm this hypothesis.

Electronic Structure Considerations

For the most part the qualitative features of the Be_{13} and Be_{13}H electronic structures are consistent with the earlier results¹⁸ for smaller systems.

For both Be_{13} clusters the highest few occupied orbitals become fairly closely spaced, these levels of course becoming continuous for the infinite cluster. As discussed earlier the singly-occupied Be_{13}H orbital is primarily of Be 2p character. The effect of the H atom is to lower the other valence orbitals of Be_{13}H relative to the Be_{13} results.

Turning to the Mulliken populations (Tables III and IV), it is of interest to compare the two Be_{13} clusters with the previously discussed planar Be_{10} cluster. While the degree of charge separation in cluster B is comparable to that predicted for Be_{10} (largest Be atom population 4.05), that for cluster A is significantly greater. For example Be atom 3 in cluster A has a population of 4.16. The difference between the two Be_{13} clusters may be related to the higher symmetry of cluster A. Our general feeling is that clusters of lower symmetry appear to yield somewhat more realistic results.

Note of course that much of the symmetry present in Be_{10} (D_{2h}) disappears in cluster A. For example, while atoms 2 and 5 are equivalent in Be_{10} , #5 has an atomic population 0.08 greater in cluster A. Similarly for cluster A, Be #3 has 0.09 more "electrons" than Be #6. Unfortunately, there appears

to be no readily visible correlation between these population changes and the positions of the three new atoms in the second layer of cluster A.

Much more subject to oscillation (as a function of position within a cluster) is 2s/2p population ratio of the different Be atoms. For example atom #4 in cluster A has a 2p population of 1.46, while its 2s population is only 0.57. This corresponds to a "hybridization" of $sp^{2.56}$, a reasonable result for a carbon atom, but a bit surprising for beryllium. On the other extreme, #2 (an edge atom) has 2s and 2p populations of 0.98 and 0.94, yielding a nearly sp hybridization. In general, we find that surface Be atoms above a second layer have larger 2p populations. Clearly one must go to a significantly larger cluster to approach the uniformity of an infinite perfectly-ordered surface.

Now turn to the effect on the Mulliken populations of bringing up the H atom. First, the hydrogen population remains close to unity, allowing us to conclude, as before,¹ that the chemisorbed bond is covalent in nature. The largest deviation from unity occurs for the directly overhead site, where the H atom population is 0.94. Note that this indicates a somewhat greater tendency toward covalency than was the case (H population 0.89) for the largest previous example [$Be_{10}(7,3)$] of the directly overhead site.

On qualitative grounds¹³ one expects Be_nH to be ionic $Be_n^+H^-$ since the hydrogen 1s orbital lies so much lower than the Be 2s and 2p orbitals. In fact, Hush³¹ has quite reasonably suggested

that a more ionic picture of the bonding might be obtained if functions capable of describing H^- were added to the basis set. For Be_4H , (3,1) we have ~~done this~~ by adding a diffuse s function ($\alpha = 0.048173$) to the hydrogen basis. However the H atom population found for the eclipsed site is 1.27, a result identical to that found in our earlier calculation. This test certainly adds weight to our conclusion that the chemisorptive bond under study here is covalent.

One prominent effect of chemisorption is an increase in the 2p populations of the Be atoms near the approaching hydrogen. As an example consider atom #4 in cluster A. For the free cluster, the open site, the eclipsed site, and the bond midpoint site, Be 2p populations of 1.46, 1.56, 1.52, and 1.60 are found. Note that the greatest enhancement (0.16) occurs for the bond midpoint site, which is closest to atom #4. This correlation between 2p population increase and nearness of the chemisorbed atom is demonstrated even more dramatically by the Be #6 population (2p increased by 0.20 electrons) for the open site. Note that this effect is usually in part compensated for by a decrease in the Be 2s population of the same atom. For example, in the case just cited the 2s population decreases by 0.13 electrons during open site chemisorption.

In our earlier study it was noted that for the directly overhead site, there is a large increase in the total atomic population for the Be atom being approached directly. Specifically for Be_{10} (7,3) an increase of 0.39 "electrons" was seen.

In the present cluster B, atom #7 increases by 0.35 in population as the hydrogen comes to within 1.41 Å. Further inspection of Table IV shows that this change is entirely due to the 2p population, which increases by 0.37.

Finally, it seems worthwhile to indicate for at least one case, "where" the H atom population resides in the electronic structure of Be_nH . For this purpose consider cluster B, the directly overhead site. The largest share, a full 54%, of the H atom population, goes to the 17a orbital ($\epsilon = -0.458$ hartree). Next is the 20a orbital ($\epsilon = -0.311$), with a 15% contribution. This is followed in importance (9%) by the 14a orbital ($\epsilon = -0.638$), which is the lowest lying valence orbital. The only other contribution in excess of 2% is the 5% contribution of the 24a orbital ($\epsilon = -0.228$). Thus we see that while the hydrogen 1s population is dominated by the 17a orbital, the remainder is spread out into several other valence orbitals.

