

**Supplementary Information:  
Convergent Energies and Anharmonic  
Vibrational Spectra of  $\text{Ca}_2\text{H}_2$  and  $\text{Ca}_2\text{H}_4$   
Constitutional Isomers**

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# 1 Basis Set Benchmarking

In this section we briefly justify the level of theory used in the present research. Table S3 shows the results from various CCSD(T) computations involving different basis sets and different levels of electron correlation. Molpro 2010 was used for these computations with a UHF reference. Spin contamination ( $\langle S^2 - S_z^2 - S_z \rangle$ ) for each computation was less than or equal to 0.003. For the pseudopotential computations we used the small-core (10 electron) DHF-adjusted pseudopotentials of Lim et al. <sup>1</sup> along with the correlation consistent basis sets designed by Hill and Peterson <sup>2</sup> to complement the small-core pseudopotentials. From Table S3 we were able to make the following observations:

1. Correlating the 3s and 3p electrons on the calcium atom dramatically improved  $R_e$ ,  $\omega_e$ , and  $D_e$ . Correlating the 1s, 2s, and 2p electrons on calcium (in addition to the 3s and 3p electrons) had a minor affect on any molecular property
2. Using a pseudopotential for the ten inner-core electrons did not appreciably change  $R_e$  or  $\omega_e$ . Due to technical limitations with using a small-core pseudopotential we chose to use regular cc-pwCVXZ basis sets instead.
3. The cc-pwCVQZ basis set slightly outperformed the cc-pCVQZ basis set at predicting  $R_e$  and  $\omega_e$ . Thus we decided to employed the weighted core valence basis sets over the core valence basis sets.
4. The higher order correlation correction ( $\delta_{TQ}$ ) has a minor impact on the value of  $D_e$  ( $\leq 0.1$  kcal mol<sup>-1</sup>). Given the same number of electrons correlated, this correction is relatively independent of the basis set.
5. The relativistic computations (e.g. cc-pwCVDZ-DK) did not considerably disagree from the non-relativistic computations (e.g. cc-pwCVDZ) in terms of  $R_e$  and  $\omega_e$ . There is a considerable difference in  $D_e$  between relativistic and non-relativistic computations, but this difference can be accounted for by a post hoc computation.
6. The addition of diffuse functions to hydrogen atoms has a more significant on molecular properties than the addition of diffuse functions to calcium atoms. This is in agreement with the relative electronegativity of hydrogen and calcium. Given the computational limitations it is lucrative to add diffuse functions to the hydrogen atoms alone.

Table S1: CCSD(T) benchmarking results for CaH.

E <sup>a</sup>	Calcium	Hydrogen	R <sub>e</sub>	ω <sub>e</sub>	D <sub>e</sub>	δ <sub>TQ</sub> <sup>b</sup>
3	cc-pVDZ	cc-pVDZ	2.0548	1247.6	34.88	0.10
11	cc-pCVDZ	cc-pVDZ	2.0321	1254.8	33.21	0.02
11	cc-pwCVDZ	cc-pVDZ	2.0319	1260.2	32.97	0.03
21	cc-pwCVDZ	cc-pVDZ	2.0315	1259.4	32.98	0.03
3	cc-pVDZ-PP	cc-pVDZ	2.0503	1251.5	34.34	0.10
11	cc-pCVDZ-PP	cc-pVDZ	2.0269	1261.6	32.74	0.03
11	cc-pwCVDZ-PP	cc-pVDZ	2.0273	1265.1	32.63	0.02
11	aug-cc-pwCVDZ-PP	cc-pVDZ	2.0282	1263.5	32.65	0.02
11	cc-pwCVDZ-PP	aug-cc-pVDZ	2.0352	1261.3	36.32	0.03
11	aug-cc-pwCVDZ-PP	aug-cc-pVDZ	2.0282	1263.5	32.65	0.02
11	cc-pwCVDZ-DK	cc-pVDZ	2.0206	1258.4	33.41	0.04
21	cc-pwCVDZ-DK	cc-pVDZ	2.0198	1258.6	33.45	0.04
3	cc-pVTZ	cc-pVTZ	2.0538	1274.8	40.62	0.10
11	cc-pCVTZ	cc-pVTZ	2.0159	1281.1	39.08	0.08
11	cc-pwCVTZ	cc-pVTZ	2.0094	1294.4	39.40	0.08
21	cc-pwCVTZ	cc-pVTZ	2.0077	1290.9	39.44	
3	cc-pVTZ-PP	cc-pVTZ	2.0517	1273.9	40.05	0.10
11	cc-pCVTZ-PP	cc-pVTZ	2.0137	1284.7	38.42	0.07
11	cc-pwCVTZ-PP	cc-pVTZ	2.0075	1299.5	38.75	0.08
11	aug-cc-pwCVTZ-PP	cc-pVTZ	2.0082	1297.6	38.80	0.08
11	cc-pwCVTZ-PP	aug-cc-pVTZ	2.0108	1290.4	39.50	0.06
11	aug-cc-pwCVTZ-PP	aug-cc-pVTZ	2.0110	1289.6	39.49	0.07
11	cc-pwCVTZ-DK	cc-pVTZ	2.0103	1296.1	38.79	0.08
21	cc-pwCVTZ-DK	cc-pVTZ	2.0083	1296.0	38.85	
3	cc-pVQZ	cc-pVQZ	2.0534	1273.8	41.93	
11	cc-pCVQZ	cc-pVQZ	2.0053	1295.1	40.83	
11	cc-pwCVQZ	cc-pVQZ	2.0033	1299.9	40.90	
3	cc-pVQZ-PP	cc-pVQZ	2.0502	1273.1	41.31	
11	cc-pCVQZ-PP	cc-pVQZ	2.0036	1297.3	40.08	
11	cc-pwCVQZ-PP	cc-pVQZ	2.0023	1302.3	40.14	
11	aug-cc-pwCVQZ-PP	cc-pVQZ	2.0028	1300.6	40.16	
11	cc-pwCVQZ-PP	aug-cc-pVQZ	2.0060	1295.1	39.81	
11	aug-cc-pwCVQZ-PP	aug-cc-pVQZ	2.0035	1298.6	40.43	
11	cc-pwCVQZ-DK	cc-pVQZ	2.0044	1299.4	40.25	
3	cc-pV5Z	cc-pV5Z	2.0541	1271.1	42.27	
11	cc-pCV5Z	cc-pV5Z	2.0028	1297.8	41.39	
11	cc-pwCV5Z	cc-pV5Z	2.0022	1300.2	41.40	
3	cc-pV5Z-PP	cc-pV5Z	2.0506	1272.7	41.69	
11	cc-pCV5Z-PP	cc-pV5Z	2.0020	1298.6	40.59	
11	cc-pwCV5Z-PP	cc-pV5Z	2.0013	1301.0	40.60	
11	aug-cc-pwCV5Z-PP	cc-pV5Z	2.0015	1300.4	40.61	
11	cc-pwCV5Z-PP	aug-cc-pV5Z	2.0015	1300.6	40.71	
11	aug-cc-pwCV5Z-PP	aug-cc-pV5Z	2.0015	1300.6	40.70	
	Experiment <sup>c</sup>		2.0025	1298.3	41.10	

<sup>a</sup> Number of electrons correlated<sup>b</sup> CCSDTQ correction to the dissociation energy ( $D_e$ )<sup>c</sup> Huber and Herzberg <sup>3</sup>

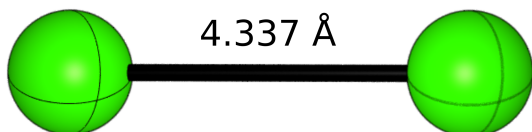
Table S2: CCSD(T) benchmarking results for Ca<sub>2</sub>H<sub>2</sub>.

E <sup>a</sup>	Calcium	Hydrogen	Ca-Ca	Ca-H	D <sub>e</sub>
6	cc-pVDZ	cc-pVDZ	3.8576	2.0649	30.12
22	cc-pCVDZ	cc-pVDZ	3.7964	2.0433	29.49
22	cc-pwCVDZ	cc-pVDZ	3.7940	2.0428	29.13
42	cc-pwCVDZ	cc-pVDZ	3.7928	2.0425	29.19
6	cc-pVDZ-PP	cc-pVDZ	3.8381	2.0594	29.88
22	cc-pCVDZ-PP	cc-pVDZ	3.7762	2.0369	29.31
22	cc-pwCVDZ-PP	cc-pVDZ	3.7757	2.0370	29.10
22	aug-cc-pwCVDZ-PP	cc-pVDZ	3.7748	2.0379	29.49
22	cc-pwCVDZ-PP	aug-cc-pVDZ	3.7873	2.0433	28.81
22	aug-cc-pwCVDZ-PP	aug-cc-pVDZ	3.7840	2.0443	36.39
22	cc-pwCVDZ-DK	cc-pVDZ	3.7892	2.0355	30.11
42	cc-pwCVDZ-DK	cc-pVDZ	3.7884	2.0348	30.16
6	cc-pVTZ	cc-pVTZ	3.8114	2.0682	32.67
22	cc-pCVTZ	cc-pVTZ	3.7342	2.0332	31.39
22	cc-pwCVTZ	cc-pVTZ	3.7312	2.0275	31.24
42	cc-pwCVTZ	cc-pVTZ	3.7210	2.0260	31.49
6	cc-pVTZ-PP	cc-pVTZ	3.7987	2.0654	32.83
22	cc-pCVTZ-PP	cc-pVTZ	3.7200	2.0296	31.74
22	cc-pwCVTZ-PP	cc-pVTZ	3.7170	2.0241	31.60
22	aug-cc-pwCVTZ-PP	cc-pVTZ	3.7179	2.0250	31.82
22	cc-pwCVTZ-PP	aug-cc-pVTZ	3.7173	2.0272	31.61
22	aug-cc-pwCVTZ-PP	aug-cc-pVTZ	3.7202	2.0270	31.83
22	cc-pwCVTZ-DK	cc-pVTZ	3.7240	2.0274	31.24
42	cc-pwCVTZ-DK	cc-pVTZ	3.7152	2.0254	31.49
6	cc-pVQZ	cc-pVQZ	3.8239	2.0686	33.35
22	cc-pCVQZ	cc-pVQZ	3.7336	2.0247	32.05
22	cc-pwCVQZ	cc-pVQZ	3.7335	2.0230	31.52
6	cc-pVQZ-PP	cc-pVQZ	3.8081	2.0647	33.36
22	cc-pCVQZ-PP	cc-pVQZ	3.7184	2.0212	31.82
22	cc-pwCVQZ-PP	cc-pVQZ	3.7144	2.0201	31.82
22	aug-cc-pwCVQZ-PP	cc-pVQZ	3.7151	2.0205	31.87
22	cc-pwCVQZ-PP	aug-cc-pVQZ	3.7139	2.0233	31.82
22	aug-cc-pwCVQZ-PP	aug-cc-pVQZ	3.7150	2.0210	31.87
22	cc-pwCVQZ-DK	cc-pVQZ	3.7254	2.0232	31.53
6	cc-pV5Z	cc-pV5Z	3.8252	2.0691	33.41
22	cc-pCV5Z	cc-pV5Z	3.7303	2.0228	31.61
22	cc-pwCV5Z	cc-pV5Z	3.7291	2.0222	31.61
6	cc-pV5Z-PP	cc-pV5Z	3.8081	2.0649	33.38
22	cc-pCV5Z-PP	cc-pV5Z	3.7107	2.0201	31.83
22	cc-pwCV5Z-PP	cc-pV5Z	3.7096	2.0195	31.84
22	aug-cc-pwCV5Z-PP	cc-pV5Z	3.7106	2.0196	31.88
22	cc-pwCV5Z-PP	aug-cc-pV5Z	3.7098	2.0196	31.84
22	aug-cc-pwCV5Z-PP	aug-cc-pV5Z	3.7106	2.0196	31.88

<sup>a</sup> Number of electrons correlated

## 2 Geometries, Frequencies, and Energies

### 2.1 Ca<sub>2</sub>

**Level of Theory:**

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

**Wavefunction Diagnostics:**

T1 = 0.019 D1 = 0.072

Figure S1: Ca<sub>2</sub>

Cartesian Coordinates of Optimized Geometry (Å):

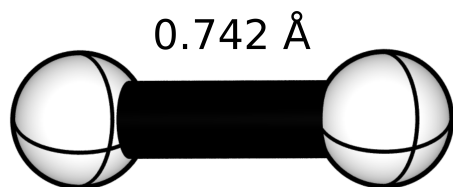
Ca	0.0000000000	0.0000000000	-2.1686786514
Ca	0.0000000000	0.0000000000	2.1686786514

Rotational Constants (GHz): 0.000 1.341 1.341

Vibrational Frequencies (cm<sup>-1</sup>):

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$\sigma_g^+$	61.1	-2.4	58.7	0.0

## 2.2 H<sub>2</sub>



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.006 D1 = 0.008

Figure S2: H<sub>2</sub>

Cartesian Coordinates of Optimized Geometry (Å):

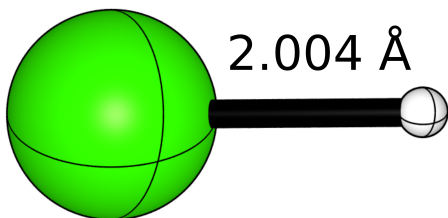
H	0.0000000000	0.0000000000	-0.3710126020
H	0.0000000000	0.0000000000	0.3710126020

Rotational Constants (GHz): 0.000, 1821.274, 1821.274

Vibrational Frequencies (cm<sup>-1</sup>):

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$\sigma_g^+$	4344.5	-254.9	4089.6	0.0

## 2.3 CaH ( $^2\Sigma^+$ )



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.026 D1 = 0.072

Figure S3: CaH

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	-0.0491723631
H	0.0000000000	0.0000000000	1.9553032053

Rotational Constants (GHz): 0.000, 127.929, 127.929

Dipole Moment (Debye): 0.0, 0.0, 2.52

Vibrational Frequencies ( $\text{cm}^{-1}$ ):

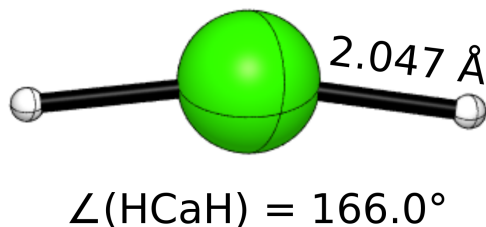
Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$\sigma^+$	1296.6	-43.9	1252.7	251.2

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) of 2 CaH ( $^2\Sigma^+$ ) relative to  $\text{Ca}_2 + \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+11.43	+20.81	-2.05	+1.85	-0.01	+0.33	[+32.36]
cc-pwCVTZ	+11.47	+19.69	-3.72	+2.83	-0.17	[+0.33]	[+30.43]
cc-pwCVQZ	+11.27	+19.39	-4.26	+3.01	[-0.17]	[+0.33]	[+29.57]
cc-pwCV5Z	+11.26	+19.31	-4.56	+3.08	[-0.17]	[+0.33]	[+29.25]
CBS Limit	[+11.26]	[+19.23]	[-4.88]	[+3.16]	[-0.17]	[+0.33]	[+28.93]



## 2.4 CaH<sub>2</sub>



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.010    D1 = 0.031

Figure S4: CaH<sub>2</sub>

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	-0.0119235058
H	0.0000000000	2.0313823586	0.2370647628
H	0.0000000000	-2.0313823586	0.2370647628

Rotational Constants (GHz): 59.896, 60.753, 4247.238

Dipole Moment (Debye): 0.0, 0.0, 0.71

Harmonic Vibrational Frequencies (cm<sup>-1</sup>):

Mode	Symmetry	$\omega$	$\delta\nu^*$	$\nu$	Intensity
1	<i>a</i> <sub>1</sub>	1330.8	-35.1	1295.7	4.8
2	<i>a</i> <sub>1</sub>	91.2			
3	<i>b</i> <sub>2</sub>	1249.6	-34.9	1214.7	859.2

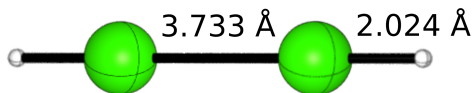
Focal Point Analysis (in kcal mol<sup>-1</sup>) of CaH<sub>2</sub> + Ca relative to Ca<sub>2</sub> + H<sub>2</sub>:

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+4.13	+7.72	-3.66	+1.36	+0.14	+0.27	[+9.97]
cc-pwCVTZ	+4.64	+6.35	-3.99	+2.01	+0.05	[+0.27]	[+9.34]
cc-pwCVQZ	+4.53	+5.86	-4.01	+2.15	[+0.05]	[+0.27]	[+8.85]
cc-pwCV5Z	+4.53	+5.71	-4.08	+2.20	[+0.05]	[+0.27]	[+8.69]
CBS Limit	[+4.54]	[+5.55]	[-4.15]	[+2.26]	[+0.05]	[+0.27]	[+8.52]

Focal Point Analysis (in kcal mol<sup>-1</sup>) of 2 CaH<sub>2</sub> relative to Ca<sub>2</sub> + 2 H<sub>2</sub>:

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+10.09	+11.97	-6.17	+1.78	+0.08	+0.36	[+18.11]
cc-pwCVTZ	+11.01	+8.57	-6.65	+2.85	-0.06	[+0.36]	[+16.07]
cc-pwCVQZ	+10.76	+7.23	-6.59	+3.00	[-0.06]	[+0.36]	[+14.69]
cc-pwCV5Z	+10.75	+6.84	-6.69	+3.07	[-0.06]	[+0.36]	[+14.27]
CBS Limit	[+10.77]	[+6.43]	[-6.80]	[+3.15]	[-0.06]	[+0.36]	[+13.85]

## 2.5 M1 [HCaCaH] $D_{\infty h}$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.011    D1 = 0.037

Figure S5: M1

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	-1.8666839110
Ca	0.0000000000	0.0000000000	1.8666839110
H	0.0000000000	0.0000000000	-3.8905587102
H	0.0000000000	0.0000000000	3.8905587102

Rotational Constants (GHz): 0.0, 1.631, 1.631

Harmonic Vibrational Frequencies ( $\text{cm}^{-1}$ ):

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$\sigma_g^+$	1300.3	-36.3	1264.0	0.0
2	$\sigma_g^+$	151.7	-0.6	151.0	0.0
3	$\pi_g$	144.4	22.9*	167.3	0.0
4	$\sigma_u^-$	1287.9	-43.0*	1244.9	1683.9
5	$\pi_u$	130.1	10.3*	140.4	428.3

\* $\nu_3$  corrected for resonance with  $\nu_4 + \nu_5$

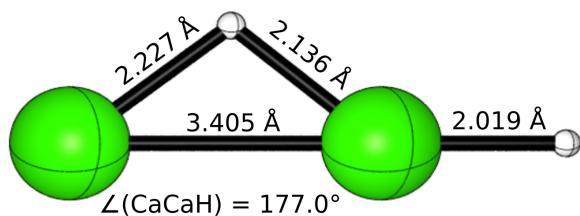
\* $\nu_4$  corrected for resonance with  $\nu_3 + \nu_5$

\* $\nu_5$  corrected for resonance with  $\nu_3 + \nu_4$

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	-2.72	+9.71	-4.78	+0.86	-0.02	+0.25	[+3.30]
cc-pwCVTZ	-2.62	+5.80	-5.63	+1.49	-0.15	[+0.25]	[-0.86]
cc-pwCVQZ	-2.77	+4.59	-5.52	+1.58	[-0.15]	[+0.25]	[-2.03]
cc-pwCV5Z	-2.78	+4.16	-5.51	+1.61	[-0.15]	[+0.25]	[-2.42]
CBS Limit	[-2.77]	[+3.72]	[-5.51]	[+1.64]	[-0.15]	[+0.25]	[-2.82]

## 2.6 M2 [Ca( $\mu_2$ -H)CaH] $C_s$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.021    D1 = 0.091

Figure S6: M2

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0207918523	0.0000000000	-1.6563291001
Ca	0.0150922579	0.0000000000	1.7490613730
H	-0.0817695443	0.0000000000	-3.6730098568
H	-1.3451359629	0.0000000000	-0.0144214354

Rotational Constants (GHz): 2.038, 2.053, 272.155

Dipole Moment (Debye): 0.0, 0.0, 2.79

Vibrational Frequencies ( $\text{cm}^{-1}$ ):

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$a'$	1304.2	-34.4	1269.7	811.1
2	$a'$	1042.3	-83.6	958.4	52.8*
3	$a'$	843.0	-46.4	796.6	729.5
4	$a'$	214.0	4.7	218.7	247.8
5	$a'$	163.9	-3.8	160.1	25.6
6	$a''$	136.9	11.4	148.3	313.4

