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Appendix I

Exponents and coefficients for STO-3G basis set

atom	shell	exponent	coefficient	
H	S 3 1.00	.3425250914D+01	.1543289673D+00	
		.6239137298D+00	.5353281423D+00	
		.1688554040D+00	.4446345422D+00	
C	S 3 1.00	.7161683735D+02	.1543289673D+00	
		.1304509632D+02	.5353281423D+00	
		.3530512160D+01	.4446345422D+00	
	SP 3 1.00	.2941249355D+01	-.9996722919D-01	.1559162750D+00
		.6834830964D+00	.3995128261D+00	.6076837186D+00
		.2222899159D+00	.7001154689D+00	.3919573931D+00
N	S 3 1.00	.9910616896D+02	.1543289673D+00	
		.1805231239D+02	.5353281423D+00	
		.4885660238D+01	.4446345422D+00	
	SP 3 1.00	.3780455879D+01	-.9996722919D-01	.1559162750D+00
		.8784922449D+00	.3995128261D+00	.6076837186D+00
		.2857143744D+00	.7001154689D+00	.3919573931D+00
O	S 3 1.00	.1307093214D+03	.1543289673D+00	
		.2380886605D+02	.5353281423D+00	
		.6443608313D+01	.4446345422D+00	
	SP 3 1.00	.5033151319D+01	-.9996722919D-01	.1559162750D+00
		.1169596125D+01	.3995128261D+00	.6076837186D+00
		.3803889600D+00	.7001154689D+00	.3919573931D+00

Exponents and coefficients for 3-21G basis set

atom	shell	exponent	coefficient	
H	S 2 1.00	.5447178000D+01	.1562850000D+00	
		.8245472400D+00	.9046910000D+00	
	S 1 1.00	.1831915800D+00	.1000000000D+01	
C	S 3 1.00	.1722560000D+03	.6176690000D-01	
		.2591090000D+02	.3587940000D+00	
		.5533350000D+01	.7007130000D+00	
	SP 2 1.00	.3664980000D+01	-.3958970000D+00	.2364600000D+00
		.7705450000D+00	.1215840000D+01	.8606190000D+00
	SP 1 1.00	.1958570000D+00	.1000000000D+01	.1000000000D+01
N	S 3 1.00	.2427660000D+03	.5986570000D-01	
		.3648510000D+02	.3529550000D+00	
		.7814490000D+01	.7065130000D+00	
	SP 2 1.00	.5425220000D+01	-.4133010000D+00	.2379720000D+00
		.1149150000D+01	.1224420000D+01	.8589530000D+00
	SP 1 1.00	.2832050000D+00	.1000000000D+01	.1000000000D+01
O	S 3 1.00	.3220370000D+03	.5923940000D-01	
		.4843080000D+02	.3515000000D+00	
		.1042060000D+02	.7076580000D+00	
	SP 2 1.00	.7402940000D+01	-.4044530000D+00	.2445860000D+00
		.1576200000D+01	.1221560000D+01	.8539550000D+00
	SP 1 1.00	.3736840000D+00	.1000000000D+01	.100000000D+01

Exponents and coefficients for 6-21G basis set

atom	shell	exponent	coefficient	
H	S 2 1.00	.5447178000D+01	.1562850000D+00	
		.8245472400D+00	.9046910000D+00	
	S 1 1.00	.1831915800D+00	.1000000000D+01	
C	S 6 1.00	.3047520000D+04	.1825880000D-02	
		.4564240000D+03	.1405660000D-01	
		.1036530000D+03	.6875700000D-01	
		.2922580000D+02	.2304220000D+00	
		.9348630000D+01	.4684630000D+00	
		.3189040000D+01	.3627800000D+00	

atom	shell	exponent	coefficient	
C	SP 2 1.00	.3664980000D+01		.2379720000D+00
		.7705450000D+00		.8589530000D+00
	SP 1 1.00	.1958570000D+00		.1000000000D+01
N	S 6 1.00	.4150110000D+04	.1845410000D-02	
		.6200840000D+03	.1416450000D-01	
		.1416880000D+03	.6863250000D-01	
		.4033670000D+02	.2285740000D+00	
		.1302670000D+02	.4661620000D+00	
		.4470030000D+01	.3656720000D+00	
	SP 2 1.00	.5425220000D+01	-.4133010000D+00	.2379720000D+00
		.1149150000D+01	.1224420000D+01	.8589530000D+00
	SP 1 1.00	.2832050000D+00	.1000000000D+01	.1000000000D+01
O	S 6 1.00	.5472270000D+04	.1832170000D-02	
		.8178060000D+03	.1410470000D-01	
		.1864460000D+03	.6862620000D-01	
		.5302300000D+02	.2293760000D+00	
		.1718000000D+02	.4663990000D+00	
		.5911960000D+01	.3641730000D+00	
	SP 2 1.00	.7402940000D+01	-.4044530000D+00	.2445860000D+00
		.1576200000D+01	.1221560000D+01	.8539550000D+00
	SP 1 1.00	.3736840000D+00	.1000000000D+01	.100000000D+01