Acknowledgments

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TABLE I. Summary of $\text{Be}_{13}\text{-H}$ Results. Distances r_e from H atom to metal surface are given in Å, and bond energies are in kcal/mole.

Site	Cluster	r_e	Chemisorbed Bond Energy
Eclipsed	A	0.90	57.2
Bond midpoint	A	1.05	44.8
Open	A	0.99	39.0
Eclipsed	B	0.94	58.3
Directly overhead	B	1.41	31.1

TABLE II. Predicted properties of several beryllium clusters and the corresponding $\text{Be}_n\text{-H}$ chemisorbed systems. Results in parentheses were obtained using the large basis set of Reference 1.

Site	Description	Ionization Potential (eV)		Singlet-Triplet Separation (eV)		Cohesive Energy (kcal/mole)		Chemisorbed Bond Energy (kcal/mole)
Directly Overhead	Be	8.44	(8.04)	1.78	(2.02)	--	(--)	46.4 (44.5)
	$\text{Be}_7(7,0)$	5.21	(5.07)	-0.73	(-0.54)	3.64	(5.69)	71.3 (62.4)
	$\text{Be}_{10}(7,3)$	6.05		0.04		8.98		27.3
	$\text{Be}_{13}(10,3)\text{B}$	4.70		-0.62		14.03		31.1
Eclipsed	$\text{Be}_4(3,1)$	7.18	(6.68)	1.15	(1.08)	4.07	(4.84)	28.7 (33.0)
	$\text{Be}_5(4,1)$	5.73	(5.11)	-0.68	(-0.40)	0.23	(1.62)	30.1 (36.4)
	$\text{Be}_7(6,1)$	5.58		-0.24		1.49		40.8
	$\text{Be}_{13}(10,3)\text{A}$	4.32		-0.62		14.15		57.2
	$\text{Be}_{13}(10,3)\text{B}$	4.70		-0.62		14.03		58.3
Bond Midpoint	$\text{Be}_4(4,0)$	5.13	(4.94)	-1.18	(-0.79)	-9.78	(-6.69)	70.1 (65.4)
	$\text{Be}_5(4,1)$	5.73	(5.11)	-0.68	(-0.40)	0.23	(1.62)	32.4 (38.1)
	$\text{Be}_{10}(10,0)$	5.17		+0.02		8.94		45.3
	$\text{Be}_{13}(10,3)\text{A}$	4.32		-0.62		14.15		44.8
Open	$\text{Be}_3(3,0)$	6.97	(6.47)	0.73	(0.98)	-5.03	(-3.24)	19.1 (22.0)
	$\text{Be}_5(4,1)$	5.73	(5.11)	-0.68	(-0.40)	0.23	(1.62)	23.2 (31.9)
	$\text{Be}_6(6,0)$	5.58		-0.24		-1.53		47.3
	$\text{Be}_6(3,3)$	5.30		-0.43		1.81		55.3
	$\text{Be}_9(6,3)$	4.81		-1.56		3.53		50.2
	$\text{Be}_{13}(10,3)\text{A}$	4.32		-0.62		14.15		39.0

TABLE III. Comparison of Be₁₃(10,3) Cluster A (see Figure 1) with three different chemisorbed species Be₁₃H.
 Energies are given in hartrees (1 hartree = 627.5 kcal/mole) and bond distances r_e in bohrs (1 bohr = 0.5292 Å).