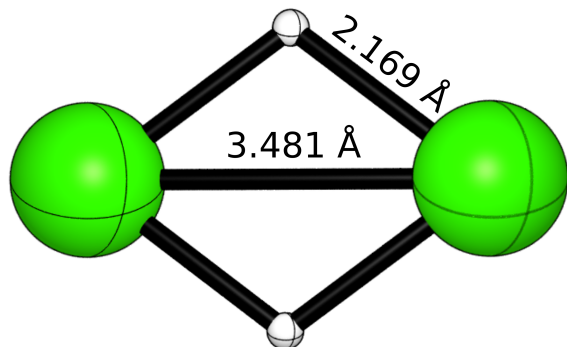
\* $\nu_1$  corrected for resonance with  $2\nu_6$

\* $\nu_2$  corrected for resonance with  $\nu_3 + \nu_4$

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	-3.24	+4.10	-3.95	+0.03	-0.08	+0.15	[-2.98]
cc-pwCVTZ	-3.22	+0.05	-4.00	+0.29	-0.21	[+0.15]	[-6.94]
cc-pwCVQZ	-3.48	-1.24	-3.89	+0.29	[-0.21]	[+0.15]	[-8.38]
cc-pwCV5Z	-3.50	-1.70	-3.93	+0.30	[-0.21]	[+0.15]	[-8.90]
CBS Limit	[-3.50]	[-2.17]	[-3.98]	[+0.30]	[-0.21]	[+0.15]	[-9.42]

## 2.7 M3 [Ca( $\mu_2$ -H) $_2$ Ca] $D_{2h}$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.026 D1 = 0.117

Figure S7: M3

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	1.7403045964
Ca	0.0000000000	0.0000000000	-1.7403045964
H	0.0000000000	1.2954015373	0.0000000000
H	0.0000000000	-1.2954015373	0.0000000000

Rotational Constants (GHz): 2.053, 2.082, 149.398

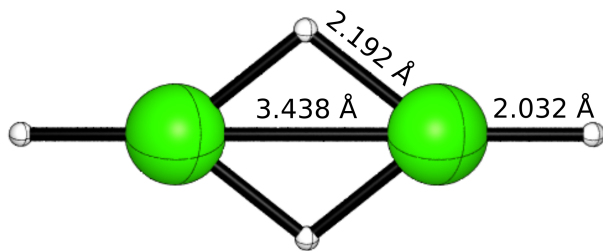
Vibrational Frequencies ( $\text{cm}^{-1}$ ):

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$a_g$	1012.0	-26.6	985.4	0.0
2	$a_g$	224.1	-7.5	216.5	0.0
3	$b_{1g}$	1030.1	-73.9	956.2	0.0
4	$b_{1u}$	434.5	-12.7	421.7	4.9
5	$b_{2u}$	829.7	-28.9	800.8	122.6
6	$b_{3u}$	1071.8	-66.9	1004.9	25.0

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+4.32	-9.43	-2.73	-4.37	+0.54	-0.40	[-12.07]
cc-pwCVTZ	+4.41	-11.98	-2.61	-4.60	+0.50	[-0.40]	[-14.67]
cc-pwCVQZ	+4.11	-12.89	-2.47	-4.72	[+0.50]	[-0.40]	[-15.87]
cc-pwCV5Z	+4.08	-13.15	-2.54	-4.77	[+0.50]	[-0.40]	[-16.27]
CBS Limit	[+4.09]	[-13.42]	[-2.61]	[-4.81]	[+0.50]	[-0.40]	[-16.66]

## 2.8 M4 [HCa( $\mu_2$ -H) $_2$ CaH] $D_{2h}$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.009 D1 = 0.028

Figure S8: M4

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	1.7191306432
Ca	0.0000000000	0.0000000000	-1.7191306432
H	0.0000000000	1.3606949333	0.0000000000
H	0.0000000000	-1.3606949333	0.0000000000
H	0.0000000000	0.0000000000	-3.7512220621
H	0.0000000000	0.0000000000	3.7512220621

Rotational Constants (GHz): 1.879, 1.905, 135.404

Vibrational Frequencies ( $\text{cm}^{-1}$ ):

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity	VCI <sup>a</sup>
1	$a_g$	1309.7	-37.3	1272.4	0.0	1264.9
2	$a_g$	1009.3	13.3	1022.6	0.0	996.6
3	$a_g$	212.0	-5.4	206.6	0.0	209.1
4	$b_{1g}$	1008.8	-57.0	951.8	0.0	933.9
5	$b_{1g}$	241.9	3.3	245.2	0.0	241.1
6	$b_{2g}$	87.8	22.8	110.6	0.0	179.0
7	$b_{1u}$	498.4	-2.4	496.0	731.9	519.9
8	$b_{1u}$	103.2	15.4	118.6	651.8	169.0
9	$b_{2u}$	904.4	-28.1	876.3	844.0	849.5
10	$b_{2u}$	223.5	5.6	229.1	611.1	236.2
11	$b_{3u}$	1299.5	-42.0	1257.5	566.3	1237.7
12	$b_{3u}$	1120.7	-64.3	1056.4	1486.1	1035.7

<sup>a</sup> Multi-level vibration configuration interaction frequencies <sup>4</sup>

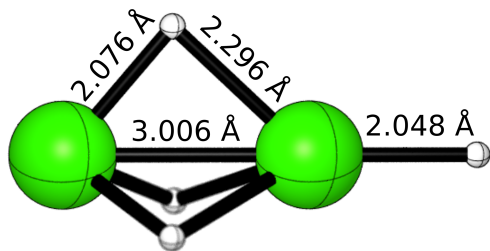
\* $\nu_2$  corrected for resonance with  $2\nu_7$

\* $\nu_{11}$  corrected for resonance with  $\nu_6 + \nu_8$

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + 2\text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	-37.87	+8.44	-5.00	+1.42	+0.03	+0.33	[-32.66]
cc-pwCVTZ	-37.07	+3.49	-5.25	+2.20	-0.13	[+0.33]	[-36.43]
cc-pwCVQZ	-37.40	+1.78	-5.15	+2.27	[-0.13]	[+0.33]	[-38.30]
cc-pwCV5Z	-37.40	+1.26	-5.25	+2.31	[-0.13]	[+0.33]	[-38.87]
CBS Limit	[-37.37]	[+0.71]	[-5.35]	[+2.36]	[-0.13]	[+0.33]	[-39.45]

## 2.9 M5 [HCa( $\mu_2$ -H)<sub>3</sub>Ca] $C_{3v}$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/DZ

### Wavefunction Diagnostics:

T1 = 0.011 D1 = 0.029

Figure S9: M5

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	1.4663417338
Ca	-0.0000000000	0.0000000000	-1.5398961593
H	1.5833387792	0.0000000000	-0.1965133772
H	-0.7916693896	-1.3712116056	-0.1965133772
H	-0.7916693896	1.3712116056	-0.1965133772
H	0.0000000000	0.0000000000	3.5143782916

Rotational Constants (GHz): 2.558, 2.558, 66.667

Dipole Moment (Debye): 0.0, 0.0, 10.72

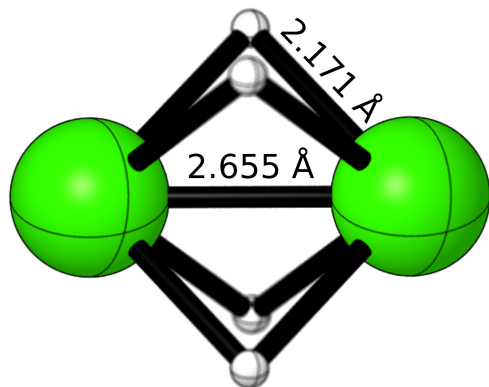
Vibrational Frequencies ( $\text{cm}^{-1}$ ):

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$a'$	1260.8	-37.8	1223.0	550.6
2	$a'$	1229.7	-61.5	1168.2	39.2
3	$a'$	911.3	-60.9	850.4	1121.8
4	$a'$	262.2	-7.5	254.7	0.0
5	$e$	1114.8	-41.2	1073.6	502.2
6	$e$	726.8	-45.0	681.8	88.6
7	$e$	622.2	-29.2	593.0	700.3
8	$e$	236.5	2.5	239.0	283.4

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + 2 \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	-33.46	+5.25	-4.08	+0.94	-0.05	+0.31	[-31.10]
cc-pwCVTZ	-33.00	-1.81	-4.15	+1.42	-0.23	[+0.31]	[-37.46]
cc-pwCVQZ	-33.49	-4.01	-4.03	+1.39	[-0.23]	[+0.31]	[-40.06]
cc-pwCV5Z	-33.51	-4.72	-4.13	+1.39	[-0.23]	[+0.31]	[-40.88]
CBS Limit	[-33.48]	[-5.46]	[-4.23]	[+1.39]	[-0.23]	[+0.31]	[-41.70]

## 2.10 M6 [Ca( $\mu_2$ -H)<sub>4</sub>Ca] $D_{4h}$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

Anharmonics: CCSD(T)/TZ

### Wavefunction Diagnostics:

T1 = 0.014 D1 = 0.041

Figure S10: M6

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	1.3277090839
Ca	0.0000000000	0.0000000000	-1.3277090839
H	1.7177315542	0.0000000000	0.0000000000
H	0.0000000000	-1.7177315542	0.0000000000
H	0.0000000000	1.7177315542	0.0000000000
H	-1.7177315542	0.0000000000	0.0000000000

Rotational Constants (GHz): 3.432, 3.432, 42.483

Vibrational Frequencies ( $\text{cm}^{-1}$ ):

Focal Point Analysis:

Mode	Symmetry	$\omega$	$\delta\nu$	$\nu$	Intensity
1	$a_{1g}$	1149.5	-50.9	1098.6	0.0
2	$a_{1g}$	325.8	-21.0	304.8	0.0
3	$b_{1g}$	906.6	-84.4	822.2	0.0
4	$b_{2g}$	912.0	-32.7	879.3	0.0
5	$e_g$	662.5	-97.1	565.4	0.0
6	$a_{2u}$	984.0	-131.6*	852.4	1150.5
7	$b_{2u}$	443.2	-83.9	359.3	0.0
8	$e_u$	1000.1	-115.9*	884.2	969.8
9	$e_u$	722.5	-41.4	681.1	687.1

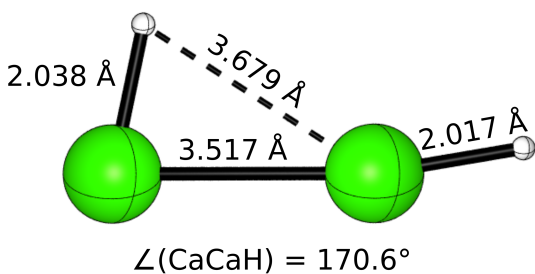
\*Corrected for resonance with  $\nu_3 + \nu_7$

\*Corrected for resonance with  $\nu_5 + \nu_7$

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + 2 \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+0.40	-0.61	-2.71	-0.02	-0.15	+0.26	[-2.84]
cc-pwCVTZ	-0.40	-10.72	-2.51	-0.02	-0.38	[+0.26]	[-13.77]
cc-pwCVQZ	-1.06	-13.87	-2.35	-0.26	[-0.38]	[+0.26]	[-17.67]
cc-pwCV5Z	-1.11	-14.85	-2.47	-0.32	[-0.38]	[+0.26]	[-18.87]
CBS Limit	[-1.10]	[-15.88]	[-2.58]	[-0.39]	[-0.38]	[+0.26]	[-20.07]

## 2.11 TS1 [M1 → M2] $C_s$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

### Wavefunction Diagnostics:

T1 = 0.018    D1 = 0.072

Figure S11: TS1

Cartesian Coordinates of Optimized Geometry (Å):

Ca	-0.0388331350	0.0000000000	-1.7879951405
Ca	-0.0185263908	0.0000000000	1.7290865569
H	1.9571521570	0.0000000000	-1.3746679637
H	0.3237076095	0.0000000000	3.7171248854

Rotational Constants (GHz): 1.887, 1.916, 125.073

Harmonic Vibrational Frequencies ( $\text{cm}^{-1}$ ):

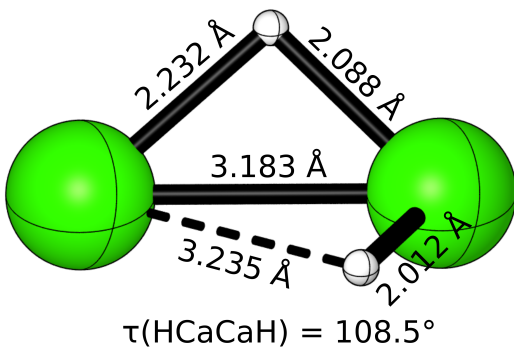
[ $a'$ ] 1300.5    [ $a''$ ] 138.0  
 [ $a'$ ] 1200.6  
 [ $a'$ ] 176.2  
 [ $a'$ ] 141.0  
 [ $a'$ ] 414.1 i

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+11.51	+7.35	-4.16	+0.23	-0.15	+0.20	[+14.98]
cc-pwCVTZ	+11.45	+2.67	-4.59	+0.67	-0.31	[+0.20]	[+10.08]
cc-pwCVQZ	+11.24	+1.28	-4.54	+0.71	[-0.31]	[+0.20]	[+8.57]
cc-pwCV5Z	+11.22	+0.73	-4.55	+0.72	[-0.31]	[+0.20]	[+8.00]
CBS Limit	[+11.22]	[+0.16]	[-4.56]	[+0.73]	[-0.31]	[+0.20]	[+7.43]



## 2.12 TS2 [M2 → M3] C<sub>1</sub>



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

### Wavefunction Diagnostics:

T1 = 0.028    D1 = 0.122

Figure S12: TS2

Cartesian Coordinates of Optimized Geometry (Å):

Ca	-0.0262236978	-0.0266326153	-1.5776078551
Ca	0.0020137363	-0.0162044547	1.6050905027
H	-0.8581004550	1.1676405901	-0.0807079782
H	1.8207919405	0.5357442965	-1.0121194880

Rotational Constants (GHz): 2.428, 2.456, 86.925

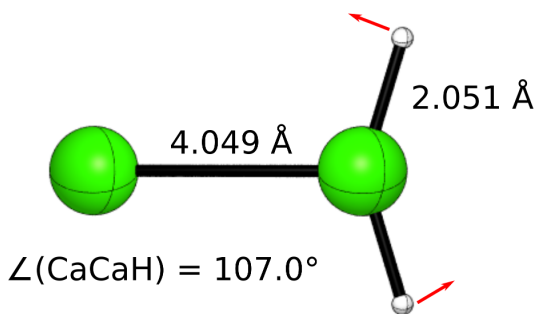
Harmonic Vibrational Frequencies (cm<sup>-1</sup>):

- [a] 1256.1
- [a] 1062.8
- [a] 786.2
- [a] 466.1
- [a] 216.4
- [a] 371.7 i

Focal Point Analysis (in kcal mol<sup>-1</sup>) relative to Ca<sub>2</sub> + H<sub>2</sub>:

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+13.34	+1.81	-3.84	-0.91	-0.35	+0.02	[+10.06]
cc-pwCVTZ	+13.03	-3.20	-3.90	-0.82	-0.21	[+0.02]	[+4.92]
cc-pwCVQZ	+12.69	-4.76	-3.81	-0.88	[-0.21]	[+0.02]	[+3.05]
cc-pwCV5Z	+12.65	-5.34	-3.87	-0.91	[-0.21]	[+0.02]	[+2.33]
CBS Limit	[+12.65]	[-5.96]	[-3.94]	[-0.94]	[-0.21]	[+0.02]	[+1.63]

### 2.13 TS3 [M2 → M2] $C_{2v}$



**Level of Theory:**

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

**Wavefunction Diagnostics:**

T1 = 0.014 D1 = 0.057

Figure S13: TS3

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	-1.9601554665
Ca	0.0000000000	0.0000000000	2.0889192444
H	0.0000000000	1.9609228149	-2.5600989227
H	0.0000000000	-1.9609228149	-2.5600989227

Rotational Constants (GHz): 11.445, 1.477, 65.198

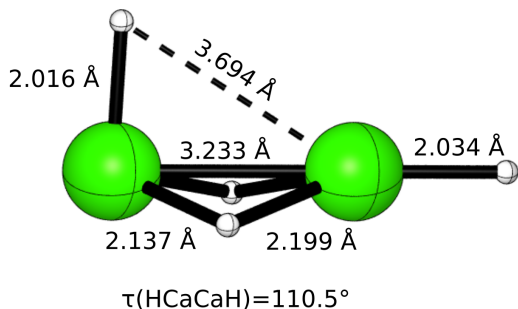
Harmonic Vibrational Frequencies ( $\text{cm}^{-1}$ ):

$[a_1]$	1289.6	$[b_1]$	142.6	$[b_2]$	1226.1
$[a_1]$	273.6			$[b_2]$	58.3 i
$[a_1]$	82.4				

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
DZ	+3.52	+4.93	-3.30	+0.81	+0.03	+0.21	[+6.21]
TZ	+3.81	+2.53	-3.34	+1.25	-0.06	[+0.21]	[+4.41]
QZ	+3.68	+1.81	-3.32	+1.32	[-0.06]	[+0.21]	[+3.64]
5Z	+3.67	+1.60	-3.38	+1.35	[-0.06]	[+0.21]	[+3.39]
CBS	[+3.67]	[+1.37]	[-3.45]	[+1.39]	[-0.06]	[+0.21]	[+3.14]

## 2.14 TS4 [M4 → M5] $C_s$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

### Wavefunction Diagnostics:

T1 = 0.011    D1 = 0.032

Figure S14: TS4

Cartesian Coordinates of Optimized Geometry (Å):

Ca	-0.0342337971	0.0000000000	1.6412469180
Ca	0.0095673719	0.0000000000	-1.5916399183
H	-0.5177970839	1.3536556151	0.0593662170
H	-0.5177970839	-1.3536556151	0.0593662170
H	0.0371173529	0.0000000000	-3.6250553028
H	1.9793192481	0.0000000000	1.5337366544

Rotational Constants (GHz): 2.201, 2.209, 61.368

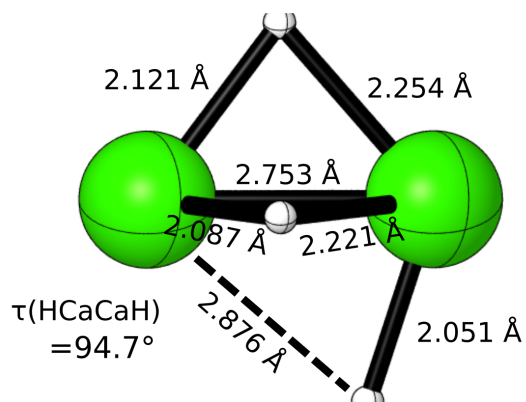
Harmonic Vibrational Frequencies ( $\text{cm}^{-1}$ ):

$[a']$	1296.7	$[a'']$	1007.7
$[a']$	1290.7	$[a'']$	906.6
$[a']$	1118.1	$[a'']$	461.6
$[a']$	1012.7	$[a'']$	242.5
$[a']$	604.9		
$[a']$	260.0		
$[a']$	168.4		
$[a']$	253.2 i		

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + 2 \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	-29.50	+6.98	-4.66	+1.16	-0.02	+0.32	[-25.72]
cc-pwCVTZ	-28.92	+1.06	-4.81	+1.81	-0.19	[+0.32]	[-30.74]
cc-pwCVQZ	-29.35	-0.90	-4.71	+1.83	[-0.19]	[+0.32]	[-33.01]
cc-pwCV5Z	-29.36	-1.50	-4.81	+1.85	[-0.19]	[+0.32]	[-33.69]
CBS Limit	[-29.34]	[-2.13]	[-4.91]	[+1.88]	[-0.19]	[+0.32]	[-34.38]

## 2.15 TS5 [M5 → M6] $C_s$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

### Wavefunction Diagnostics:

T1 = 0.014 D1 = 0.042

Figure S15: TS5

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0088970719	0.0000000000	1.3815011294
Ca	-0.0213019239	0.0000000000	-1.3712506861
H	0.1306651205	1.6493635592	0.1087810383
H	0.1306651205	-1.6493635592	0.1087810383
H	-1.7031456868	0.0000000000	0.1288988145
H	1.9350853520	0.0000000000	-0.7540623039

Rotational Constants (GHz): 3.174, 3.199, 41.297

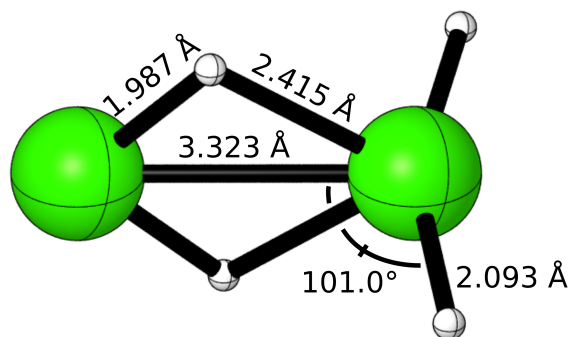
Harmonic Vibrational Frequencies ( $\text{cm}^{-1}$ ):