Exponents and coefficients for 6-31G basis set

atom	shell	exponent	coefficient	
H	S 3 1.00	.1873113696D+02	.3349460434D-01	
		.2825394365D+01	.2347269535D+00	
		.6401216923D+00	.8137573262D+00	
	S 1 1.00	.1612777588D+00	.1000000000D+01	
C	S 6 1.00	.3047524880D+04	.1834737130D-02	
		.4573651800D+03	.1403732280D-01	
		.1039486850D+03	.6884262220D-01	
		.2921015530D+02	.2321844430D+00	
		.9286662960D+01	.4679413480D+00	
		.3163926960D+01	.3623119850D+00	
	SP 3 1.00	.7868272350D+01	-.1193324200D+00	.6899906660D-01
		.1881288540D+01	-.1608541520D+00	.3164239610D+00
		.5442492580D+00	.1143456440D+01	.7443082910D+00
	SP 1 1.00	.1687144782D+00	.1000000000D+01	.1000000000D+01

atom	shell	exponent	coefficient	
N	S 6 1.00	.4171351146D+04	.1834772160D-02	
		.6274579110D+03	.1399462700D-01	
		.1429020930D+03	.6858655180D-01	
		.4023432930D+02	.2322408730D+00	
		.1282021290D+02	.4690699480D+00	
		.4390437010D+01	.3604551990D+00	
	SP 3 1.00	.1162636186D+02	-.1149611820D+00	.6757974390D-01
		.2716279807D+01	-.1691174790D+00	.3239072960D+00
		.7722183966D+00	.1145851950D+01	.7408951400D+00
	SP 1 1.00	.2120314975D+00	.1000000000D+01	.1000000000D+01
O	S 6 1.00	.5484671660D+04	.1831074430D-02	
		.8252349460D+03	.1395017220D-01	
		.1880469580D+03	.6844507810D-01	
		.5296450000D+02	.2327143360D+00	
		.1689757040D+02	.4701928980D+00	
		.5799635340D+01	.3585208530D+00	
	SP 3 1.00	.1553961625D+02	-.1107775490D+00	.7087426820D-01
		.3599933586D+01	-.1480262620D+00	.3397528390D+00
		.1013761750D+01	.1130767010D+01	.7271585770D+00
	SP 1 1.00	.3736840000D+00	.1000000000D+01	.100000000D+01

Exponents and coefficients for DZV basis set

atom	shell	exponent	coefficient
H	S 3 1.00	.1924060000D+02	.3282800000D-01
		.2899200000D+01	.2312080000D+00
		.6534000000D+00	.8172380000D+00
	S 1 1.00	.1776000000D+00	.1000000000D+01
C	S 7 1.00	.4233000000D+04	.1220000000D-02
		.6349000000D+03	.9342000000D-02
		.1461000000D+03	.4545200000D-01
		.4250000000D+02	.1546570000D+00
		.1419000000D+02	.3588660000D+00
		.5148000000D+01	.4386320000D+00
		.1967000000D+01	.1459180000D+00
	S 2 1.00	.5148000000D+01	-.1683670000D+00
		.4962000000D+00	.1060091000D+01
	S 1 1.00	.1533000000D+00	.1000000000D+01

atom	shell	exponent	coefficient
C	P 4 1.00	.1816000000D+02	.1853900000D-01
		.3986000000D+01	.1154360000D+00
		.1143000000D+01	.3861880000D+00
		.3594000000D+00	.6401140000D+00
	P 1 1.00	.1146000000D+00	.1000000000D+01
N	S 7 1.00	.5909000000D+04	.1190000000D-02
		.8875000000D+03	.9099000000D-02
		.2047000000D+03	.4414500000D-01
		.5984000000D+02	.1504640000D+00
		.2000000000D+02	.3567410000D+00
		.7193000000D+01	.4465330000D+00
		.2686000000D+01	.1456030000D+00
	S 2 1.00	.7193000000D+01	-.1604050000D+00
		.7000000000D+00	.1058215000D+01
	S 1 1.00	.2133000000D+00	.1000000000D+01
	P 4 1.00	.2679000000D+02	.1825400000D-01
		.5956000000D+01	.1164610000D+00
		.1707000000D+01	.3901780000D+00
		.5314000000D+00	.6371020000D+00
	P 1 1.00	.1654000000D+00	.1000000000D+01
O	S 7 1.00	.7817000000D+04	.1176000000D-02
		.1176000000D+04	.8968000000D-02
		.2732000000D+03	.4286800000D-01
		.8117000000D+02	.1439300000D+00
		.2718000000D+02	.3556300000D+00
		.9532000000D+01	.4612480000D+00
		.3414000000D+01	.1402060000D+00
	S 2 1.00	.9532000000D+01	.1541530000D+00
		.9398000000D+00	.1056914000D+01
	S 1 1.00	.2846000000D+00	.1000000000D+01
	P 4 1.00	.3518000000D+02	.1958000000D-01
		.7904000000D+01	.1242000000D+00
		.2305000000D+01	.3947140000D+00
		.7171000000D+00	.6273760000D+00
	P 1 1.00	.2137000000D+00	.1000000000D+01