	Be ₁₃ + H		Open Site		Eclipsed Site		Bond Midpoint Site	
Total Energy	-187.8713		-187.9334		-187.9624		-187.9427	
Relative Energy	0.0000		- 0.0621		- 0.0911		- 0.0714	
r _e	---		1.868		1.708		1.981	
Valence	9a'	-0.615	9a'	-0.662	9a'	-0.659	9a'	-0.652
Orbital	6a''	-0.502	6a''	-0.512	10a''	-0.544	10a''	-0.512
Energies	10a'	-0.477	10a'	-0.492	6a''	-0.507	6a''	-0.508
	11a''	-0.415	11a''	-0.477	11a''	-0.425	11a''	-0.455
	7a''	-0.390	12a''	-0.422	12a''	-0.419	12a''	-0.421
	12a''	-0.349	7a''	-0.394	7a''	-0.392	7a''	-0.393
	13a''	-0.289	13a''	-0.306	13a''	-0.299	13a''	-0.309
	8a''	-0.285	8a''	-0.291	8a''	-0.288	8a''	-0.289
	14a''	-0.265	14a''	-0.284	14a''	-0.283	14a''	-0.283
	9a''	-0.227	9a''	-0.232	15a''	-0.259	15a''	-0.244
	10a''	-0.216	13a''	-0.231	9a''	-0.228	9a''	-0.230
	15a''	-0.208	10a''	-0.218	10a''	-0.218	10a''	-0.218
	16a''	-0.182	16a''	-0.192	16a''	-0.198	16a''	-0.187
	1s _H	-0.484	17a''	-0.215	17a''	-0.208	17a''	-0.218
Populations								
Be #1	s	2.93		2.96		2.94		2.97
	p	1.04		1.01		1.02		1.00
	Total	3.97		3.97		3.96		3.97
Be #2	s	2.94		2.96		2.95		2.95
	p	0.98		0.97		0.97		0.99
	Total	3.92		3.93		3.92		3.94
Be #3	s	2.80		2.80		2.79		2.80
	p	1.36		1.32		1.36		1.27
	Total	4.16		4.12		4.15		4.07
Be #4	s	2.57		2.50		2.51		2.49
	p	1.46		1.56		1.52		1.60
	Total	4.03		4.06		4.03		4.09
Be #5	s	2.88		2.96		2.88		2.92
	p	1.13		1.04		1.13		1.09
	Total	4.01		4.00		4.01		4.01
Be #6	s	2.78		2.65		2.71		2.69
	p	1.29		1.49		1.40		1.40
	Total	4.07		4.14		4.11		4.09
Be #7	s	2.79		2.78		2.76		2.73
	p	1.11		1.08		1.13		1.15
	Total	3.90		3.86		3.89		3.88
Be #8	s	2.84		2.79		2.90		2.86
	p	1.16		1.18		1.08		1.13
	Total	4.00		3.97		3.98		3.99
Hydrogen	s	1.00		1.00		1.02		0.95

TABLE IV. Comparison of Be₁₃(10,3) Cluster B (see Figure 2) with two models for Be₁₃H. All entries are given in atomic units.

	Be ₁₃ + H	Directly Overhead Site	Eclipsed Site
Total Energy	-187.8688	-187.9183	-187.9617
Relative Energy	0.0000	- 0.0495	- 0.0929
r _e	---	2.66	1.77
Valence	14a -0.621	-0.638	-0.662
Orbital	15a -0.508	-0.515	-0.553
Energies	16a -0.477	-0.483	-0.496
	17a -0.426	-0.458	-0.455
	18a -0.381	-0.427	-0.418
	19a -0.374	-0.391	-0.391
	20a -0.282	-0.311	-0.312
	21a -0.272	-0.291	-0.287
	22a -0.260	-0.276	-0.273
	23a -0.240	-0.251	-0.263
	24a -0.214	-0.228	-0.241
	25a -0.204	-0.217	-0.211
	26a -0.193	-0.198	-0.200
	1s _H -0.484	27a -0.221	27a -0.228
Populations			
Be #1	s 2.97	2.96	2.97
	p 1.02	1.02	1.00
	Total 3.99	3.98	3.97
Be #2	s 2.92	2.92	2.91
	p 1.02	1.01	1.01
	Total 3.94	3.93	3.92
Be #3	s 2.81	2.80	2.79
	p 1.22	1.19	1.24
	Total 4.03	3.99	4.03
Be #4	s 2.61	2.58	2.55
	p 1.39	1.38	1.45
	Total 4.00	3.96	4.00
Be #5	s 2.95	2.89	2.97
	p 1.02	1.04	0.97
	Total 3.97	3.93	3.94
Be #6	s 2.78	2.82	2.75
	p 1.27	1.19	1.33
	Total 4.05	4.01	4.08
Be #7	s 2.68	2.66	2.63
	p 1.31	1.68	1.43
	Total 3.99	4.34	4.06
Be #8	s 2.89	2.98	2.94
	p 1.10	0.97	1.06
	Total 3.99	3.95	4.00
Be #9	s 2.83	2.92	2.92
	p 1.16	1.05	1.07
	Total 3.99	3.98	3.99
Be #10	s 2.88	2.91	2.97
	p 1.09	1.02	1.02
	Total 3.97	3.93	3.99
Be #11	s 3.00	3.04	2.97
	p 1.06	0.98	1.06
	Total 4.06	4.02	4.03
Be #12	s 2.82	2.86	2.73
	p 1.17	1.13	1.22
	Total 3.99	3.99	3.95
Be #13	s 2.92	2.91	2.90
	p 1.13	1.12	1.14
	Total 4.05	4.03	4.04
Hydrogen	s 1.0	0.94	1.01

FIGURE CAPTIONS

Figure 1. Picture of Cluster A, thirteen atom model for the (0001) face of metallic beryllium. Atoms are numbered to aid in visualization of the Mulliken populations.

Figure 2. The second thirteen atom model, Cluster B, for the (0001) face of beryllium.

XBB 757-5390A

Fig. 1

XBB 757-5391A

Fig. 2

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