$[a']$	1184.6	$[a'']$	1077.4
$[a']$	1168.9	$[a'']$	843.5
$[a']$	998.5	$[a'']$	743.6
$[a']$	891.0	$[a'']$	581.3
$[a']$	722.1		
$[a']$	552.0		
$[a']$	332.9		
$[a']$	415.6 i		

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + 2 \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	+0.86	+0.75	-3.28	+0.16	-0.16	+0.27	[-1.40]
cc-pwCVTZ	+0.36	-8.45	-3.14	+0.28	-0.37	[+0.27]	[-11.07]
cc-pwCVQZ	-0.25	-11.30	-3.00	+0.10	[-0.37]	[+0.27]	[-14.55]
cc-pwCV5Z	-0.29	-12.20	-3.11	+0.06	[-0.37]	[+0.27]	[-15.65]
CBS Limit	[-0.28]	[-13.15]	[-3.21]	[+0.01]	[-0.37]	[+0.27]	[-16.74]

## 2.16 TS6 [M5 → M5] $C_{2v}$



### Level of Theory:

Geometry: CCSD(T)/QZ

Harmonics: CCSD(T)/QZ

### Wavefunction Diagnostics:

T1 = 0.012 D1 = 0.037

Figure S16: TS6

Cartesian Coordinates of Optimized Geometry (Å):

Ca	0.0000000000	0.0000000000	-1.7041825128
Ca	0.0000000000	0.0000000000	1.6191248212
H	0.0000000000	1.4310774680	-0.3261232328
H	0.0000000000	-1.4310774680	-0.3261232328
H	-2.0548888039	0.0000000000	2.0172518114
H	2.0548888039	0.0000000000	2.0172518114

Rotational Constants (GHz): 2.120, 2.160, 39.980

Harmonic Vibrational Frequencies ( $\text{cm}^{-1}$ ):

[a <sub>1</sub> ]	1378.7	[a <sub>2</sub> ]	389.7	[b <sub>1</sub> ]	1146.8	[b <sub>2</sub> ]	1312.3
[a <sub>1</sub> ]	1218.8			[b <sub>1</sub> ]	526.4	[b <sub>2</sub> ]	506.5
[a <sub>1</sub> ]	739.6			[b <sub>1</sub> ]	258.7 i	[b <sub>2</sub> ]	259.5
[a <sub>1</sub> ]	272.1						
[a <sub>1</sub> ]	112.4						

Focal Point Analysis (in  $\text{kcal mol}^{-1}$ ) relative to  $\text{Ca}_2 + 2 \text{H}_2$ :

Basis	$\Delta E_e$ HF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ (T)	$+\delta$ T	$+\delta$ (Q)	$\Delta E_e$ Net
cc-pwCVDZ	-3.01	+7.07	-5.01	+1.11	-0.06	+0.32	[+0.42]
cc-pwCVTZ	-2.43	+1.47	-5.17	+1.78	-0.22	[+0.32]	[-4.25]
cc-pwCVQZ	-2.86	-0.35	-5.07	+1.82	[-0.22]	[+0.32]	[-6.36]
cc-pwCV5Z	-2.88	-0.92	-5.16	+1.85	[-0.22]	[+0.32]	[-7.02]
CBS Limit	[-2.86]	[-1.52]	[-5.27]	[+1.88]	[-0.22]	[+0.32]	[-7.68]

### 3 M5 vs. M4 Thermodynamical Analysis

Using the rigid rotor harmonic oscillator approximation we have computed the difference in Gibbs free energy ( $\Delta G_T$ ) between the tribridged (M5) and dibridged (M4) isomers of  $\text{Ca}_2\text{H}_4$ . The CCSD(T)/QZ rotational constants and fundamental frequencies were used for this analysis.

Temp (K)	$\Delta H(T)$ (kcal mol <sup>-1</sup> )	$\Delta S(T)$ (cal mol <sup>-1</sup> )	$\Delta G(T)$ (kcal mol <sup>-1</sup> )	$K_{\text{eq}}$
100	-0.970	-1.933	-0.777	2484.6
200	-1.315	-4.341	-0.446	3.073
300	-1.548	-5.306	0.044	0.929
400	-1.682	-5.696	0.596	0.472
500	-1.760	-5.872	1.176	0.306
600	-1.809	-5.961	1.768	0.227
700	-1.841	-6.011	2.367	0.182
800	-1.863	-6.041	2.970	0.154
900	-1.880	-6.060	3.575	0.136
1000	-1.892	-6.074	4.181	0.122

## 4 Relaxed Surface Scans

### 4.1 2 CaH $\rightarrow$ M1

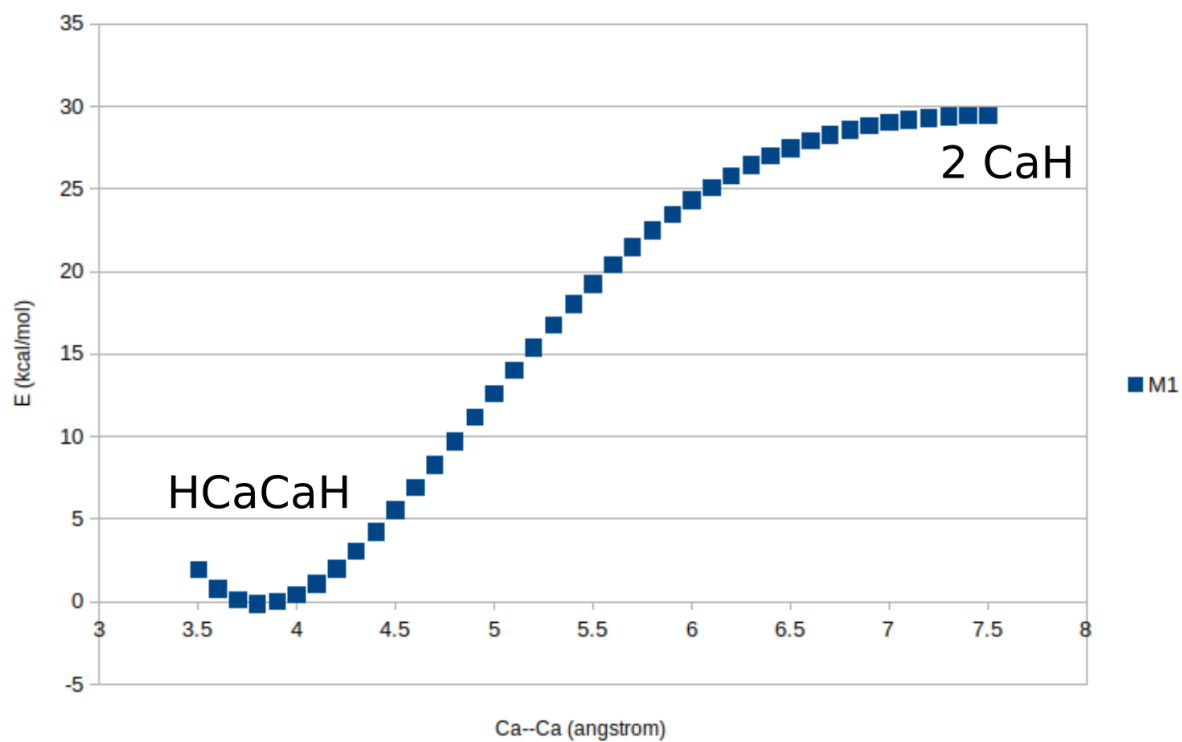


Figure S17: CCSD(T)/DZ//MP2/DZ relaxed surface scan of 2 CaH  $\rightarrow$  M1 approach

## 4.2 $\text{CaH}_2 + \text{Ca} \rightarrow \text{M2}$

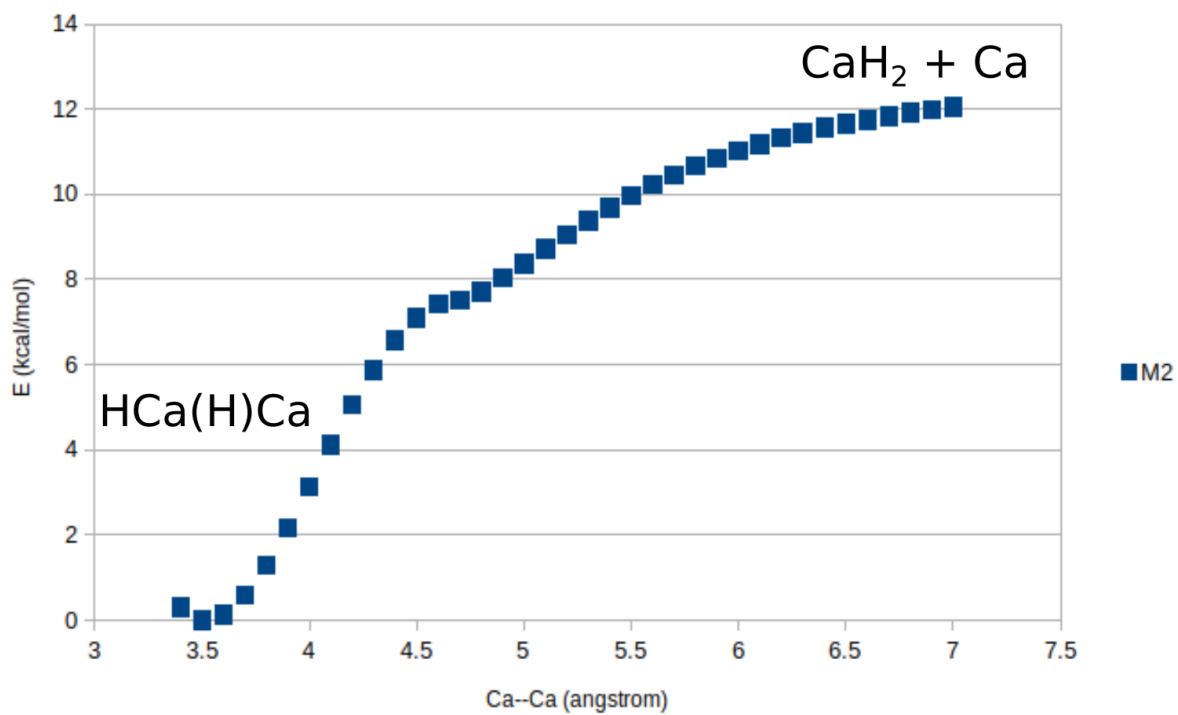


Figure S18: CCSD(T)/DZ//MP2/DZ relaxed surface scan of  $\text{CaH}_2 + \text{Ca} \rightarrow \text{M2}$  approach



### 4.3 $2 \text{CaH}_2 \rightarrow \text{Ca}_2\text{H}_4$

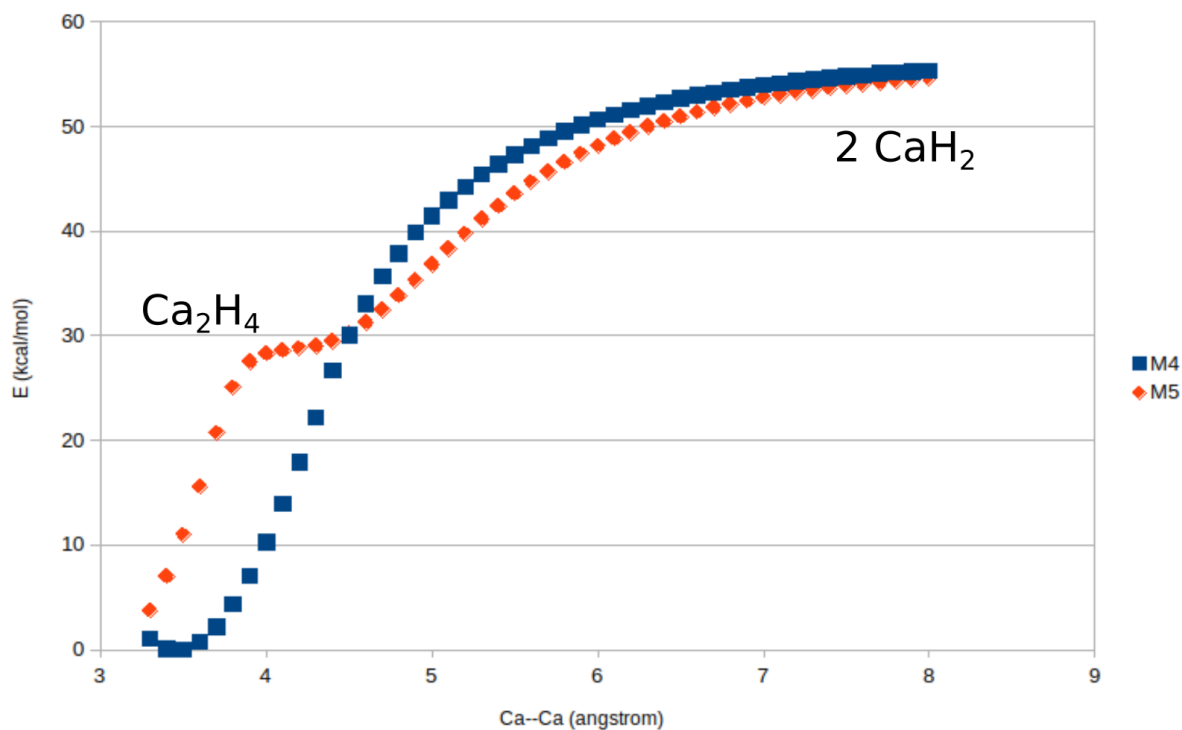


Figure S19: CCSD(T)/DZ//MP2/DZ relaxed surface scan of  $2 \text{CaH}_2 \rightarrow \text{Ca}_2\text{H}_4$

Notice that while both approaches appear barrierless, the steeper slope in the 4-5 Å region suggests that the formation of dibridged  $\text{Ca}_2\text{H}_4$  will be more rapid than tribridged  $\text{Ca}_2\text{H}_4$  which is in agreement with experiment.

## 5 QSD Reaction Paths

### 5.1 M1 → TS1 → M2

4			
QSD point 1			
Ca	-0.0000025339	0.0000000000	-1.9019348901
Ca	0.0000231298	0.0000000000	1.9019347037
H	-0.0001638705	0.0000000000	-3.9510865200
H	-0.0006551102	0.0000005813	3.9510939314
4			
QSD point 2			
Ca	-0.0002114596	0.0000000000	-1.9020149334
Ca	0.0002726777	0.0000000000	1.9020087782
H	0.0034165302	0.0000000000	-3.9509555416
H	-0.0058508199	0.0000000000	3.9512003005
4			
QSD point 3			
Ca	-0.0015381690	0.0000000000	-1.9019743084
Ca	0.0010710155	0.0000000000	1.9019666470
H	0.0342614004	0.0000000000	-3.9507877987
H	-0.0156853832	0.0000000000	3.9510924506
4			
QSD point 4			
Ca	-0.0087885290	0.0000000000	-1.8992942710
Ca	0.0015892758	0.0000000000	1.8989270621
H	0.2428538780	0.0000000000	-3.9330401738
H	0.0434191814	0.0000000000	3.9476419678
4			
QSD point 5			
Ca	-0.0190710771	0.0000000000	-1.8933083087
Ca	0.0015218367	0.0000000000	1.8914234370
H	0.5511123835	0.0000000000	-3.8607127022
H	0.1467203791	0.0000000000	3.9356632502
4			
QSD point 6			
Ca	-0.0290204841	0.0000000000	-1.8858915490
Ca	0.0013327621	0.0000000000	1.8811545216
H	0.8617220014	0.0000000000	-3.7288073260
H	0.2392601016	0.0000000000	3.9171717704
4			
QSD point 7			
Ca	-0.0378661979	0.0000000000	-1.8776262730
Ca	0.0006629228	0.0000000000	1.8685518066
H	1.1628572838	0.0000000000	-3.5335664717
H	0.3165038532	0.0000000000	3.8944060160
4			
QSD point 8			
Ca	-0.0447134356	0.0000000000	-1.8690653567
Ca	-0.0009219582	0.0000000000	1.8541801374
H	1.4379330679	0.0000000000	-3.2775861658
H	0.3767251308	0.0000000000	3.8694860670
4			
QSD point 9			
Ca	-0.0489525699	0.0000000000	-1.8605415990
Ca	-0.0037642868	0.0000000000	1.8383915098
H	1.6754106035	0.0000000000	-2.9628783282
H	0.4208368091	0.0000000000	3.8436604948
4			

QSD point 10			
Ca	-0.0500547272	0.0000000000	-1.8517665984
Ca	-0.0083116851	0.0000000000	1.8206635465
H	1.8671208493	0.0000000000	-2.5791461055
H	0.4537770255	0.0000000000	3.8159363128
4			
QSD point 11			
Ca	-0.0471288877	0.0000000000	-1.8423387954
Ca	-0.0148699585	0.0000000000	1.7995731579
H	1.9964617226	0.0000004613	-2.0855795113
H	0.4688772412	-0.0000020243	3.7861239371
4			
QSD point 12			
Ca	-0.0382450185	0.0000000000	-1.8332618760
Ca	-0.0228455633	0.0000000000	1.7742738540
H	1.9920100069	0.0000000000	-1.4160775397
H	0.4372124823	0.0000009173	3.7616932717
4			
QSD point 13			
Ca	-0.0369317404	0.0000000000	-1.8322116500
Ca	-0.0237113390	0.0000000000	1.7713660036
H	1.9780708075	0.0000000000	-1.3394470071
H	0.4333570804	0.0000009177	3.7589298242
4			
QSD point 14			
Ca	-0.0248208586	0.0000000000	-1.8229237199
Ca	-0.0293022955	0.0000000000	1.7471281127
H	1.7505474895	0.0000000000	-0.7220073268
H	0.4016203137	0.0000009956	3.7359644473
4			
QSD point 15			
Ca	-0.0152462364	0.0000000000	-1.8148839624
Ca	-0.0297524508	0.0000000000	1.7282535421
H	1.4286627765	0.0000000000	-0.2790980772
H	0.3606772484	0.0000004468	3.7238936456
4			
QSD point 16			
Ca	-0.0093051718	0.0000000000	-1.8060538185
Ca	-0.0278623730	0.0000000000	1.7128536298
H	1.1444002558	0.0000000000	-0.0082128736
H	0.3335400956	0.0000003678	3.7142504997
4			
QSD point 17			
Ca	-0.0149724627	0.0000000000	-1.7957456564
Ca	-0.0205894563	0.0000000000	1.7026624637
H	1.3150154604	0.0000000000	-0.0344151961
H	0.0990783500	-0.0000003011	3.7358005598
4			
QSD point 18			
Ca	-0.0143087608	0.0000000000	-1.7936060878
Ca	-0.0201558351	0.0000000000	1.6984077627
H	1.2961031287	0.0000000000	0.0484931520
H	0.0743564262	0.0000000000	3.7369989100
4			
QSD point 19			
Ca	-0.0156012956	0.0000000000	-1.8046790617
Ca	-0.0206812005	0.0000000000	1.7093856371
H	1.3804285093	0.0000000000	0.0379590384
H	0.0623185237	0.0000005317	3.7513145882

## 5.2 M2 → TS2 → M3

4
QSD Point 1
Ca 0.0170817298 0.0006801828 -1.7108018037
Ca 0.0161216135 -0.0002508203 1.8061490148
H -1.3331614210 0.0000607318 -0.0393228315
H 0.0128546551 -0.0171340167 -3.7520895770
4
QSD Point 2
Ca 0.0170785727 0.0007350899 -1.7109473820
Ca 0.0161209429 -0.0002711589 1.8062741464
H -1.3326291850 0.0000708187 -0.0381607931
H 0.0124746301 -0.0185186972 -3.7524385620
4
QSD Point 3
Ca 0.0162837693 -0.0025176869 -1.7104223418
Ca 0.0164578168 0.0009105270 1.8057615394
H -1.3360272164 0.0008347773 -0.0401259357
H 0.0340818929 0.0630727640 -3.7509678197
4
QSD Point 4
Ca 0.0142668910 -0.0098073549 -1.7091527343
Ca 0.0172504548 0.0033642106 1.8040737416
H -1.3395065607 0.0132139101 -0.0404240576
H 0.0862422611 0.2429930296 -3.7340406638
4
QSD Point 5
Ca 0.0121242437 -0.0162783389 -1.7074704216
Ca 0.0180652631 0.0052401041 1.8016454218
H -1.3432357396 0.0394229412 -0.0428183820
H 0.1427719907 0.3995044254 -3.7019819119
4
QSD Point 6
Ca 0.0081812893 -0.0246345179 -1.7044776015
Ca 0.0194273389 0.0069744021 1.7970088415
H -1.3439093063 0.1070300888 -0.0450942291
H 0.2460723148 0.5952115536 -3.6343431357
4
QSD Point 7
Ca -0.0018389291 -0.0349372128 -1.6980658761
Ca 0.0222022847 0.0066278208 1.7869270562
H -1.3175274953 0.3177690341 -0.0506854725
H 0.5077934891 0.8079333204 -3.4828146358
4
QSD Point 8
Ca -0.0156084591 -0.0387995436 -1.6912475350
Ca 0.0245550830 0.0025189787 1.7758679733
H -1.2174938058 0.6106796117 -0.0557723836
H 0.8617378212 0.8319906266 -3.3090977171
4
QSD Point 9
Ca -0.0298114694 -0.0369457171 -1.6827672525
Ca 0.0251204469 -0.0031011360 1.7618614448
H -1.0529151651 0.8787611030 -0.0625997622
H 1.2394502594 0.7136728451 -3.0825231865
4
QSD Point 10
Ca -0.0381328603 -0.0338211141 -1.6739690274

