



Reference:N:\hobbies\WINMCAD\AA-Default.mcd

a_{sub_0} is the Bohr radius.

p is the shrinkage level.

$$a(p) := \frac{a_0}{p} \cdot \left(1 + \sqrt{\frac{3}{4}} \right) \quad \text{Hydrinohydride radius according to Mills}$$

$$s(p) := 2 \cdot a(p) \quad \text{Length of the side of a regular tetrahedron comprising 4 Hydrinohydride ions}$$

$$R_{\text{Li1}} := \frac{a_0}{3} \cdot \left(1 + \sqrt{\frac{3}{4}} \right) \quad \text{Radius of Li+ (2 electrons around a central charge of 3)}$$

$$R_{\text{Li2}} := \frac{a_0}{3} \quad \text{Radius of Li++ (1 electron around a central charge of 3)}$$

ce is the charge of an electron

$$\text{HH}(p) := \frac{ce^2}{4 \cdot \pi \cdot \epsilon \cdot s(p)} \quad \text{Repulsion between a pair of Hydrinohydride ions}$$

$$\text{HLi}(p) := \frac{3 \cdot ce^2}{4 \cdot \pi \cdot \epsilon \cdot \sqrt{\frac{3}{8}} \cdot s(p)} \quad \text{Attraction between each Hydrinohydride ion & Li+++ ion at the core of the tetrahedron.}$$

$p := 1..24$ p takes values from 1 to 24 for Hydrinohydride

$$E1(p) := \frac{ce^2}{4 \cdot \pi \cdot \epsilon \cdot (a(p) + R_{\text{Li1}})} \quad \text{1 Hy- and Li+ ion side by side}$$

$$E2(p) := \frac{4 \cdot ce^2}{4 \cdot \pi \cdot \epsilon \cdot (a(p) + R_{\text{Li2}})} - \frac{ce^2}{4 \cdot \pi \cdot \epsilon \cdot (s(p) + 2 \cdot R_{\text{Li2}})} \quad \text{2 Hy- ions on opposite sides of Li+++}$$

$$E3(p) := 9 \cdot \frac{ce^2}{4 \cdot \pi \cdot \epsilon \cdot \frac{s(p)}{\sqrt{3}}} - 3 \cdot \text{HH}(p) \quad \text{3 Hy- in an equilateral triangle with Li+++ at the center}$$

$$E4(p) := 4 \cdot \text{HLi}(p) - 6 \cdot \text{HH}(p) \quad \text{4 Hy- in a tetrahedron with Li+++ at the center}$$

$$I_{p,0} := E1(p) - 520.2 \cdot \frac{\text{kJ}}{\text{mole}} \quad \text{Reaction energy for addition of 1st Hy- to Li}$$

$$I_{p,1} := E2(p) - E1(p) - 7298.1 \cdot \frac{\text{kJ}}{\text{mole}} \quad \text{Reaction energy for addition of 2nd Hy- to LiHy}$$

$$I_{p,2} := E3(p) - E2(p) - 11815 \cdot \frac{\text{kJ}}{\text{mole}} \quad \text{Reaction energy for addition of 3rd Hy- to LiHy2}$$

$$I_{p,3} := E4(p) - E3(p) \quad \text{Reaction energy for addition of 4th Hy- to LiHy3}$$

$$I_{p,4} := I_{p,0} + I_{p,1} + I_{p,2} + I_{p,3} \quad \text{Total reaction energy for formation of LiHy4-}$$

Column 0 is net energy released when first Hy- is added.
 Column 1 when second Hy- is added.
 Column 2 when third Hy- is added.
 Column 3 when the fourth Hy- is added.
 Column 4 is the total for all 4 Hy-.
 The row numbers are the "p" values.

With removal of each electron, the effective central charge increases which also increases the binding force on the existing Hy- ions.

	0	1	2	3	4
0	0	0	0	0	0
1	5.545	-43.273	-73.972	7.346	-104.353
2	12.108	-17.93	-14.091	14.691	-5.222
3	16.482	2.179	53.212	22.037	93.909
4	19.607	18.435	125.616	29.383	193.041
5	21.951	31.816	201.677	36.728	292.172
6	23.774	43.006	280.45	44.074	391.304
7	25.232	52.494	361.289	51.42	490.435
8	26.425	60.638	443.738	58.765	589.567
9	27.419	67.701	527.467	66.111	688.698
10	28.261	73.885	612.228	73.457	787.83
11	28.982	79.341	697.836	80.802	886.961
12	29.607	84.192	784.146	88.148	986.093
I = 13	30.153	88.533	871.045	95.494	$1.085 \cdot 10^3$
14	30.636	92.438	958.442	102.839	$1.184 \cdot 10^3$
15	31.065	95.972	$1.046 \cdot 10^3$	110.185	$1.283 \cdot 10^3$
16	31.449	99.183	$1.134 \cdot 10^3$	117.531	$1.383 \cdot 10^3$
17	31.794	102.115	$1.223 \cdot 10^3$	124.876	$1.482 \cdot 10^3$
18	32.106	104.802	$1.312 \cdot 10^3$	132.222	$1.581 \cdot 10^3$
19	32.391	107.273	$1.401 \cdot 10^3$	139.568	$1.68 \cdot 10^3$
20	32.65	109.554	$1.49 \cdot 10^3$	146.913	$1.779 \cdot 10^3$
21	32.888	111.666	$1.579 \cdot 10^3$	154.259	$1.878 \cdot 10^3$
22	33.106	113.626	$1.669 \cdot 10^3$	161.605	$1.977 \cdot 10^3$
23	33.308	115.451	$1.759 \cdot 10^3$	168.95	$2.077 \cdot 10^3$
24	33.495	117.153	$1.849 \cdot 10^3$	176.296	$2.176 \cdot 10^3$