Ca	0.0238563104	-0.0068527255	1.7468805110
H	-0.9377701550	1.0149131567	-0.0693075369
H	1.5054667613	0.6024524550	-2.8299645065
4			
QSD Point 11			
Ca	-0.0423211112	-0.0310772997	-1.6624487065
Ca	0.0207076792	-0.0096793266	1.7268210015
H	-0.8695596449	1.0953940517	-0.0793383846
H	1.7290020269	0.5252635089	-2.4803790403
4			
QSD Point 12			
Ca	-0.0418274597	-0.0293938631	-1.6508158405
Ca	0.0162244774	-0.0116231277	1.7059526081
H	-0.8471722717	1.1368569805	-0.0896691594
H	1.8652562166	0.4941537854	-2.1028042461
4			
QSD Point 13			
Ca	-0.0386223317	-0.0284210374	-1.6408639193
Ca	0.0116973768	-0.0130240517	1.6876898112
H	-0.8490197933	1.1562408530	-0.0973001129
H	1.9196710154	0.4917929302	-1.7646973749
4			
QSD Point 14			
Ca	-0.0345385198	-0.0277857485	-1.6330007689
Ca	0.0078879563	-0.0141070115	1.6729048696
H	-0.8618591509	1.1621526917	-0.1011795600
H	1.9215994009	0.5036824006	-1.4855779438
4			
QSD Point 15			
Ca	-0.0310746330	-0.0275970880	-1.6267942270
Ca	0.0054862980	-0.0148153466	1.6621941314
H	-0.8813361090	1.1629695383	-0.1079481630
H	1.8988376147	0.5235300344	-1.2997032550
4			
QSD Point 16			
Ca	-0.0253181237	-0.0262752602	-1.6201290790
Ca	0.0018339898	-0.0160382481	1.6474118609
H	-0.8987381491	1.1381731371	-0.0867346144
H	1.8325676322	0.5443927040	-0.9981453389
4			
QSD Point 17			
Ca	-0.0237649697	-0.0259503708	-1.6185501471
Ca	0.0010740899	-0.0163317609	1.6438567732
H	-0.9060097210	1.1288877278	-0.0810347682
H	1.8082960298	0.5524304427	-0.9252647892
4			
QSD Point 18			
Ca	-0.0171585699	-0.0245773895	-1.6123463018
Ca	-0.0011770732	-0.0174795009	1.6298746959
H	-0.9488962860	1.0749605602	-0.0554870031
H	1.6779997806	0.5974010570	-0.6415168225
4			
QSD Point 19			
Ca	-0.0126996303	-0.0224452564	-1.6131364350
Ca	-0.0020476971	-0.0179512056	1.6245086531
H	-0.9722265443	0.9943225679	-0.0088849145
H	1.5586432786	0.6120133210	-0.4433230540
4			
QSD Point 20			

Ca	-0.0061947188	-0.0202217527	-1.6181527092
Ca	-0.0011655928	-0.0179052546	1.6237032301
H	-1.0750835630	0.8512467584	0.0087841551
H	1.3677609929	0.6648459192	-0.2294965744
4			
QSD Point 21			
Ca	-0.0004990841	-0.0183806898	-1.6257146028
Ca	0.0007542555	-0.0170289925	1.6287551690
H	-1.2198254440	0.7010197305	-0.0268135037
H	1.2096787387	0.7070205001	-0.0940923982
4			
QSD Point 22			
Ca	0.0000749475	-0.0163944911	-1.6385622873
Ca	0.0008182529	-0.0156236065	1.6404841349
H	-1.2418991701	0.6271255239	-0.0178489418
H	1.2063817087	0.6460508065	-0.0585719258
4			
QSD Point 23			
Ca	0.0002844379	-0.0148232591	-1.6552530552
Ca	0.0007525269	-0.0139577661	1.6576861869
H	-1.2760794530	0.5625980675	-0.0352822218
H	1.2348453015	0.5818584394	-0.0614694888
4			
QSD Point 24			
Ca	0.0001922804	-0.0128768915	-1.6745588166
Ca	0.0006071838	-0.0120220220	1.6773747073
H	-1.2889365965	0.4887098484	-0.0444092302
H	1.2571464838	0.5013773132	-0.0675626115
4			
QSD Point 25			
Ca	0.0002733191	-0.0116986659	-1.6919594541
Ca	0.0005234886	-0.0102699173	1.6973622397
H	-1.3438687748	0.4314435526	-0.0997582050
H	1.3121842967	0.4421211600	-0.1150796328

### 5.3 M2 → TS3 → M2'

4
QSD Point 1
Ca -0.0000002105 -0.0184376293 -1.7107791619
Ca 0.0000000801 -0.0155831403 1.8060911660
H -0.0000001687 1.3304393608 -0.0384806579
H 0.0000053517 0.0223717640 -3.7515317657
4
QSD Point 2
Ca -0.0000002127 -0.0184363879 -1.7107710544
Ca 0.0000000810 -0.0155834870 1.8060833506
H -0.0000001703 1.3304399989 -0.0384998674
H 0.0000054098 0.0223355474 -3.7515241728
4
QSD Point 3
Ca -0.0000002000 -0.0183859837 -1.7107431108
Ca 0.0000000760 -0.0156035300 1.8060560620
H -0.0000001548 1.3305328245 -0.0385010078
H 0.0000050828 0.0210354288 -3.7515490781
4
QSD Point 4
Ca -0.0000001736 -0.0184724342 -1.7109357069
Ca 0.0000000661 -0.0155667330 1.8062584089
H -0.0000001421 1.3303326305 -0.0387918924
H 0.0000044146 0.0232100654 -3.7516459272
4
QSD Point 5
Ca -0.0000001221 -0.0183447003 -1.7140148006
Ca 0.0000000464 -0.0155721177 1.8094418657
H -0.0000000934 1.3282021573 -0.0399044964
H 0.0000031068 0.0204754051 -3.7546832494
4
QSD Point 6
Ca -0.0000004104 -0.0185043658 -1.7030348119
Ca 0.0000001560 -0.0157595709 1.7983073903
H -0.0000002902 1.3446005306 -0.0440453396
H 0.0000104052 0.0178799552 -3.7443993510
4
QSD Point 7
Ca -0.0000004697 -0.0184917434 -1.7049311420
Ca 0.0000001823 -0.0152343196 1.7993519873
H -0.0000005543 1.3005469504 -0.0090547784
H 0.0000119850 0.0405453807 -3.7455213658
4
QSD Point 8
Ca 0.0000000000 -0.0179490541 -1.7263533128
Ca 0.0000000000 -0.0159442160 1.8228375235
H 0.0000000000 1.3524472842 -0.0696384015
H 0.0000015827 -0.0047060842 -3.7669859640
4
QSD Point 9
Ca 0.0000000000 -0.0149294691 -1.7454972372
Ca 0.0000000000 -0.0162429224 1.8416165605
H 0.0000000000 1.2922155186 -0.0357327522
H -0.0000024174 -0.0526680750 -3.7863821333
4
QSD Point 10
Ca 0.0000004093 -0.0126858576 -1.7647792349

Ca	-0.0000001331	-0.0171260889	1.8620557544
H	-0.0000008529	1.3069437365	-0.0644847215
H	-0.0000101283	-0.1214933972	-3.8036452304
4			
QSD Point 11			
Ca	0.0000005917	-0.0092106657	-1.7839982037
Ca	-0.0000001750	-0.0179090971	1.8814903996
H	-0.0000021772	1.2781650660	-0.0595087918
H	-0.0000143915	-0.1997674476	-3.8171973738
4			
QSD Point 12			
Ca	0.0000010421	-0.0061082563	-1.8040193627
Ca	-0.0000002767	-0.0189693077	1.9024130422
H	-0.0000055572	1.2863119951	-0.0853025072
H	-0.0000248779	-0.2891209283	-3.8272504990
4			
QSD Point 13			
Ca	0.0000020807	-0.0019459284	-1.8233770593
Ca	-0.0000004778	-0.0198863442	1.9217323843
H	-0.0000151381	1.2544192299	-0.0805640645
H	-0.0000485991	-0.3862748122	-3.8304638028
4			
QSD Point 14			
Ca	0.0000004859	0.0009836542	-1.8427032347
Ca	-0.0000000980	-0.0210520691	1.9420801089
H	-0.0000042881	1.2827935681	-0.1232645946
H	-0.0000111384	-0.4847876639	-3.8283844306
4			
QSD Point 15			
Ca	0.0000005947	0.0061160808	-1.8624085455
Ca	-0.0000000934	-0.0218736043	1.9609265992
H	-0.0000066623	1.2242023576	-0.1002452666
H	-0.0000132697	-0.5976159116	-3.8172533840
4			
QSD Point 16			
Ca	0.0000007007	0.0092941996	-1.8828667911
Ca	-0.0000000905	-0.0231758410	1.9823641420
H	-0.0000089388	1.2711562208	-0.1620704354
H	-0.0000153238	-0.7191628587	-3.7943692571
4			
QSD Point 17			
Ca	0.0000008273	0.0160354169	-1.9099060993
Ca	-0.0000000563	-0.0242506318	2.0080139404
H	-0.0000132343	1.2196359947	-0.1559442158
H	-0.0000174242	-0.8929639592	-3.7452426337
4			
QSD Point 18			
Ca	0.0000007882	0.0199086037	-1.9369803855
Ca	-0.0000000297	-0.0254659141	2.0355989376
H	-0.0000139322	1.2765893475	-0.2336119085
H	-0.0000162293	-1.0556069487	-3.6878829875
4			
QSD Point 19			
Ca	0.0000009500	0.0184219459	-1.9596515190
Ca	-0.0000000562	-0.0264075739	2.0628323512
H	-0.0000159570	1.5059159152	-0.4729041792
H	-0.0000195855	-1.1883732341	-3.6300064633
4			
QSD Point 20			



Ca	0.0000006642	0.0148454041	-1.9785538672
Ca	-0.0000000559	-0.0255582744	2.0880917265
H	-0.0000105584	1.7451980837	-0.8014452095
H	-0.0000136276	-1.3192085957	-3.5542479882
4			
QSD Point 21			
Ca	0.0000028482	0.0116484364	-1.9934144450
Ca	-0.0000002788	-0.0232144029	2.1085237571
H	-0.0000445448	1.9053821076	-1.1180859228
H	-0.0000576271	-1.4454698757	-3.4591520359
4			
QSD Point 22			
Ca	-0.0000024013	0.0093889753	-2.0043858875
Ca	0.0000002498	-0.0205152852	2.1234144883
H	0.0000377468	1.9930257108	-1.3710678348
H	0.0000478074	-1.5505961019	-3.3620177856
4			
QSD Point 23			
Ca	0.0000089337	0.0077303944	-2.0129071718
Ca	-0.0000009542	-0.0178712301	2.1346794880
H	-0.0001421890	2.0408038837	-1.5750589410
H	-0.0001751114	-1.6375609359	-3.2671285218
4			
QSD Point 24			
Ca	0.0000014415	0.0064163095	-2.0197401561
Ca	-0.0000001557	-0.0153536184	2.1434814176
H	-0.0000232804	2.0661447740	-1.7458193808
H	-0.0000278460	-1.7107591945	-3.1746617605
4			
QSD Point 25			
Ca	0.0000024501	0.0052916077	-2.0254082126
Ca	-0.0000002660	-0.0129435876	2.1506132372
H	-0.0000401621	2.0776600866	-1.8945617835
H	-0.0000466851	-1.7733846771	-3.0841248308
4			
QSD Point 26			
Ca	0.0000001644	0.0042656824	-2.0302211324
Ca	-0.0000000179	-0.0105750618	2.1565303885
H	-0.0000027351	2.0796931880	-2.0299708442
H	-0.0000030910	-1.8288053110	-2.9926247310
4			
QSD Point 27			
Ca	0.0000046660	0.0032329843	-2.0341512438
Ca	-0.0000005064	-0.0080728474	2.1613011062
H	-0.0000788699	2.0737219801	-2.1634509063
H	-0.0000865331	-1.8812683467	-2.8925707674
4			
QSD Point 28			
Ca	0.0001369209	0.0025912550	-2.0361910052
Ca	-0.0000148435	-0.0064892347	2.1637440881
H	-0.0023370820	2.0661552523	-2.2440653780
H	-0.0025172401	-1.9111549293	-2.8279900655
4			
QSD Point 29			
Ca	-0.0008317497	0.0022201326	-2.0372406463
Ca	0.0000901532	-0.0055726989	2.1649995899
H	0.0142750143	2.0604679868	-2.2897879528
H	0.0152140302	-1.9271556311	-2.7904533883
4			

QSD Point 30			
Ca	0.0003366292	0.0017056823	-2.0382786360
Ca	-0.0000364570	-0.0042852966	2.1662447732
H	-0.0058222730	2.0511944903	-2.3521416965
H	-0.0061138561	-1.9486180037	-2.7363385504
4			
QSD Point 31			
Ca	-0.0000642375	0.0014184144	-2.0387955249
Ca	0.0000069551	-0.0035660543	2.1668596874
H	0.0011157643	2.0452604101	-2.3864687012
H	0.0011620309	-1.9598610741	-2.7059094502
4			
QSD Point 32			
Ca	0.0000118811	0.0012007429	-2.0391328221
Ca	-0.0000012862	-0.0030202777	2.1672600692
H	-0.0002070275	2.0404118988	-2.4122392442
H	-0.0002142718	-1.9680594214	-2.6826474173
4			
QSD Point 33			
Ca	-0.0000022461	0.0010227084	-2.0393699468
Ca	0.0000002431	-0.0025733384	2.1675411326
H	0.0000392409	2.0362272186	-2.4331622472
H	0.0000404075	-1.9745675452	-2.6634716082
4			
QSD Point 34			
Ca	0.0000003934	0.0008744907	-2.0395405696
Ca	-0.0000000426	-0.0022009585	2.1677431091
H	-0.0000068885	2.0325947761	-2.4504745672
H	-0.0000070632	-1.9798487528	-2.6474060448
4			
QSD Point 35			
Ca	0.0000000000	0.0007492986	-2.0396784146
Ca	0.0000000000	-0.0018863088	2.1679055333
H	0.0000016888	2.0294167274	-2.4650542566
H	0.0000016888	-1.9842043460	-2.6338037272
4			
QSD Point 36			
Ca	0.0000000000	0.0006417239	-2.0399072453
Ca	0.0000000000	-0.0016167727	2.1681663639
H	0.0000000000	2.0265838022	-2.4777464676
H	0.0000000000	-1.9878116961	-2.6223839688
4			
QSD Point 37			
Ca	0.0000000000	0.0002395261	-2.0400035154
Ca	0.0000000000	-0.0006035992	2.1682886173
H	0.0000000000	2.0155207917	-2.5235941334
H	0.0000000000	-2.0010436868	-2.5775695129
4			
QSD Point 38			
Ca	0.0000000000	-0.0002396178	-2.0400035162
Ca	0.0000000000	0.0006038217	2.1682886164
H	0.0000000000	2.0010409553	-2.5775794079
H	0.0000000000	-2.0155232563	-2.5235841713
4			
QSD Point 39			
Ca	0.0000000000	-0.0006418614	-2.0399072080
Ca	0.0000000000	0.0016171153	2.1681663193
H	0.0000000000	1.9878070835	-2.6223991554
H	0.0000000000	-2.0265873446	-2.4777309896

4			
QSD Point 40			
Ca	0.0000000000	-0.0007494535	-2.0396782851
Ca	0.0000000000	0.0018866908	2.1679053786
H	-0.0000002879	1.9841991940	-2.6338203160
H	-0.0000002879	-2.0294206054	-2.4650366694
4			
QSD Point 41			
Ca	-0.0000007873	-0.0008746728	-2.0395403385
Ca	0.0000000852	0.0022014046	2.1677428407
H	0.0000141339	1.9798426061	-2.6474252648
H	0.0000137842	-2.0325991310	-2.4504538648
4			
QSD Point 42			
Ca	0.0000039659	-0.0010228961	-2.0393697076
Ca	-0.0000004293	0.0025738073	2.1675408631
H	-0.0000713455	1.9745607192	-2.6634920313
H	-0.0000692854	-2.0362315708	-2.4331406178
4			
QSD Point 43			
Ca	-0.0000213243	-0.0012010591	-2.0391324004
Ca	0.0000023084	0.0030210638	2.1672595549
H	0.0003845793	1.9680479119	-2.6826808429
H	0.0003715737	-2.0404190748	-2.4122021390
4			
QSD Point 44			
Ca	0.0001149830	-0.0014204381	-2.0387929649
Ca	-0.0000124494	0.0035711481	2.1668566046
H	-0.0020800555	1.9597818523	-2.7061282995
H	-0.0019971207	-2.0453032697	-2.3862290621
4			
QSD Point 45			
Ca	-0.0005395515	-0.0017399692	-2.0382257790
Ca	0.0000584376	0.0043715855	2.1661809034
H	0.0098040007	1.9472100259	-2.7400152289
H	0.0093271425	-2.0518543319	-2.3480271011
4			
QSD Point 46			
Ca	0.0004895029	-0.0022062718	-2.0372801858
Ca	-0.0000530546	0.0055372516	2.1650454400
H	-0.0089520295	1.9278147396	-2.7889640970
H	-0.0084030207	-2.0602687253	-2.2915281799
4			
QSD Point 47			
Ca	-0.0000228877	-0.0025526474	-2.0362437177
Ca	0.0000024810	0.0063924212	2.1638134281
H	0.0004205587	1.9129310265	-2.8238935759
H	0.0003909020	-2.0656168322	-2.2488230479
4			
QSD Point 48			
Ca	0.0000065925	-0.0032327069	-2.0340987474
Ca	-0.0000007153	0.0080677281	2.1612386978
H	-0.0001222590	1.8814647721	-2.8920989102
H	-0.0001114434	-2.0737258670	-2.1635286192
4			
QSD Point 49			
Ca	0.0000005906	-0.0042758349	-2.0302075142
Ca	-0.0000000642	0.0106017381	2.1565110912
H	-0.0000111065	1.8281641419	-2.9937962420

H	-0.0000098244	-2.0797090748	-2.0285735106
4			
QSD Point 50			
Ca	-0.0000022808	-0.0053001522	-2.0253656922
Ca	0.0000002476	0.0129636714	2.1505613810
H	0.0000434642	1.7728709521	-3.0849245098
H	0.0000373819	-2.0776052096	-1.8933908765
4			
QSD Point 51			
Ca	0.0000009046	-0.0064250332	-2.0196946553
Ca	-0.0000000977	0.0153713027	2.1434235736
H	-0.0000174771	1.7102772831	-3.1753125436
H	-0.0000146086	-2.0660191756	-1.7446777780
4			
QSD Point 52			
Ca	-0.0000077084	-0.0077438927	-2.0128302908
Ca	0.0000008231	0.0178936343	2.1345807131
H	0.0001511124	1.6369060632	-3.2678838510
H	0.0001226737	-2.0405031439	-1.5734330186
4			
QSD Point 53			
Ca	0.0000019982	-0.0094086954	-2.0042827791
Ca	-0.0000002078	0.0205432128	2.1232776031
H	-0.0000397881	1.5496091110	-3.3630104557
H	-0.0000314065	-1.9923650874	-1.3687320537
4			
QSD Point 54			
Ca	-0.0000022727	-0.0116748973	-1.9932865289
Ca	0.0000002223	0.0232404620	2.1083494836
H	0.0000459890	1.4443291757	-3.4601089645
H	0.0000355440	-1.9042254307	-1.1152856285
4			
QSD Point 55			
Ca	-0.0000004421	-0.0148820415	-1.9783791066
Ca	0.0000000371	0.0255763619	2.0878533159
H	0.0000090719	1.3178747738	-3.5551323868
H	0.0000070305	-1.7431266355	-0.7980298137
4			
QSD Point 56			
Ca	-0.0000006750	-0.0184519031	-1.9594475596
Ca	0.0000000398	0.0264059033	2.0625708724
H	0.0000139163	1.1871441556	-3.6306085856
H	0.0000113458	-1.5034291802	-0.4700148424
4			
QSD Point 57			
Ca	-0.0000005475	-0.0199010938	-1.9367399684
Ca	0.0000000206	0.0254529424	2.0353323847
H	0.0000112742	1.0542543766	-3.6884015492
H	0.0000096782	-1.2750195924	-0.2320540781
4			
QSD Point 58			
Ca	-0.0000005897	-0.0159688894	-1.9095746568
Ca	0.0000000405	0.0242377676	2.0076906376
H	0.0000124246	0.8909673590	-3.7458548471
H	0.0000094143	-1.2197732787	-0.1556556693
4			
QSD Point 59			
Ca	-0.0000004878	-0.0092237739	-1.8825389205
Ca	0.0000000633	0.0231592848	1.9820402636

H	0.0000106728	0.7171222367	-3.7948544237
H	0.0000062072	-1.2712576749	-0.1617440171
4			
QSD Point 60			
Ca	-0.0000004230	-0.0060461404	-1.8620363639
Ca	0.0000000667	0.0218528070	1.9605475273
H	0.0000094437	0.5954951975	-3.8175408699
H	0.0000047248	-1.2240357807	-0.0996837960
4			
QSD Point 61			
Ca	-0.0000004556	-0.0009138857	-1.8423841149
Ca	0.0000000921	0.0210364204	1.9417632712
H	0.0000104479	0.4830636773	-3.8284817992
H	0.0000040060	-1.2832216134	-0.1232579725
4			
QSD Point 62			
Ca	-0.0000003438	0.0020013212	-1.8230947453
Ca	0.0000000791	0.0198718710	1.9214463903
H	0.0000080319	0.3848440993	-3.8304557163
H	0.0000024918	-1.2546156603	-0.0804258160
4			
QSD Point 63			
Ca	-0.0000002506	0.0061528908	-1.8037500350
Ca	0.0000000666	0.0189551126	1.9021337399
H	0.0000059835	0.2878724438	-3.8271517174
H	0.0000013305	-1.2862739127	-0.0850046516
4			
QSD Point 64			
Ca	-0.0000001094	0.0092619577	-1.7837180256
Ca	0.0000000324	0.0178972397	1.8812065414
H	0.0000026616	0.1985793392	-3.8170255408
H	0.0000003999	-1.2785450431	-0.0595342847
4			
QSD Point 65			
Ca	0.0000000000	0.0127255371	-1.7644763302
Ca	0.0000000000	0.0171120848	1.8617371727
H	0.0000018986	0.1203484323	-3.8033982146
H	0.0000000000	-1.3068197347	-0.0641083491
4			
QSD Point 66			
Ca	0.0000000000	0.0149776126	-1.7451716825
Ca	0.0000000000	0.0162346097	1.8412881287
H	0.0000007498	0.0516996135	-3.7860642589
H	0.0000000000	-1.2928309020	-0.0359362221

## 5.4 M4 → TS4 → M5

6

QSD Point 1

Ca	0.0000350396	0.0000057121	1.7478044669
Ca	-0.0000181352	-0.0000184404	-1.7477984144
H	0.0000629135	1.3652736772	0.0000010867
H	0.0000629609	-1.3652687541	-0.0001615058
H	0.0000870947	0.0005006019	-3.8011861738
H	-0.0008851596	0.0000006057	3.8011059204

6

QSD Point 2

Ca	0.0000550651	0.0000093699	1.7479517730
Ca	-0.0000197399	-0.0000188498	-1.7479528881
H	0.0001825379	1.3659708649	-0.0001743509
H	0.0001828928	-1.3655209308	0.0000306387
H	-0.0002011596	0.0001846871	-3.8010660029
H	-0.0015689539	-0.0002576600	3.8012540562

6

QSD Point 3

Ca	-0.0005135058	0.0000474947	1.7483615323
Ca	0.0002063204	-0.0001620068	-1.7483597407
H	-0.0018767589	1.3658214341	-0.0002376115
H	-0.0018772740	-1.3650616465	-0.0011037415
H	0.0014032807	0.0039685883	-3.8004212693
H	0.0145657569	-0.0001748832	3.8016913819

6

QSD Point 4

Ca	0.0013912254	0.0002619405	1.7481505052
Ca	-0.0006851915	-0.0008597161	-1.7481620044
H	0.0007802564	1.3634877707	0.0016846804
H	0.0008799130	-1.3626611173	-0.0054378923
H	0.0041180832	0.0230160204	-3.7974563685
H	-0.0338531774	-0.0000725640	3.8016668370

6

QSD Point 5

Ca	-0.0005316558	-0.0017421059	1.7515622264
Ca	0.0003549167	0.0049153782	-1.7505031520
H	0.0064682596	1.3460411577	-0.0272361859
H	0.0073039633	-1.3863989748	-0.0160423214
H	-0.0115240620	-0.1057228531	-3.8041580817
H	0.0047797405	0.0198978094	3.8053232651

6

QSD Point 6

Ca	-0.0068651123	0.0028436745	1.7464752133
Ca	0.0028530361	-0.0074834951	-1.7481022667
H	-0.0116796544	1.4127704147	0.0320570066
H	-0.0199915125	-1.3160671458	0.0436490953
H	0.0063641299	0.1367814670	-3.8007891336
H	0.1848443289	-0.0489856488	3.7897816268

6

QSD Point 7

Ca	-0.0116260298	-0.0001986068	1.7473262606
Ca	0.0049158059	0.0004288340	-1.7465982561
H	-0.0289420722	1.3664792417	-0.0044897559
H	-0.0287565390	-1.3638837562	0.0012009363
H	0.0099843319	-0.0126363154	-3.7995474718
H	0.3145414451	0.0008860134	3.7738877260

6

QSD Point 8			
Ca	-0.0167480808	-0.0002241304	1.7472390196
Ca	0.0070968166	0.0005104886	-1.7458621007
H	-0.0418632784	1.3698789178	-0.0054944527
H	-0.0423812895	-1.3621063481	0.0050731663
H	0.0127224516	-0.0181883251	-3.7982734505
H	0.4552976076	-0.0009710703	3.7439425594
6			
QSD Point 9			
Ca	-0.0219167415	-0.0002892788	1.7463363946
Ca	0.0092307801	0.0005889226	-1.7438956369
H	-0.0575233605	1.3700822862	-0.0064993136
H	-0.0580574606	-1.3605363398	0.0060289598
H	0.0175944240	-0.0210024311	-3.7962622125
H	0.6024344160	-0.0004586335	3.6996776137
6			
QSD Point 10			
Ca	-0.0265417194	-0.0004296925	1.7456194444
Ca	0.0111395103	0.0009884842	-1.7419809011
H	-0.0708019646	1.3722055455	-0.0084042123
H	-0.0717582084	-1.3601111067	0.0097071606
H	0.0188327197	-0.0333533358	-3.7938694668
H	0.7361850821	-0.0009610490	3.6478824926
6			
QSD Point 11			
Ca	-0.0309854648	-0.0005449049	1.7442265067
Ca	0.0128697339	0.0011214000	-1.7389881154
H	-0.0880383154	1.3720991145	-0.0088962017
H	-0.0878565295	-1.3597379791	0.0103971633
H	0.0232147000	-0.0363550272	-3.7917472970
H	0.8730389891	0.0010699841	3.5819455213
6			
QSD Point 12			
Ca	-0.0349576837	-0.0005083145	1.7445451216
Ca	0.0143958990	0.0010143008	-1.7377681641
H	-0.1057504703	1.3766843307	-0.0066610028
H	-0.1069899188	-1.3606791070	0.0145782228
H	0.0265875961	-0.0357972513	-3.7854554551
H	1.0037771848	-0.0003281494	3.5080574537
6			
QSD Point 13			
Ca	-0.0383981840	0.0006659368	1.7417290261
Ca	0.0155558563	-0.0022842091	-1.7334132560
H	-0.1250248162	1.3896627548	0.0104026933
H	-0.1430416733	-1.3450465142	0.0238408784
H	0.0390855566	0.0352101917	-3.7801363688
H	1.1372894543	-0.0154770129	3.4152222563
6			
QSD Point 14			
Ca	-0.0417450355	-0.0044196003	1.7393765851
Ca	0.0170101259	0.0096224322	-1.7265604032
H	-0.1854552851	1.3325301225	-0.0445398606
H	-0.1075392809	-1.4051778315	-0.0141009345
H	0.0277327391	-0.2045783097	-3.7741221946
H	1.2488274897	0.0703391993	3.3231368515
6			
QSD Point 15			
Ca	-0.0439454229	-0.0006416288	1.7353763484
Ca	0.0178758560	0.0011055946	-1.7224184946

H	-0.1691839839	1.3864844719	-0.0021747937
H	-0.1761114246	-1.3546274145	0.0316959252
H	0.0279358250	-0.0469157175	-3.7703183966
H	1.3539969249	-0.0033906033	3.2255376449
6			
QSD Point 16			
Ca	-0.0460915284	-0.0016030665	1.7316923097
Ca	0.0186080884	0.0029356344	-1.7157275637
H	-0.2089206873	1.3790173352	-0.0071798392
H	-0.1914925331	-1.3655142524	0.0300029578
H	0.0274238523	-0.0827126485	-3.7621920745
H	1.4658483414	0.0162209734	3.1045424590
6			
QSD Point 17			
Ca	-0.0476312669	-0.0018488921	1.7267950526
Ca	0.0190315118	0.0032806825	-1.7078091957
H	-0.2444854352	1.3803398470	-0.0044102000
H	-0.2195271297	-1.3675620846	0.0362764047
H	0.0267093919	-0.0911180476	-3.7528352577
H	1.5745516015	0.0214061815	2.9660102826
6			
QSD Point 18			
Ca	-0.0484398529	-0.0025633145	1.7210322935
Ca	0.0190636323	0.0038954142	-1.6986543312
H	-0.2948696060	1.3773571041	-0.0014133294
H	-0.2393670302	-1.3729498609	0.0415632538
H	0.0267559192	-0.1005265211	-3.7423145275
H	1.6756047342	0.0431493036	2.8123212311
6			
QSD Point 19			
Ca	-0.0484980993	-0.0032651548	1.7149321506
Ca	0.0187406723	0.0044276346	-1.6892217934
H	-0.3473691733	1.3725596220	0.0023301767
H	-0.2546557024	-1.3786392343	0.0473828609
H	0.0265507197	-0.1077911549	-3.7319097429
H	1.7587565689	0.0676456060	2.6598430741
6			
QSD Point 20			
Ca	-0.0472038383	-0.0090571800	1.7084763206
Ca	0.0174665264	0.0067730561	-1.6793381468
H	-0.5425143125	1.3147455863	0.0065990700
H	-0.1213772414	-1.4059234821	0.0516174235
H	0.0388016792	-0.1085105416	-3.7216033627
H	1.8075724223	0.2905149584	2.5047286127
6			
QSD Point 21			
Ca	-0.0468856314	0.0034459474	1.7019384511
Ca	0.0178527372	0.0021509441	-1.6695524159
H	-0.2151620374	1.4138196552	0.0121026579
H	-0.5137310784	-1.3227950241	0.0578417243
H	0.0069961493	-0.1165794801	-3.7115267831
H	1.8763688614	-0.1970014655	2.3537752972
6			
QSD Point 22			
Ca	-0.0451003503	0.0003109350	1.6968662157
Ca	0.0162185371	0.0017050809	-1.6611992511
H	-0.3608438379	1.3958155794	0.0271227379
H	-0.4493971808	-1.3543148292	0.0590432582
H	0.0257504579	-0.0679944706	-3.7011228108



H	1.9329548278	-0.0536716832	2.1966859412
6			
QSD Point 23			
Ca	-0.0438017399	0.0015994061	1.6886633549
Ca	0.0165080898	0.0087075396	-1.6477736148
H	-0.2996216036	1.3753794460	-0.0108551000
H	-0.5640842575	-1.3588208359	0.0313303542
H	-0.0094001648	-0.2427849207	-3.6902199719
H	1.9584181438	-0.1836218784	2.0437939834
6			
QSD Point 24			
Ca	-0.0409083057	-0.0010572812	1.6803888243
Ca	0.0136521053	0.0004707855	-1.6386027919
H	-0.4745316183	1.3875692859	0.0489461860
H	-0.4542244567	-1.3564131247	0.0813799613
H	0.0226752378	-0.0284380335	-3.6848519898
H	1.9899037962	0.0206034494	1.8929346977
6			
QSD Point 25			
Ca	-0.0383117575	-0.0003383570	1.6735047147
Ca	0.0122906719	0.0024134311	-1.6275474507
H	-0.4702903385	1.3789397493	0.0426844744
H	-0.5204646493	-1.3602614009	0.0669698307
H	0.0223683097	-0.0714569219	-3.6754484804
H	2.0030961935	-0.0297352382	1.7383370408
6			
QSD Point 26			
Ca	-0.0324465842	-0.0000811000	1.6593355301
Ca	0.0089664126	0.0002286500	-1.6071717342
H	-0.5511038957	1.3656034709	0.0655681886
H	-0.5506177345	-1.3656673535	0.0677105990
H	0.0332513905	-0.0061261271	-3.6605075654
H	2.0021421637	0.0003227897	1.4529734287
6			
QSD Point 27			
Ca	-0.0306796822	0.0001577911	1.6553883767
Ca	0.0080573491	-0.0004413940	-1.6015228749
H	-0.5654532210	1.3643586350	0.0719637337
H	-0.5664944947	-1.3641812770	0.0678382090
H	0.0358697936	0.0118063329	-3.6561651802
H	1.9956385198	-0.0007064260	1.3744407897
6			
QSD Point 28			
Ca	-0.0239850332	0.0004826258	1.6411338567
Ca	0.0049927026	-0.0006028238	-1.5806405394
H	-0.6488786110	1.3312918966	0.0846612461
H	-0.5903848899	-1.3851216710	0.0564581233
H	0.0450141826	0.0354879155	-3.6397852555
H	1.9494655107	0.0231214423	1.0931931808
6			
QSD Point 29			
Ca	-0.0194812386	0.0033464828	1.6304790452
Ca	0.0020211390	-0.0141190082	-1.5701992098
H	-0.5994432351	1.4245437705	0.1611680313
H	-0.6920488482	-1.2866335510	0.1115080031
H	0.0714866275	0.3194921167	-3.6214051616
H	1.9142935981	-0.0290407100	0.9517453761
6			
QSD Point 30			

Ca	-0.0156118342	0.0022819333	1.6249624077
Ca	0.0015031822	-0.0063143269	-1.5585672024
H	-0.6933818141	1.3424737980	0.1271796675
H	-0.6638310187	-1.3644109344	0.0651162014
H	0.0613928191	0.1735314093	-3.6162286538
H	1.8568402839	0.0087509244	0.7837758043
6			
QSD Point 31			
Ca	-0.0095008779	0.0033714670	1.6099200801
Ca	-0.0005851196	-0.0092599598	-1.5391412554
H	-0.7348259799	1.3388262788	0.1533075683
H	-0.6988001431	-1.3630974982	0.0670761932
H	0.0725011436	0.2503776072	-3.5982509141
H	1.7621873264	0.0080452386	0.5633987375
6			
QSD Point 32			
Ca	-0.0054115485	0.0035930946	1.5986465832
Ca	-0.0012795325	-0.0101622170	-1.5251601149
H	-0.7790490370	1.3293246566	0.1692032899
H	-0.7054444957	-1.3701255592	0.0792557821
H	0.0672101047	0.2716862980	-3.5834500921
H	1.6833493905	0.0303309755	0.4128551286
6			
QSD Point 33			
Ca	-0.0033264091	0.0025581661	1.5874819107
Ca	0.0001643302	-0.0088098007	-1.5125103861
H	-0.9864794659	1.2012282581	0.1750003047
H	-0.5087518034	-1.4591622769	0.1060254602
H	0.0149459568	0.2328362786	-3.5734463920
H	1.6060230753	0.2736894371	0.3112325516
6			
QSD Point 34			
Ca	-0.0024184316	0.0010723376	1.5766372688
Ca	0.0012029171	-0.0053129468	-1.5016470343
H	-1.1495589199	1.0738598468	0.1732856103
H	-0.3303979814	-1.5161036359	0.1438591485
H	-0.0167010832	0.1343939872	-3.5648677401
H	1.5449920337	0.4764745398	0.2657909211
6			
QSD Point 35			
Ca	0.0000891379	0.0011520380	1.5677888588
Ca	-0.0021376111	-0.0016327355	-1.4927317783
H	0.7208904553	1.4284707960	0.1765567418
H	-1.5734197518	-0.0970604112	0.1732130883
H	0.0515867156	0.0296849257	-3.5568260246
H	0.8823986248	-1.3419807239	0.2224660543
6			
QSD Point 36			
Ca	0.0009338927	0.0000645118	1.5673523392
Ca	-0.0020243812	0.0024757624	-1.4941211032
H	1.4355428121	-0.7618251614	0.2006354023
H	-0.0620279305	1.5777062350	0.2132620932
H	0.0387666651	-0.0450819590	-3.5562889570
H	-1.3689190645	-0.8718112662	0.2304046950

## 5.5 M5 → TS5 → M6

6

QSD Point 1

Ca	-1.1855190556	0.1376994346	1.5752605205
Ca	0.6851409317	-0.0781657234	-0.8447986828
H	0.4736374673	1.3120226496	1.0256349219
H	0.0694002991	-1.4366073873	0.9583562584
H	-1.6022621898	0.2494518106	-0.4863056115
H	1.9438336172	-0.2232981756	-2.4777624967

6

QSD Point 2

Ca	-1.1852342456	0.1376430387	1.5757551722
Ca	0.6847251812	-0.0780907917	-0.8454457683
H	0.4733594531	1.3118797608	1.0253305800
H	0.0691688899	-1.4363701199	0.9580628811
H	-1.6026500769	0.2494897300	-0.4856485315
H	1.9448618681	-0.2234490094	-2.4776694237

6

QSD Point 3

Ca	-1.1848294985	0.1375705815	1.5762521923
Ca	0.6842086679	-0.0779990491	-0.8461643411
H	0.4731904180	1.3118010752	1.0247781636
H	0.0690288991	-1.4362172235	0.9575178906
H	-1.6032860903	0.2495629193	-0.4848797102
H	1.9459186738	-0.2236156949	-2.4771192855

6

QSD Point 4

Ca	-1.1843678828	0.1374904599	1.5768413248
Ca	0.6836596102	-0.0778973027	-0.8470765379
H	0.4731267446	1.3117992404	1.0239571811
H	0.0689739135	-1.4361602494	0.9566999968
H	-1.6042188970	0.2496767280	-0.4839371670
H	1.9470575814	-0.2238062677	-2.4760998881

6

QSD Point 5

Ca	-1.1842867112	0.1374744346	1.5772845593
Ca	0.6836271244	-0.0778742532	-0.8478077764
H	0.4732465386	1.3119337508	1.0233158478
H	0.0690633979	-1.4363042511	0.9560531715
H	-1.6049849910	0.2497769527	-0.4833121482
H	1.9475657112	-0.2239040252	-2.4751487444

6

QSD Point 6

Ca	-1.1849476000	0.1375828718	1.5772337606
Ca	0.6845361239	-0.0780052881	-0.8478002436
H	0.4735129706	1.3121737559	1.0234958590
H	0.0692660013	-1.4366380410	0.9562190914
H	-1.6048600077	0.2497720321	-0.4836231271
H	1.9467235818	-0.2237827223	-2.4751404306

6

QSD Point 7

Ca	-1.1858879532	0.1377369527	1.5768338214
Ca	0.6857663383	-0.0781977803	-0.8471972393
H	0.4737328758	1.3123534704	1.0242625410
H	0.0694319701	-1.4369221261	0.9569733969
H	-1.6040946771	0.2496849189	-0.4844984091
H	1.9452825160	-0.2235528271	-2.4759892011

6

QSD Point 8			
Ca	-1.1869927074	0.1379174621	1.5762407197
Ca	0.6871917340	-0.0784286122	-0.8462081746
H	0.4738964474	1.3124646603	1.0253809407
H	0.0695584904	-1.4371366607	0.9580812579
H	-1.6029864022	0.2495536565	-0.4856735176
H	1.9435635077	-0.2232678974	-2.4774363164
6			
QSD Point 9			
Ca	-1.1887668184	0.1382000475	1.5754093418
Ca	0.6895034501	-0.0788120002	-0.8442999481
H	0.4741158706	1.3124587185	1.0270254623
H	0.0697673754	-1.4372766735	0.9597178426
H	-1.6018653988	0.2494297755	-0.4872460028
H	1.9414765911	-0.2228972593	-2.4802217861
6			
QSD Point 10			
Ca	-1.1910203503	0.1385152630	1.5757205343
Ca	0.6926366724	-0.0793541191	-0.8411510051
H	0.4746879591	1.3118135145	1.0270244226
H	0.0704987977	-1.4368048649	0.9597301224
H	-1.6058600883	0.2499983442	-0.4865363216
H	1.9432880793	-0.2230655291	-2.4844028429
6			
QSD Point 11			
Ca	-1.1898317523	0.1382575117	1.5785788332
Ca	0.6913671620	-0.0791722548	-0.8415557427
H	0.4751652923	1.3109409738	1.0223571633
H	0.0712196726	-1.4358513857	0.9550989823
H	-1.6155062322	0.2512759430	-0.4810567105
H	1.9518169276	-0.2243481796	-2.4830376158
6			
QSD Point 12			
Ca	-1.1839560479	0.1372459472	1.5841318373
Ca	0.6839291555	-0.0779614100	-0.8473053930
H	0.4754061933	1.3101972718	1.0125334832
H	0.0716985955	-1.4347046771	0.9453255232
H	-1.6297148681	0.2531011358	-0.4706885698
H	1.9668680416	-0.2267756592	-2.4736119711
6			
QSD Point 13			
Ca	-1.1720435826	0.1352669674	1.5931098880
Ca	0.6684283671	-0.0754034389	-0.8600797911
H	0.4753972525	1.3097589111	0.9962126606
H	0.0718803034	-1.4334700228	0.9290669566
H	-1.6494655830	0.2555893590	-0.4542575492
H	1.9900343124	-0.2306391673	-2.4536672552
6			
QSD Point 14			
Ca	-1.1591246988	0.1331547637	1.6018287213
Ca	0.6512975565	-0.0725608037	-0.8745246806
H	0.4752371962	1.3099041943	0.9802267027
H	0.0717539713	-1.4327846572	0.9131245142
H	-1.6667713967	0.2577404267	-0.4386195923
H	2.0118384415	-0.2343513153	-2.4316507556
6			
QSD Point 15			
Ca	-1.1454420287	0.1309465372	1.6102529494
Ca	0.6327720691	-0.0694743067	-0.8903665024

H	0.4750590735	1.3107256395	0.9647274413
H	0.0714206099	-1.4327841513	0.8976443764
H	-1.6819899468	0.2596087809	-0.4238311157
H	2.0324112929	-0.2379198911	-2.4080422392
6			
QSD Point 16			
Ca	-1.1312083616	0.1286739770	1.6183860230
Ca	0.6130619900	-0.0661811136	-0.9073436400
H	0.4749644590	1.3122931287	0.9498153013
H	0.0709581043	-1.4335704402	0.8827222802
H	-1.6955377776	0.2612557312	-0.4098719616
H	2.0519926558	-0.2413686746	-2.3833230932
6			
QSD Point 17			
Ca	-1.1165922085	0.1263603415	1.6262688243
Ca	0.5922963638	-0.0627042681	-0.9252537078
H	0.4750261609	1.3146981338	0.9355861872
H	0.0704101252	-1.4352562321	0.8684480576
H	-1.7078166620	0.2627394974	-0.3966973832
H	2.0709072905	-0.2447348641	-2.3579670685
6			
QSD Point 18			
Ca	-1.1017504390	0.1240277526	1.6339164960
Ca	0.5706275853	-0.0590720945	-0.9438731451
H	0.4753168488	1.3180223267	0.9220903499
H	0.0698226341	-1.4379426881	0.8548677808
H	-1.7192644351	0.2641228159	-0.3842166321
H	2.0894788758	-0.2480555041	-2.3323999399
6			
QSD Point 19			
Ca	-1.0869388573	0.1217164120	1.6411008317
Ca	0.5487219212	-0.0553995520	-0.9625858749
H	0.4760315539	1.3220229392	0.9089448754
H	0.0694530522	-1.4414309713	0.8416093442
H	-1.7308582776	0.2655388221	-0.3719817649
H	2.1078216775	-0.2513450415	-2.3067025019
6			
QSD Point 20			
Ca	-1.0724412305	0.1194700676	1.6475452655
Ca	0.5275042324	-0.0518447733	-0.9806133549
H	0.4773698131	1.3261607460	0.8954923144
H	0.0696479867	-1.4452227688	0.8280395898
H	-1.7437632301	0.2671427869	-0.3593561229
H	2.1259134983	-0.2546034499	-2.2807227822
6			
QSD Point 21			
Ca	-1.0620053970	0.1178630954	1.6517026100
Ca	0.5127282420	-0.0493717785	-0.9931355472
H	0.4788844031	1.3288681525	0.8847872223
H	0.0704013969	-1.4478028274	0.8172643633
H	-1.7549248986	0.2685504967	-0.3492695082
H	2.1391473235	-0.2570045302	-2.2609642305
6			
QSD Point 22			
Ca	-1.0570401814	0.1171029042	1.6534233347
Ca	0.5060740731	-0.0482593885	-0.9987881350
H	0.4799110516	1.3298159824	0.8789615476
H	0.0711545309	-1.4487552208	0.8114212736
H	-1.7614238079	0.2693787929	-0.3437918654

H	2.145554036	-0.2581804617	-2.2508412458
6			
QSD Point 23			
Ca	-1.0455892294	0.1156113307	1.6558294427
Ca	0.4950460496	-0.0458118927	-1.0079488768
H	0.4791926156	1.3315641566	0.8632232407
H	0.0699076385	-1.4487790149	0.7951132019
H	-1.7723084374	0.2713771415	-0.3318367480
H	2.1586087870	-0.2602387529	-2.2242684769
6			
QSD Point 24			
Ca	-1.0335588327	0.1139198247	1.6579954878
Ca	0.4837785338	-0.0435148131	-1.0172514846
H	0.4785180673	1.3333782990	0.8472940416
H	0.0687081811	-1.4491312777	0.7787173807
H	-1.7830418971	0.2731236778	-0.3196902452
H	2.1708360318	-0.2623613940	-2.1971059170
6			
QSD Point 25			
Ca	-1.0210570336	0.1121157203	1.6599541854
Ca	0.4722829530	-0.0413057216	-1.0267546687
H	0.4778689440	1.3353896224	0.8314300663
H	0.0675020952	-1.4498224186	0.7624880127
H	-1.7933209889	0.2746665439	-0.3076594108
H	2.1822211215	-0.2644747639	-2.1695986378
6			
QSD Point 26			
Ca	-1.0081470082	0.1102313293	1.6617125522
Ca	0.4605562913	-0.0391394775	-1.0364611984
H	0.4772393708	1.3376211673	0.8156528274
H	0.0662698818	-1.4508162061	0.7464150434
H	-1.8029642978	0.2760309406	-0.2958053775
H	2.1927257551	-0.2665352352	-2.1417252939
6			
QSD Point 27			
Ca	-0.9948160536	0.1082754239	1.6632650996
Ca	0.4485883365	-0.0369929379	-1.0463631805
H	0.4766106524	1.3400771547	0.7999654840
H	0.0649886845	-1.4520864567	0.7304842995
H	-1.8118687453	0.2772299455	-0.2841732603
H	2.2023104440	-0.2685176099	-2.1134431939
6			
QSD Point 28			
Ca	-0.9810690309	0.1062541657	1.6646104373
Ca	0.4363849541	-0.0348492700	-1.0564414336
H	0.4759753978	1.3427566245	0.7843599476
H	0.0636480338	-1.4536118245	0.7146701842
H	-1.8199779384	0.2782758343	-0.2727825853
H	2.2109520266	-0.2704043398	-2.0847233226
6			
QSD Point 29			
Ca	-0.9668995391	0.1041698583	1.6657435855
Ca	0.4239601564	-0.0326980746	-1.0666747117
H	0.4753248003	1.3456610424	0.7688357839
H	0.0622363436	-1.4553791928	0.6989587656
H	-1.8272644720	0.2791789882	-0.2616533564
H	2.2186338451	-0.2721831955	-2.0555515185
6			
QSD Point 30			

Ca	-0.9523103789	0.1020248559	1.6666612962
Ca	0.4113360619	-0.0305322235	-1.0770383089
H	0.4746542109	1.3487933235	0.7533930592
H	0.0607459433	-1.4573803700	0.6833381201
H	-1.8337207335	0.2799493484	-0.2507978674
H	2.2253493899	-0.2738455071	-2.0259277934
6			
QSD Point 31			
Ca	-0.9373002746	0.0998202633	1.6673577704
Ca	0.3985391068	-0.0283476482	-1.0875078034
H	0.4739579879	1.3521589444	0.7380352813
H	0.0591678562	-1.4596117115	0.6678020428
H	-1.8393516115	0.2805957284	-0.2402267773
H	2.2310963466	-0.2753851322	-1.9958592676
6			
QSD Point 32			
Ca	-0.9218722020	0.0975573190	1.6678282050
Ca	0.3855987756	-0.0261422017	-1.0980582915
H	0.4732318691	1.3557646795	0.7227664712
H	0.0574943673	-1.4620725819	0.6523463943
H	-1.8441711966	0.2811263862	-0.2299466426
H	2.2358788088	-0.2767980116	-1.9653606972
6			
QSD Point 33			
Ca	-0.9060264317	0.0952366383	1.6680661865
Ca	0.3725457284	-0.0239155326	-1.1086662127
H	0.4724704811	1.3596189095	0.7075918541
H	0.0557165029	-1.4647648688	0.6369698133
H	-1.8481990080	0.2815486483	-0.2199621280
H	2.2397035963	-0.2780815803	-1.9344493622
6			
QSD Point 34			
Ca	-0.8897651917	0.0928589147	1.6680661403
Ca	0.3594108652	-0.0216683205	-1.1193088476
H	0.4716688171	1.3637307934	0.6925166648
H	0.0538256794	-1.4676923053	0.6216722458
H	-1.8514586451	0.2818692712	-0.2102753915
H	2.2425817740	-0.2792346195	-1.9031461097
6			
QSD Point 35			
Ca	-0.8730881208	0.0904243598	1.6678211898
Ca	0.3462243610	-0.0194023024	-1.1299650645
H	0.4708207655	1.3681103991	0.6775460902
H	0.0518121860	-1.4708599835	0.6064547743
H	-1.8539755452	0.2820941921	-0.2008869534
H	2.2445258661	-0.2802568277	-1.8714713907
6			
QSD Point 36			
Ca	-0.8559955530	0.0879332006	1.6673250053
Ca	0.3330155123	-0.0171198696	-1.1406153136
H	0.4699198995	1.3727680452	0.6626857252
H	0.0496661206	-1.4742738481	0.5913198229
H	-1.8557763507	0.2822287371	-0.1917960437
H	2.2455511474	-0.2811487961	-1.8394475037
6			
QSD Point 37			
Ca	-0.8384860067	0.0853853895	1.6665707337
Ca	0.3198120629	-0.0148239987	-1.1512418278
H	0.4689587484	1.3777143152	0.6479411565

H	0.0473767472	-1.4779405139	0.5762707176
H	-1.8568880496	0.2822776471	-0.1830009626
H	2.2456743866	-0.2819118151	-1.8070961583
6			
QSD Point 38			
Ca	-0.8205570202	0.0827806948	1.6655515786
Ca	0.3066400932	-0.0125180122	-1.1618281548
H	0.4679293060	1.3829597380	0.6333177435
H	0.0449328838	-1.4818668156	0.5613112671
H	-1.8573377504	0.2822451335	-0.1744993739
H	2.2449137714	-0.2825476974	-1.7744385837
6			
QSD Point 39			
Ca	-0.8022032669	0.0801184865	1.6642600063
Ca	0.2935243950	-0.0102055714	-1.1723589687
H	0.4668222779	1.3885146063	0.6188209542
H	0.0423223904	-1.4860595165	0.5464460193
H	-1.8571525610	0.2821350730	-0.1662891013
H	2.2432878716	-0.2830586413	-1.7414947756
6			
QSD Point 40			
Ca	-0.7834195557	0.0773981371	1.6626891643
Ca	0.2804882787	-0.0078905086	-1.1828197860
H	0.4656280169	1.3943887416	0.6044564337
H	0.0395330056	-1.4905251198	0.5316801025
H	-1.8563593247	0.2819510274	-0.1583679717
H	2.2408168801	-0.2834472565	-1.7082852740
6			
QSD Point 41			
Ca	-0.7641987087	0.0746187632	1.6608309564
Ca	0.2675532864	-0.0055767475	-1.1931973822
H	0.4643359757	1.4005919292	0.5902292046
H	0.0365517021	-1.4952701621	0.5170185046
H	-1.8549838495	0.2816961428	-0.1507329532
H	2.2375212022	-0.2837164039	-1.6748281623
6			
QSD Point 42			
Ca	-0.7445324213	0.0717793577	1.6586766741
Ca	0.2547393341	-0.0032684110	-1.2034797866
H	0.4629346695	1.4071332324	0.5761449932
H	0.0333648808	-1.5003005984	0.5024673549
H	-1.8530513362	0.2813732030	-0.1433811834
H	2.2334224321	-0.2838693352	-1.6411412927
6			
QSD Point 43			
Ca	-0.7244107470	0.0688787024	1.6562168682
Ca	0.2420645514	-0.0009696147	-1.2136561195
H	0.4614119167	1.4140208526	0.5622098305
H	0.0299586071	-1.5056216891	0.4880335100
H	-1.8505869012	0.2809848441	-0.1363100973
H	2.2285431160	-0.2839095790	-1.6072413918
6			
QSD Point 44			
Ca	-0.7038210552	0.0659152425	1.6534404733
Ca	0.2295452622	0.0013155166	-1.2237163035
H	0.4597548289	1.4212619799	0.5484300274
H	0.0263186416	-1.5112377695	0.4737244316
H	-1.8476158190	0.2805335789	-0.1295176457
H	2.2229059622	-0.2838408646	-1.5731431151



6			
QSD Point 45			
Ca	-0.6827490862	0.0628872322	1.6503351104
Ca	0.2171961945	0.0035829699	-1.2336509251
H	0.4579504074	1.4288623126	0.5348125522
H	0.0224309792	-1.5171518913	0.4595485416
H	-1.8441641825	0.2800218563	-0.1230025022
H	2.2165342330	-0.2836670788	-1.5388599970
6			
QSD Point 46			
Ca	-0.6611786870	0.0597926225	1.6468866703
Ca	0.2050303216	0.0058285474	-1.2434510634
H	0.4559849958	1.4368257978	0.5213649127
H	0.0182823569	-1.5233658700	0.4455151612
H	-1.8402588475	0.2794528712	-0.1167639808
H	2.2094516931	-0.2833923866	-1.5044041954
6			
QSD Point 47			
Ca	-0.6390918769	0.0566294573	1.6430788411
Ca	0.1930585263	0.0080486783	-1.2531082766
H	0.4538466122	1.4451539759	0.5080950660
H	0.0138603488	-1.5298792180	0.4316341305
H	-1.8359287044	0.2788287877	-0.1108021728
H	2.2016817849	-0.2830208226	-1.4697853023
6			
QSD Point 48			
Ca	-0.6164694125	0.0533953586	1.6388932581
Ca	0.1812899106	0.0102396445	-1.2626142348
H	0.4515231495	1.4538459336	0.4950113554
H	0.0091543266	-1.5366896614	0.4179160957
H	-1.8312040661	0.2781530222	-0.1051177478
H	2.1932482148	-0.2825566565	-1.4350113885
6			
QSD Point 49			
Ca	-0.5932905640	0.0500879371	1.6343089072
Ca	0.1697315125	0.0123980695	-1.2719605450
H	0.4490038492	1.4628975067	0.4821223161
H	0.0041555897	-1.5437922297	0.4043720603
H	-1.8261175033	0.2774290189	-0.0997119404
H	2.1841742172	-0.2820041475	-1.4000879213
6			
QSD Point 50			
Ca	-0.5695345481	0.0467048521	1.6293027095
Ca	0.1583884022	0.0145208462	-1.2811384256
H	0.4462795680	1.4723007903	0.4694365742
H	-0.0011419086	-1.5511789121	0.3910133343
H	-1.8207038940	0.2766606341	-0.0945863971
H	2.1744829868	-0.2813675656	-1.3650186821
6			
QSD Point 51			
Ca	-0.5451800432	0.0432437675	1.6238488524
Ca	0.1472635531	0.0166051702	-1.2901383824
H	0.4433429819	1.4820438452	0.4569623940
H	-0.0067413160	-1.5588383764	0.3778510668
H	-1.8150004530	0.2758520906	-0.0897429644
H	2.1641969028	-0.2806511105	-1.3298047137
6			
QSD Point 52			
Ca	-0.5202072429	0.0397026076	1.6179198173

Ca	0.1363581328	0.0186485413	-1.2989497775
H	0.4401889467	1.4921100958	0.4447075775
H	-0.0126423172	-1.5667554912	0.3648961632
H	-1.8090467139	0.2750080494	-0.0851833987
H	2.1533383742	-0.2798589797	-1.2944458889
6			
QSD Point 53			
Ca	-0.4945976516	0.0360795720	1.6114859363
Ca	0.1256714015	0.0206487515	-1.3075604723
H	0.4368146536	1.5024782487	0.4326788629
H	-0.0188410063	-1.5749112231	0.3521586123
H	-1.8028841091	0.2741335057	-0.0809089859
H	2.1419290428	-0.2789952609	-1.2589399375
6			
QSD Point 54			
Ca	-0.4683364604	0.0323734161	1.6045166637
Ca	0.1152010114	0.0226039355	-1.3159564984
H	0.4332201719	1.5131218863	0.4208819043
H	-0.0253292654	-1.5832823544	0.3396474982
H	-1.7965558350	0.2732337852	-0.0769203089
H	2.1299905798	-0.2780639863	-1.2232842667
6			
QSD Point 55			
Ca	-0.4414126622	0.0285834957	1.5969804114
Ca	0.1049430579	0.0245125095	-1.3241217719
H	0.4294084472	1.5240095108	0.4093205748
H	-0.0320947513	-1.5918415018	0.3273702494
H	-1.7901060405	0.2723144349	-0.0732166557
H	2.1175439326	-0.2770690363	-1.1874752335
6			
QSD Point 56			
Ca	-0.4138226032	0.0247102221	1.5888466260
Ca	0.0948926322	0.0263731559	-1.3320379995
H	0.4253860563	1.5351042315	0.3979972954
H	-0.0391201107	-1.6005569843	0.3153329380
H	-1.7835795846	0.2713811931	-0.0697957758
H	2.1046105650	-0.2760142239	-1.1515111892
6			
QSD Point 57			
Ca	-0.3855702782	0.0207550953	1.5800860614
Ca	0.0850439224	0.0281848223	-1.3396847652
H	0.4211633260	1.5463641028	0.3869122395
H	-0.0463829866	-1.6093931347	0.3035394747
H	-1.7770211655	0.2704398372	-0.0666531706
H	2.0912116706	-0.2749031785	-1.1153917733
6			
QSD Point 58			
Ca	-0.3566713159	0.0167212286	1.5706734750
Ca	0.0753910616	0.0299465796	-1.3470396211
H	0.4167550979	1.5577417349	0.3760637559
H	-0.0538551555	-1.6183101275	0.2919919626
H	-1.7704749738	0.2694961639	-0.0637818407
H	2.0773693531	-0.2737394169	-1.0791215537
6			
QSD Point 59			
Ca	-0.3271557285	0.0126136666	1.5605903744
Ca	0.0659287613	0.0316576811	-1.3540786247
H	0.4121811338	1.5691845286	0.3654482942
H	-0.0615022094	-1.6272642989	0.2806906116

H	-1.7639840550	0.2685559033	-0.0611719833
H	2.0631074062	-0.2725263997	-1.0427123832
6			
QSD Point 60			
Ca	-0.2970701344	0.0084396730	1.5498272616
Ca	0.0566528154	0.0333174063	-1.3607772846
H	0.4074667061	1.5806348635	0.3550601163
H	-0.0692830873	-1.6362084507	0.2696333717
H	-1.7575896111	0.2676245893	-0.0588102938
H	2.0484512719	-0.2712674499	-1.0061847400
6			
QSD Point 61			
Ca	-0.2664831544	0.0042093646	1.5383891207
Ca	0.0475616126	0.0349249434	-1.3671112982
H	0.4026431121	1.5920299479	0.3448921253
H	-0.0771495477	-1.6450918549	0.2588167512
H	-1.7513307417	0.2667075376	-0.0566801685
H	2.0334306441	-0.2699659761	-0.9695739251
6			
QSD Point 62			
Ca	-0.2354879112	-0.0000640364	1.5262997564
Ca	0.0386567741	0.0364793591	-1.3730579369
H	0.3977477788	1.6033024212	0.3349357088
H	-0.0850462318	-1.6538608522	0.2482356140
H	-1.7452437335	0.2658097526	-0.0547616177
H	2.0180805844	-0.2686255687	-0.9329327455
6			
QSD Point 63			
Ca	-0.2042046934	-0.0043639455	1.5136066579
Ca	0.0299441040	0.0379794654	-1.3785974357
H	0.3928241005	1.6143811935	0.3251809388
H	-0.0929110645	-1.6624596204	0.2378833081
H	-1.7393614584	0.2649358493	-0.0530314465
H	2.0024431976	-0.2672501446	-0.8963351370
6			
QSD Point 64			
Ca	-0.1727855055	-0.0086699168	1.5003874659
Ca	0.0214346959	0.0394234274	-1.3837142147
H	0.3879212105	1.6251918404	0.3156175105
H	-0.1006757198	-1.6708307399	0.2277527112
H	-1.7337132041	0.2640902928	-0.0514639203
H	1.9865715968	-0.2658440373	-0.8598827022
6			
QSD Point 65			
Ca	-0.1414123911	-0.0129577583	1.4867528103
Ca	0.0131448889	0.0408101963	-1.3883979702
H	0.3830922868	1.6356595465	0.3062347560
H	-0.1082670332	-1.6789161369	0.2178354469
H	-1.7283241372	0.2632759329	-0.0500317213
H	1.9705308314	-0.2644142621	-0.8237048287
6			
QSD Point 66			
Ca	-0.1102999951	-0.0171997960	1.4728500960
Ca	0.0050962243	0.0421368157	-1.3926431534
H	0.3783950517	1.6457082060	0.2970204649
H	-0.1156088936	-1.6866593080	0.2081219312
H	-1.7232151280	0.2624968444	-0.0487058426
H	1.9544017819	-0.2629663028	-0.7879618246
6			

QSD Point 67			
Ca	-0.0797010019	-0.0213637103	1.4588685859
Ca	-0.0026845512	0.0434005535	-1.3964529679
H	0.3738879821	1.6552632756	0.2879750963
H	-0.1226239177	-1.6940051881	0.1986148315
H	-1.7184055880	0.2617561053	-0.0474644180
H	1.9382946099	-0.2615103581	-0.7528649378
6			
QSD Point 68			
Ca	-0.0498451407	-0.0254203218	1.4449901479
Ca	-0.0101803657	0.0446026703	-1.3998012208
H	0.3696447636	1.6642400209	0.2789993879
H	-0.1292174697	-1.7008849560	0.1892134706
H	-1.7139143221	0.2610573564	-0.0462239605
H	1.9222749118	-0.2600514586	-0.7185063163
6			
QSD Point 69			
Ca	-0.0218896724	-0.0292197779	1.4319118920
Ca	-0.0171593786	0.0457092451	-1.4028065858
H	0.3657639566	1.6724935566	0.2707468666
H	-0.1352579039	-1.7072300790	0.1805789623
H	-1.7098186788	0.2604169706	-0.0452620095
H	1.9071139491	-0.2586619613	-0.6865029100
6			
QSD Point 70			
Ca	0.0214470274	-0.0350895768	1.4113167397
Ca	-0.0279086937	0.0473996498	-1.4064088561
H	0.3601876058	1.6841929514	0.2559136218
H	-0.1438705616	-1.7160123472	0.1652018615
H	-1.7040254998	0.2594824481	-0.0423597694
H	1.8829146696	-0.2564473392	-0.6350001794
6			
QSD Point 71			
Ca	0.0320870263	-0.0365304296	1.4062596424
Ca	-0.0305477872	0.0478146288	-1.4072910048
H	0.3588192699	1.6870632782	0.2522666366
H	-0.1459837471	-1.7181660597	0.1614215861
H	-1.7026043221	0.2592532200	-0.0416435282
H	1.8769720718	-0.2559035125	-0.6223505705
6			
QSD Point 72			
Ca	0.0753527324	-0.0423904555	1.3856940004
Ca	-0.0412785024	0.0495017791	-1.4108686173
H	0.3532581847	1.6987239623	0.2374156572
H	-0.1545704651	-1.7269146359	0.1460283963
H	-1.6968296448	0.2583209151	-0.0387145639
H	1.8528034276	-0.2536920644	-0.5708949209
6			
QSD Point 73			
Ca	0.1011809188	-0.0458923561	1.3732954388
Ca	-0.0476733556	0.0504625175	-1.4121854328
H	0.3501205629	1.7048536957	0.2265259850
H	-0.1592629283	-1.7313202080	0.1348826335
H	-1.6937269226	0.2577572418	-0.0354278778
H	1.8380662232	-0.2523861385	-0.5384280394
6			
QSD Point 74			
Ca	0.1276938817	-0.0494847490	1.3606137245
Ca	-0.0542896091	0.0514398159	-1.4132218756

H	0.3468905456	1.7110048819	0.2143531729
H	-0.1640385109	-1.7356556028	0.1224678272
H	-1.6904695974	0.2571435597	-0.0312915303
H	1.8228790657	-0.2510633283	-0.5042511431
6			
QSD Point 75			
Ca	0.1516847753	-0.0527358707	1.3491836385
Ca	-0.0603558485	0.0522815618	-1.4133878016
H	0.3439283967	1.7160610009	0.2008871052
H	-0.1682259928	-1.7389817001	0.1088543496
H	-1.6875165923	0.2565139744	-0.0255905522
H	1.8090810720	-0.2499311566	-0.4712574407
6			
QSD Point 76			
Ca	0.1723993354	-0.0555422852	1.3393079317
Ca	-0.0656952442	0.0529629925	-1.4126765007
H	0.3411555243	1.7199759361	0.1860007626
H	-0.1718872677	-1.7412246982	0.0939167869
H	-1.6847672482	0.2558433026	-0.0178789070
H	1.7972916923	-0.2490659747	-0.4399506177
6			
QSD Point 77			
Ca	0.1890136576	-0.0577865139	1.3311637060
Ca	-0.0700576513	0.0534334851	-1.4109696546
H	0.3384578994	1.7225029709	0.1691090320
H	-0.1750542430	-1.7420955356	0.0770973854
H	-1.6821692521	0.2550917298	-0.0071841930
H	1.7881677178	-0.2485669029	-0.4104516790
6			
QSD Point 78			
Ca	0.1998603896	-0.0592323227	1.3251741616
Ca	-0.0729227934	0.0535820836	-1.4080638807
H	0.3357367008	1.7230926189	0.1495614223
H	-0.1776537977	-1.7410333674	0.0578106076
H	-1.6797198800	0.2542047578	0.0078807752
H	1.7828500211	-0.2485965890	-0.3835277923
6			
QSD Point 79			
Ca	0.2026248252	-0.0595567766	1.3221317892
Ca	-0.0736850885	0.0532514564	-1.4041426206
H	0.3331401489	1.7212868120	0.1281656466
H	-0.1794079198	-1.7377538258	0.0369751637
H	-1.6774687872	0.2531375289	0.0275996086
H	1.7825947897	-0.2493092706	-0.3617715778
6			
QSD Point 80			
Ca	0.2057611967	-0.0599233805	1.3186000221
Ca	-0.0749805996	0.0529286020	-1.4021154041
H	0.3308315633	1.7212357206	0.1091932250
H	-0.1814024342	-1.7364870282	0.0186171891
H	-1.6741149410	0.2518792308	0.0457908751
H	1.7812228144	-0.2498837198	-0.3409641381

## 5.6 M5 → TS6 → M5'

6

QSD Point 1

Ca	1.2141857380	0.0000000000	-1.0668137357
Ca	-0.5344164320	-0.0000000000	1.4705829326
H	-0.2043602837	1.4084620205	-0.3451862483
H	-0.2043602837	-1.4084620205	-0.3451862483
H	-2.0992376216	0.0000000000	2.8260968395
H	1.7712931125	-0.0000000000	0.9431455993

6

QSD Point 2

Ca	1.1849076225	0.0000000000	-1.0774780447
Ca	-0.5155177082	-0.0000000000	1.4749234135
H	-0.1969936630	1.4057774765	-0.3401976539
H	-0.1969936630	-1.4057774765	-0.3401976539
H	-2.1113153250	0.0000000000	2.8055977695
H	1.7801815803	-0.0000000000	0.9599907494

6

QSD Point 3

Ca	1.1813330804	-0.0000000000	-1.0759730818
Ca	-0.5011211663	0.0000000000	1.4874071882
H	-0.1970258862	1.4069887194	-0.3268251205
H	-0.1970258862	-1.4069887194	-0.3268251205
H	-2.1273839634	-0.0000000000	2.7733619255
H	1.7911728601	0.0000000000	0.9514919414

6

QSD Point 4

Ca	1.1699647811	-0.0000000000	-1.0763798841
Ca	-0.4834834508	-0.0000000000	1.4996864375
H	-0.1975549818	1.4084825684	-0.3161632838
H	-0.1975549818	-1.4084825684	-0.3161632838
H	-2.1386788944	-0.0000000000	2.7409266173
H	1.8008945610	0.0000000000	0.9507307721

6

QSD Point 5

Ca	1.1556949495	-0.0000000000	-1.0758508791
Ca	-0.4639160677	-0.0000000000	1.5133225212
H	-0.2004469148	1.4128427512	-0.3076508566
H	-0.2004469148	-1.4128427512	-0.3076508566
H	-2.1452971943	-0.0000000000	2.7073632536
H	1.8098088225	0.0000000000	0.9531040547

6

QSD Point 6

Ca	1.1361020027	-0.0000000000	-1.0784273708
Ca	-0.4434489893	-0.0000000000	1.5278125914
H	-0.2035174204	1.4191527909	-0.3033225870
H	-0.2035174204	-1.4191527909	-0.3033225870
H	-2.1473964199	-0.0000000000	2.6759877713
H	1.8178440097	0.0000000000	0.9639093638

6

QSD Point 7

Ca	1.1121025264	-0.0000000000	-1.0878944055
Ca	-0.4238311745	-0.0000000000	1.5408476259
H	-0.2049884515	1.4249177701	-0.3026527369
H	-0.2049884515	-1.4249177701	-0.3026527369
H	-2.1470774465	-0.0000000000	2.6504020379
H	1.8253537851	0.0000000000	0.9845873797

6

QSD Point 8			
Ca	1.0860509249	-0.0000000000	-1.1036148187
Ca	-0.4059507860	-0.0000000000	1.5518263355
H	-0.2049368293	1.4295703990	-0.3037294634
H	-0.2049368293	-1.4295703990	-0.3037294634
H	-2.1459132886	-0.0000000000	2.6299663999
H	1.8330157894	0.0000000000	1.0119181741
6			
QSD Point 9			
Ca	1.0591272804	-0.0000000000	-1.1238781411
Ca	-0.3897686030	-0.0000000000	1.5610557455
H	-0.2037715204	1.4333079927	-0.3054365653
H	-0.2037715204	-1.4333079927	-0.3054365653
H	-2.1444945247	-0.0000000000	2.6131026696
H	1.8410639944	0.0000000000	1.0432300295
6			
QSD Point 10			
Ca	1.0317752882	-0.0000000000	-1.1472404402
Ca	-0.3749537415	-0.0000000000	1.5689717527
H	-0.2017978505	1.4363794216	-0.3073080770
H	-0.2017978505	-1.4363794216	-0.3073080770
H	-2.1429985429	-0.0000000000	2.5985924932
H	1.8494563782	0.0000000000	1.0769295347
6			
QSD Point 11			
Ca	1.0041447040	-0.0000000000	-1.1726647567
Ca	-0.3611742086	-0.0000000000	1.5759241630
H	-0.1992040131	1.4389614633	-0.3091716947
H	-0.1992040131	-1.4389614633	-0.3091716947
H	-2.1414741022	-0.0000000000	2.5856401832
H	1.8580703381	0.0000000000	1.1120810025
6			
QSD Point 12			
Ca	0.9762851662	0.0000000000	-1.1994187720
Ca	-0.3481685656	-0.0000000000	1.5821616345
H	-0.1961054275	1.4411703653	-0.3109709347
H	-0.1961054275	-1.4411703653	-0.3109709347
H	-2.1399320295	-0.0000000000	2.5737359028
H	1.8667805884	0.0000000000	1.1481003240
6			
QSD Point 13			
Ca	0.9482152202	0.0000000000	-1.2269754641
Ca	-0.3357448705	-0.0000000000	1.5878554503
H	-0.1925763897	1.4430828054	-0.3126936337
H	-0.1925763897	-1.4430828054	-0.3126936337
H	-2.1383718876	-0.0000000000	2.5625458115
H	1.8754812490	0.0000000000	1.1845987069
6			
QSD Point 14			
Ca	0.9199465645	0.0000000000	-1.2549451724
Ca	-0.3237652056	0.0000000000	1.5931236128
H	-0.1886684084	1.4447507363	-0.3143442174
H	-0.1886684084	-1.4447507363	-0.3143442174
H	-2.1367901671	0.0000000000	2.5518441846
H	1.8840891235	0.0000000000	1.2213030637
6			
QSD Point 15			
Ca	0.8914912385	-0.0000000000	-1.2830323022
Ca	-0.3121305460	0.0000000000	1.5980479987

H	-0.1844202406	1.4462106733	-0.3159329405
H	-0.1844202406	-1.4462106733	-0.3159329405
H	-2.1351826338	0.0000000000	2.5414728148
H	1.8925415619	0.0000000000	1.2580146393
6			
QSD Point 16			
Ca	0.8628635636	-0.0000000000	-1.3110067912
Ca	-0.3007694753	-0.0000000000	1.6026855358
H	-0.1798635598	1.4474891046	-0.3174714095
H	-0.1798635598	-1.4474891046	-0.3174714095
H	-2.1335451524	0.0000000000	2.5313168364
H	1.9007932225	0.0000000000	1.2945845217
6			
QSD Point 17			
Ca	0.8340809856	-0.0000000000	-1.3386858588
Ca	-0.2896301542	-0.0000000000	1.6070758427
H	-0.1750263453	1.4486061808	-0.3189708417
H	-0.1750263453	-1.4486061808	-0.3189708417
H	-2.1318736746	0.0000000000	2.5212899473
H	1.9088126821	0.0000000000	1.3308990480
6			
QSD Point 18			
Ca	0.8051624487	-0.0000000000	-1.3659214175
Ca	-0.2786745138	-0.0000000000	1.6112459142
H	-0.1699343227	1.4495776454	-0.3204414628
H	-0.1699343227	-1.4495776454	-0.3204414628
H	-2.1301641932	0.0000000000	2.5113248822
H	1.9165797890	0.0000000000	1.3668708523
6			
QSD Point 19			
Ca	0.7761293971	-0.0000000000	-1.3925915680
Ca	-0.2678746280	-0.0000000000	1.6152137149
H	-0.1646123990	1.4504164020	-0.3218919483
H	-0.1646123990	-1.4504164020	-0.3218919483
H	-2.1284127437	0.0000000000	2.5013676411
H	1.9240832277	0.0000000000	1.4024314215
6			
QSD Point 20			
Ca	0.7470038904	-0.0000000000	-1.4185950089
Ca	-0.2572095614	-0.0000000000	1.6189904952
H	-0.1590848725	1.4511332924	-0.3233296266
H	-0.1590848725	-1.4511332924	-0.3233296266
H	-2.1266152007	0.0000000000	2.4913732308
H	1.9313188164	0.0000000000	1.4375278531
6			
QSD Point 21			
Ca	0.7178087351	-0.0000000000	-1.4438468517
Ca	-0.2466635083	-0.0000000000	1.6225827012
H	-0.1533757853	1.4517377169	-0.3247603116
H	-0.1533757853	-1.4517377169	-0.3247603116
H	-2.1247674050	0.0000000000	2.4813031513
H	1.9382879047	0.0000000000	1.4721189397
6			
QSD Point 22			
Ca	0.6885665423	-0.0000000000	-1.4682758162
Ca	-0.2362240169	-0.0000000000	1.6259933182
H	-0.1475089190	1.4522380659	-0.3261884221
H	-0.1475089190	-1.4522380659	-0.3261884221
H	-2.1228651481	0.0000000000	2.4711234582



H	1.9449961238	0.0000000000	1.5061731979
6			
QSD Point 23			
Ca	0.6592993837	-0.0000000000	-1.4918222001
Ca	-0.2258810267	-0.0000000000	1.6292233162
H	-0.1415076798	1.4526420197	-0.3276170084
H	-0.1415076798	-1.4526420197	-0.3276170084
H	-2.1209042451	0.0000000000	2.4608034972
H	1.9514523208	0.0000000000	1.5396667093
6			
QSD Point 24			
Ca	0.6300278524	-0.0000000000	-1.5144365684
Ca	-0.2156256513	-0.0000000000	1.6322725203
H	-0.1353948489	1.4529567464	-0.3290478663
H	-0.1353948489	-1.4529567464	-0.3290478663
H	-2.1188805243	0.0000000000	2.4503147942
H	1.9576675948	0.0000000000	1.5725822793
6			
QSD Point 25			
Ca	0.6007703065	-0.0000000000	-1.5360782164
Ca	-0.2054495391	-0.0000000000	1.6351403718
H	-0.1291922600	1.4531891216	-0.3304816114
H	-0.1291922600	-1.4531891216	-0.3304816114
H	-2.1167900144	0.0000000000	2.4396304687
H	1.9636545435	0.0000000000	1.6049078727
6			
QSD Point 26			
Ca	0.5715435392	-0.0000000000	-1.5567145467
Ca	-0.1953448118	-0.0000000000	1.6378265724
H	-0.1229207391	1.4533457997	-0.3319174782
H	-0.1229207391	-1.4533457997	-0.3319174782
H	-2.1146289605	0.0000000000	2.4287252301
H	1.9694263595	0.0000000000	1.6366349496
6			
QSD Point 27			
Ca	0.5423609074	-0.0000000000	-1.5763205005
Ca	-0.1853032636	-0.0000000000	1.6403316031
H	-0.1165995782	1.4534334126	-0.3333536165
H	-0.1165995782	-1.4534334126	-0.3333536165
H	-2.1123938928	0.0000000000	2.4175744684
H	1.9749967077	0.0000000000	1.6677588792
6			
QSD Point 28			
Ca	0.5132325644	-0.0000000000	-1.5948775913
Ca	-0.1753165224	-0.0000000000	1.6426569891
H	-0.1102463288	1.4534585599	-0.3347871397
H	-0.1102463288	-1.4534585599	-0.3347871397
H	-2.1100816281	0.0000000000	2.4061545044
H	1.9803790340	0.0000000000	1.6982775549
6			
QSD Point 29			
Ca	0.4841655873	-0.0000000000	-1.6123731441
Ca	-0.1653760830	-0.0000000000	1.6448050883
H	-0.1038766965	1.4534278171	-0.3362139557
H	-0.1038766965	-1.4534278171	-0.3362139557
H	-2.1076894132	0.0000000000	2.3944426765
H	1.9855862456	0.0000000000	1.7281904206
6			
QSD Point 30			

Ca	0.4551637908	-0.0000000000	-1.6287995276
Ca	-0.1554735684	-0.0000000000	1.6467793493
H	-0.0975043209	1.4533476838	-0.3376289950
H	-0.0975043209	-1.4533476838	-0.3376289950
H	-2.1052149135	0.0000000000	2.3824174227
H	1.9906305337	0.0000000000	1.7574978187
6			
QSD Point 31			
Ca	0.4262282448	0.0000000000	-1.6441533517
Ca	-0.1456007871	-0.0000000000	1.6485839816
H	-0.0911409664	1.4532249255	-0.3390262896
H	-0.0911409664	-1.4532249255	-0.3390262896
H	-2.1026561118	0.0000000000	2.3700584350
H	1.9955231608	0.0000000000	1.7862005211
6			
QSD Point 32			
Ca	0.3973566743	0.0000000000	-1.6584346076
Ca	-0.1357501135	-0.0000000000	1.6502238707
H	-0.0847959679	1.4530659420	-0.3403992332
H	-0.0847959679	-1.4530659420	-0.3403992332
H	-2.1000113578	0.0000000000	2.3573469128
H	2.0002742013	0.0000000000	1.8142992205
6			
QSD Point 33			
Ca	0.3685461217	0.0000000000	-1.6716457279
Ca	-0.1259151545	-0.0000000000	1.6517042679
H	-0.0784771366	1.4528773553	-0.3417404836
H	-0.0784771366	-1.4528773553	-0.3417404836
H	-2.0972796678	0.0000000000	2.3442665807
H	2.0048926095	0.0000000000	1.8417926887
6			
QSD Point 34			
Ca	0.3397919940	0.0000000000	-1.6837911685
Ca	-0.1160907460	-0.0000000000	1.6530304953
H	-0.0721902785	1.4526654692	-0.3430422597
H	-0.0721902785	-1.4526654692	-0.3430422597
H	-2.0944603603	0.0000000000	2.3308034179
H	2.0093859482	0.0000000000	1.8686785175
6			
QSD Point 35			
Ca	0.3110891826	0.0000000000	-1.6948765777
Ca	-0.1062732049	-0.0000000000	1.6542078024
H	-0.0659395901	1.4524365184	-0.3442967564
H	-0.0659395901	-1.4524365184	-0.3442967564
H	-2.0915532875	0.0000000000	2.3169464622
H	2.0137604408	0.0000000000	1.8949524569
6			
QSD Point 36			
Ca	0.2824345099	0.0000000000	-1.7049088054
Ca	-0.0964613426	-0.0000000000	1.6552412922
H	-0.0597280875	1.4521964841	-0.3454960118
H	-0.0597280875	-1.4521964841	-0.3454960118
H	-2.0885590829	0.0000000000	2.3026888172
H	2.0180209696	0.0000000000	1.9206072261
6			
QSD Point 37			
Ca	0.2538247940	0.0000000000	-1.7138951737
Ca	-0.0866555463	-0.0000000000	1.6561353183
H	-0.0535572819	1.4519511139	-0.3466326141

H	-0.0535572819	-1.4519511139	-0.3466326141
H	-2.0854786179	0.0000000000	2.2880269719
H	2.0221708963	0.0000000000	1.9456344806
6			
QSD Point 38			
Ca	0.2252607428	0.0000000000	-1.7218435461
Ca	-0.0768588503	-0.0000000000	1.6568937545
H	-0.0474282009	1.4517059843	-0.3476996630
H	-0.0474282009	-1.4517059843	-0.3476996630
H	-2.0823135438	0.0000000000	2.2729625493
H	2.0262120691	0.0000000000	1.9700227859
6			
QSD Point 39			
Ca	0.1967463753	-0.0000000000	-1.7287627633
Ca	-0.0670767365	-0.0000000000	1.6575196601
H	-0.0413410365	1.4514664174	-0.3486912127
H	-0.0413410365	-1.4514664174	-0.3486912127
H	-2.0790658888	0.0000000000	2.2575022643
H	2.0301445280	0.0000000000	1.9937593166
6			
QSD Point 40			
Ca	0.1682889741	0.0000000000	-1.7346621853
Ca	-0.0573165400	-0.0000000000	1.6580146110
H	-0.0352955257	1.4512377235	-0.3496025163
H	-0.0352955257	-1.4512377235	-0.3496025163
H	-2.0757377472	0.0000000000	2.2416575519
H	2.0339665676	0.0000000000	2.0168309275
6			
QSD Point 41			
Ca	0.1398999222	0.0000000000	-1.7395515876
Ca	-0.0475884078	-0.0000000000	1.6583790486
H	-0.0292906260	1.4510253943	-0.3504305957
H	-0.0292906260	-1.4510253943	-0.3504305957
H	-2.0723318788	0.0000000000	2.2254471014
H	2.0376741842	0.0000000000	2.0392223066
6			
QSD Point 42			
Ca	0.1116029745	0.0000000000	-1.7434465495
Ca	-0.0379039101	-0.0000000000	1.6586117759
H	-0.0233272348	1.4508367887	-0.3511738978
H	-0.0233272348	-1.4508367887	-0.3511738978
H	-2.0688490314	0.0000000000	2.2088941681
H	2.0412597810	0.0000000000	2.0609238668
6			
QSD Point 43			
Ca	0.0833582773	-0.0000000000	-1.7463400844
Ca	-0.0282870908	0.0000000000	1.6587111649
H	-0.0173835775	1.4506775688	-0.3518339392
H	-0.0173835775	-1.4506775688	-0.3518339392
H	-2.0653035784	0.0000000000	2.1920598074
H	2.0447152398	0.0000000000	2.0818722599
6			
QSD Point 44			
Ca	0.0555464628	-0.0000000000	-1.7487853090
Ca	-0.0187586912	0.0000000000	1.6587051035
H	-0.0115233955	1.4505315685	-0.3525140605
H	-0.0115233955	-1.4505315685	-0.3525140605
H	-2.0617085821	0.0000000000	2.1752412890
H	2.0480172844	0.0000000000	2.1025019061

6			
QSD Point 45			
Ca	0.0068667851	-0.0000000000	-1.7488262474
Ca	-0.0023189545	0.0000000000	1.6587038137
H	-0.0014244836	1.4505290153	-0.3525272565
H	-0.0014244836	-1.4505290153	-0.3525272565
H	-2.0557053609	-0.0000000000	2.1434018208
H	2.0540127935	0.0000000000	2.1344099868
6			
QSD Point 46			
Ca	0.0000000000	0.0000000000	-1.7488055676
Ca	0.0000000000	0.0000000000	1.6587039703
H	0.0000000000	1.4505284981	-0.3525164304
H	0.0000000000	-1.4505284981	-0.3525164304
H	-2.0548562403	0.0000000000	2.1388846555
H	2.0548562403	0.0000000000	2.1388846555
6			
QSD Point 47			
Ca	-0.0068667403	-0.0000000000	-1.7488262909
Ca	0.0023189967	0.0000000000	1.6587037947
H	0.0014245099	1.4505289952	-0.3525272847
H	0.0014245099	-1.4505289952	-0.3525272847
H	-2.0540127431	0.0000000000	2.1344100288
H	2.0557053892	0.0000000000	2.1434018779
6			
QSD Point 48			
Ca	-0.0555460688	-0.0000000000	-1.7487852991
Ca	0.0187589992	-0.0000000000	1.6587051129
H	0.0115235722	1.4505315774	-0.3525140601
H	0.0115235722	-1.4505315774	-0.3525140601
H	-2.0480169801	0.0000000000	2.1025019120
H	2.0617089015	-0.0000000000	2.1752412427
6			
QSD Point 49			
Ca	-0.0833586961	-0.0000000000	-1.7463400957
Ca	0.0282856217	0.0000000000	1.6587111786
H	0.0173829979	1.4506775801	-0.3518339490
H	0.0173829979	-1.4506775801	-0.3518339490
H	-2.0447170334	-0.0000000000	2.0818710391
H	2.0653017880	-0.0000000000	2.1920610085
6			
QSD Point 50			
Ca	-0.1116033114	-0.0000000000	-1.7434465229
Ca	0.0379008880	0.0000000000	1.6586117971
H	0.0233258984	1.4508368079	-0.3511738730
H	0.0233258984	-1.4508368079	-0.3511738730
H	-2.0412632511	-0.0000000000	2.0609219241
H	2.0688455271	-0.0000000000	2.2088959729
6			
QSD Point 51			
Ca	-0.1399003951	-0.0000000000	-1.7395516412
Ca	0.0475831387	-0.0000000000	1.6583790962
H	0.0292882765	1.4510253839	-0.3504305428
H	0.0292882765	-1.4510253839	-0.3504305428
H	-2.0376801231	0.0000000000	2.0392192524
H	2.0723258509	0.0000000000	2.2254500111
6			
QSD Point 52			
Ca	-0.1682899204	0.0000000000	-1.7346623366

Ca	0.0573086830	-0.0000000000	1.6580147101
H	0.0352919957	1.4512377246	-0.3496024377
H	0.0352919957	-1.4512377246	-0.3496024377
H	-2.0339754124	0.0000000000	2.0168262876
H	2.0757286839	0.0000000000	2.2416620386
6			
QSD Point 53			
Ca	-0.1967474454	0.0000000000	-1.7287630144
Ca	0.0670656855	-0.0000000000	1.6575197843
H	0.0413360214	1.4514664296	-0.3486910943
H	0.0413360214	-1.4514664296	-0.3486910943
H	-2.0301567979	0.0000000000	1.9937530822
H	2.0790531583	0.0000000000	2.2575083380
6			
QSD Point 54			
Ca	-0.2252625591	-0.0000000000	-1.7218440418
Ca	0.0768443029	-0.0000000000	1.6568940018
H	0.0474216415	1.4517060012	-0.3476994756
H	0.0474216415	-1.4517060012	-0.3476994756
H	-2.0262282124	0.0000000000	1.9700144200
H	2.0822966673	0.0000000000	2.2729707356
6			
QSD Point 55			
Ca	-0.2824373528	-0.0000000000	-1.7049098491
Ca	0.0964383710	0.0000000000	1.6552417644
H	0.0597176705	1.4521964960	-0.3454956823
H	0.0597176705	-1.4521964960	-0.3454956823
H	-2.0180461134	-0.0000000000	1.9205942588
H	2.0885322100	-0.0000000000	2.3027016406
6			
QSD Point 55			
Ca	-0.3110931080	-0.0000000000	-1.6948780254
Ca	0.1062455371	0.0000000000	1.6542084739
H	0.0659270826	1.4524365330	-0.3442962720
H	0.0659270826	-1.4524365330	-0.3442962720
H	-2.0137906334	-0.0000000000	1.8949365287
H	2.0915207750	-0.0000000000	2.3169621404
6			
QSD Point 56			
Ca	-0.3397965900	-0.0000000000	-1.6837930100
Ca	0.1160578717	0.0000000000	1.6530313287
H	0.0721753990	1.4526654786	-0.3430416497
H	0.0721753990	-1.4526654786	-0.3430416497
H	-2.0094215154	-0.0000000000	1.8686597388
H	2.0944216440	-0.0000000000	2.3308219261
6			
QSD Point 57			
Ca	-0.3685514435	-0.0000000000	-1.6716481462
Ca	0.1258767261	0.0000000000	1.6517053294
H	0.0784597286	1.4528773660	-0.3417396999
H	0.0784597286	-1.4528773660	-0.3417396999
H	-2.0049339087	-0.0000000000	1.8417709889
H	2.0972342933	-0.0000000000	2.3442880109
6			
QSD Point 58			
Ca	-0.3973630544	-0.0000000000	-1.6584377724
Ca	0.1357058692	0.0000000000	1.6502252840
H	0.0847759387	1.4530659559	-0.3403982585
H	0.0847759387	-1.4530659559	-0.3403982585

H	-2.0003215002	-0.0000000000	1.8142742799
H	2.0999589654	-0.0000000000	2.3573715962
6			
QSD Point 59			
Ca	-0.4262357737	-0.0000000000	-1.6441572352
Ca	0.1455504532	0.0000000000	1.6485857178
H	0.0911181420	1.4532249471	-0.3390250682
H	0.0911181420	-1.4532249471	-0.3390250682
H	-1.9955766596	-0.0000000000	1.7861720184
H	2.1025963120	-0.0000000000	2.3700865827
6			
QSD Point 60			
Ca	-0.4551725849	-0.0000000000	-1.6288041854
Ca	0.1554168097	0.0000000000	1.6467813982
H	0.0974786018	1.4533477281	-0.3376274922
H	0.0974786018	-1.4533477281	-0.3376274922
H	-1.9906904635	-0.0000000000	1.7574656203
H	2.1051472993	-0.0000000000	2.3824491653
6			
QSD Point 61			
Ca	-0.4841757836	-0.0000000000	-1.6123787399
Ca	0.1653126698	0.0000000000	1.6448076319
H	0.1038479249	1.4534278690	-0.3362121536
H	0.1038479249	-1.4534278690	-0.3362121536
H	-1.9856528265	-0.0000000000	1.7281543279
H	2.1076136154	-0.0000000000	2.3944781581
6			
QSD Point 62			
Ca	-0.5132441222	-0.0000000000	-1.5948842113
Ca	0.1752461127	0.0000000000	1.6426599728
H	0.1102143437	1.4534586277	-0.3347850299
H	0.1102143437	-1.4534586277	-0.3347850299
H	-1.9804524550	-0.0000000000	1.6982375450
H	2.1099972468	-0.0000000000	2.4061938723
6			
QSD Point 63			
Ca	-0.5423740124	-0.0000000000	-1.5763283015
Ca	0.1852255860	0.0000000000	1.6403351277
H	0.1165642763	1.4534335056	-0.3333511279
H	0.1165642763	-1.4534335056	-0.3333511279
H	-1.9750771867	-0.0000000000	1.6677147716
H	2.1123005650	-0.0000000000	2.4176178170
6			
QSD Point 64			
Ca	-0.5715585441	-0.0000000000	-1.5567235360
Ca	0.1952596812	0.0000000000	1.6378306670
H	0.1228820354	1.4533459315	-0.3319145420
H	0.1228820354	-1.4533459315	-0.3319145420
H	-1.9695140496	-0.0000000000	1.6365863119
H	2.1145263555	-0.0000000000	2.4287728327
6			
QSD Point 65			
Ca	-0.6007873274	-0.0000000000	-1.5360884527
Ca	0.2053566758	0.0000000000	1.6351450712
H	0.1291500016	1.4531892829	-0.3304782128
H	0.1291500016	-1.4531892829	-0.3304782128
H	-1.9637495882	-0.0000000000	1.6048545321
H	2.1166777566	-0.0000000000	2.4396824923
6			

QSD Point 66			
Ca	-0.6300466033	-0.0000000000	-1.5144483187
Ca	0.2155246278	0.0000000000	1.6322779000
H	0.1353487998	1.4529569080	-0.3290440320
H	0.1353487998	-1.4529569080	-0.3290440320
H	-1.9577702155	-0.0000000000	1.5725245302
H	2.1187581809	-0.0000000000	2.4503711893
6			
QSD Point 67			
Ca	-0.6593208224	-0.0000000000	-1.4918355397
Ca	0.2257718450	0.0000000000	1.6292294893
H	0.1414578934	1.4526422589	-0.3276125668
H	0.1414578934	-1.4526422589	-0.3276125668
H	-1.9515626353	-0.0000000000	1.5396037268
H	2.1207715330	-0.0000000000	2.4608647079
6			
QSD Point 68			
Ca	-0.6885904576	-0.0000000000	-1.4682906268
Ca	0.2361063176	0.0000000000	1.6260002299
H	0.1474551392	1.4522383214	-0.3261833898
H	0.1474551392	-1.4522383214	-0.3261833898
H	-1.9451142306	-0.0000000000	1.5061048710
H	2.1227216681	-0.0000000000	2.4711895653
6			
QSD Point 69			
Ca	-0.7178355168	-0.0000000000	-1.4438633618
Ca	0.2465370517	0.0000000000	1.6225904696
H	0.1533179400	1.4517380189	-0.3247546475
H	0.1533179400	-1.4517380189	-0.3247546475
H	-1.9384139361	-0.0000000000	1.4720451408
H	2.1246127676	-0.0000000000	2.4813743106
6			
QSD Point 70			
Ca	-0.7470336338	-0.0000000000	-1.4186132757
Ca	0.2570741215	0.0000000000	1.6189991761
H	0.1590227790	1.4511336159	-0.3233232925
H	0.1590227790	-1.4511336159	-0.3233232925
H	-1.9314528881	-0.0000000000	1.4374483746
H	2.1264490482	-0.0000000000	2.4914495747
6			
QSD Point 71			
Ca	-0.7761622984	-0.0000000000	-1.3926118080
Ca	0.2677299461	0.0000000000	1.6152233758
H	0.1645459333	1.4504167468	-0.3218849177
H	0.1645459333	-1.4504167468	-0.3218849177
H	-1.9242254309	-0.0000000000	1.4023462318
H	2.1282347097	-0.0000000000	2.5014492975
6			
QSD Point 72			
Ca	-0.8051986599	-0.0000000000	-1.3659438413
Ca	0.2785203685	0.0000000000	1.6112566228
H	0.1698633446	1.4495780057	-0.3204337015
H	0.1698633446	-1.4495780057	-0.3204337015
H	-1.9167301956	-0.0000000000	1.3667799115
H	2.1299739510	-0.0000000000	2.5114119655
6			
QSD Point 73			
Ca	-0.8341207025	-0.0000000000	-1.3387106464
Ca	0.2894663926	0.0000000000	1.6070876861

H	0.1749507298	1.4486065386	-0.3189623177
H	0.1749507298	-1.4486065386	-0.3189623177
H	-1.9089713067	-0.0000000000	1.3308022778
H	2.1316709211	-0.0000000000	2.5213825647
6			
QSD Point 74			
Ca	-0.8629075102	-0.0000000000	-1.3110339578
Ca	0.3005961445	0.0000000000	1.6026985823
H	0.1797833119	1.4474894754	-0.3174620013
H	0.1797833119	-1.4474894754	-0.3174620013
H	-1.9009599384	-0.0000000000	1.2944813461
H	2.1333297081	-0.0000000000	2.5314152674
6			
QSD Point 75			
Ca	-0.8915391742	-0.0000000000	-1.2830620127
Ca	0.3119475066	-0.0000000000	1.5980622517
H	0.1843351546	1.4462109711	-0.3159226914
H	0.1843351546	-1.4462109711	-0.3159226914
H	-1.8927162774	-0.0000000000	1.2579053370
H	2.1349542812	-0.0000000000	2.5415770292
6			
QSD Point 76			
Ca	-0.9199991131	-0.0000000000	-1.2549776917
Ca	0.3235726076	-0.0000000000	1.5931391811
H	0.1885785378	1.4447509838	-0.3143330496
H	0.1885785378	-1.4447509838	-0.3143330496
H	-1.8842715893	-0.0000000000	1.2211874956
H	2.1365488288	-0.0000000000	2.5519543220
6			
QSD Point 77			
Ca	-0.9482722121	-0.0000000000	-1.2270110193
Ca	0.3355428771	-0.0000000000	1.5878723443
H	0.1924816159	1.4430828962	-0.3126815626
H	0.1924816159	-1.4430828962	-0.3126815626
H	-1.8756711909	-0.0000000000	1.1844771647
H	2.1381175810	-0.0000000000	2.5626618276
6			
QSD Point 78			
Ca	-0.9763470842	-0.0000000000	-1.1994576923
Ca	0.3479576321	-0.0000000000	1.5821798979
H	0.1960058540	1.4411702939	-0.3109578998
H	0.1960058540	-1.4411702939	-0.3109578998
H	-1.8669775086	-0.0000000000	1.1479728963
H	2.1396649791	-0.0000000000	2.5738578733
6			
QSD Point 79			
Ca	-1.0042114570	-0.0000000000	-1.1727074032
Ca	0.3609549133	0.0000000000	1.5759437889
H	0.1990996784	1.4389610868	-0.3091577338
H	0.1990996784	-1.4389610868	-0.3091577338
H	-1.8582735815	-0.0000000000	1.1119482137
H	2.1411947039	-0.0000000000	2.5857680277
6			
QSD Point 80			
Ca	-1.0318468026	-0.0000000000	-1.1472874203
Ca	0.3747269417	0.0000000000	1.5689926704
H	0.2016889528	1.4363786268	-0.3072932394
H	0.2016889528	-1.4363786268	-0.3072932394
H	-1.8496651042	-0.0000000000	1.0767923140



H	2.1427074576	-0.0000000000	2.5987260590
6			
QSD Point 81			
Ca	-1.0592035970	-0.0000000000	-1.1239300297
Ca	0.3895357263	0.0000000000	1.5610778435
H	0.2036583613	1.4333066112	-0.3054209202
H	0.2036583613	-1.4333066112	-0.3054209202
H	-1.8412769976	-0.0000000000	1.0430892094
H	2.1441928419	-0.0000000000	2.6132419491
6			
QSD Point 82			
Ca	-1.0861313555	-0.0000000000	-1.1036724911
Ca	0.4057135230	0.0000000000	1.5518492845
H	0.2048197251	1.4295681239	-0.3037133028
H	0.2048197251	-1.4295681239	-0.3037133028
H	-1.8332315321	-0.0000000000	1.0117755921
H	2.1456024493	-0.0000000000	2.6301113449
6			
QSD Point 83			
Ca	-1.1121859236	-0.0000000000	-1.0879589616
Ca	0.4235914928	0.0000000000	1.5408711641
H	0.2048678504	1.4249143147	-0.3026367370
H	0.2048678504	-1.4249143147	-0.3026367370
H	-1.8255705025	-0.0000000000	0.9844457382
H	2.1467591218	-0.0000000000	2.6505526608
6			
QSD Point 84			
Ca	-1.1361860686	-0.0000000000	-1.0784995484
Ca	0.4432081954	0.0000000000	1.5278365655
H	0.2033936085	1.4191480307	-0.3033080639
H	0.2033936085	-1.4191480307	-0.3033080639
H	-1.8180602184	-0.0000000000	0.9637719287
H	2.1470716790	-0.0000000000	2.6761443311
6			
QSD Point 85			
Ca	-1.1557767656	-0.0000000000	-1.0759294680
Ca	0.4636718912	0.0000000000	1.5133480173
H	0.2003199837	1.4128378141	-0.3076393359
H	0.2003199837	-1.4128378141	-0.3076393359
H	-1.8100261565	-0.0000000000	0.9529726602
H	2.1449635208	-0.0000000000	2.7075246698
6			
QSD Point 86			
Ca	-1.1700487958	0.0000000000	-1.0764602652
Ca	0.4832286250	-0.0000000000	1.4997159162
H	0.1974246959	1.4084797292	-0.3161535248
H	0.1974246959	-1.4084797292	-0.3161535248
H	-1.8011216184	-0.0000000000	0.9505976060
H	2.1383283618	0.0000000000	2.7410911256
6			
QSD Point 87			
Ca	-1.1814200574	-0.0000000000	-1.0760589845
Ca	0.5008442197	0.0000000000	1.4874389513
H	0.1968854895	1.4069851295	-0.3268174447
H	0.1968854895	-1.4069851295	-0.3268174447
H	-1.7914204544	-0.0000000000	0.9513582627
H	2.1270045112	-0.0000000000	2.7735343233
6			
QSD Point 88			

Ca	-1.1850328576	0.0000000000	-1.0775608206
Ca	0.5152143173	-0.0000000000	1.4749660163
H	0.1968415945	1.4057757524	-0.3401842462
H	0.1968415945	-1.4057757524	-0.3401842462
H	-1.7804631112	-0.0000000000	0.9598298103
H	2.1109000068	-0.0000000000	2.8057719843
6			
QSD Point 89			
Ca	-1.2142428940	0.0000000000	-1.0669446343
Ca	0.5340947459	-0.0000000000	1.4706016060
H	0.2041856580	1.4084453776	-0.3452039594
H	0.2041856580	-1.4084453776	-0.3452039594
H	-1.7715628996	-0.0000000000	0.9430629898
H	2.0987910052	0.0000000000	2.8263269599

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