Exponents and coefficients for DZ basis set

atom	shell	exponent	coefficient
H	S 3 1.00	.1924060000D+02	.3282800000D-01
		.2899200000D+01	.2312080000D+00
		.6534000000D+00	.8172380000D+00
	S 1 1.00	.1776000000D+00	.1000000000D+01
C	S 6 1.00	.4232610000D+04	.2029000000D-02
		.6348820000D+03	.1553500000D-01
		.1460970000D+03	.7541099936D-01
		.4249740000D+02	.2571210000D+00
		.1418920000D+02	.5965550000D+00
		.1966600000D+01	.2425169945D+00
	S 1 1.00	.5147700000D+01	.1000000000D+01
	S 1 1.00	.4962000000D+00	.1000000000D+01
	S 1 1.00	.1533000000D+00	.1000000000D+01
	P 4 1.00	.1815570000D+02	.1853400000D-01
		.3986400000D+01	.1154420000D+00
		.1142900000D+01	.3862060000D+00
		.3594000000D+00	.6400890000D+00
	P 1 1.00	.1146000000D+00	.1000000000D+01
N	S 6 1.00	.5909440000D+04	.2004000000D-02
		.8874510000D+03	.1531000000D-02
		.2047900000D+03	.7429300000D-01
		.5983760000D+02	.2533640000D+00
		.1999810000D+02	.6005760000D+00
		.2686000000D+01	.2451110000D+00
	S 1 1.00	.7192700000D+01	.1000000000D+01
	S 1 1.00	.7000000000D+00	.1000000000D+01
	S 1 1.00	.2133000000D+00	.1000000000D+01
	P 4 1.00	.2678600000D+02	.1825700000D-01
		.5956400000D+01	.1164070000D+00
		.1707400000D+01	.3901110000D+00
		.5314000000D+00	.6372210000D+00
	P 1 1.00	.1654000000D+00	.1000000000D+01
O	S 6 1.00	.7816540000D+04	.2031000000D-02
		.1175820000D+04	.1543600000D-01
		.2731880000D+03	.7377100000D-01
		.8116960000D+02	.2476060000D+00
		.2718360000D+02	.6118320000D+00
		.3413600000D+01	.2412050000D+00
	S 1 1.00	.9532000000D+01	.1000000000D+01
	S 1 1.00	.9398000000D+00	.1000000000D+01

atom	shell	exponent	coefficient
O	S 1 1.00	.2846000000D+00	.1000000000D+01
	P 4 1.00	.3518320000D+02	.1958000000D-01
		.7904000000D+01	.1241890000D+00
		.2305100000D+01	.3947270000D+00
		.7171000000D+00	.6273750000D+00
	P 1 1.00	.2137000000D+00	.1000000000D+01

Exponents and coefficients for DZP basis set

atom	shell	exponent	coefficient
H	S 3 1.00	.1924060000D+02	.3282800000D-01
		.2899200000D+01	.2312080000D+00
		.6534000000D+00	.8172380000D+00
	S 1 1.00	.1776000000D+00	.1000000000D+01
	P 1 1.00	.1000000000D+01	.1000000000D+01
C	S 6 1.00	.4232610000D+04	.2029000000D-02
		.6348820000D+03	.1553500000D-01
		.1460970000D+03	.7541099936D-01
		.4249740000D+02	.2571210000D+00
		.1418920000D+02	.5965550000D+00
		.1966600000D+01	.2425169945D+00
	S 1 1.00	.5147700000D+01	.1000000000D+01
	S 1 1.00	.4962000000D+00	.1000000000D+01
	S 1 1.00	.1533000000D+00	.1000000000D+01
	P 4 1.00	.1815570000D+02	.1853400000D-01
		.3986400000D+01	.1154420000D+00
		.1142900000D+01	.3862060000D+00
		.3594000000D+00	.6400890000D+00
	P 1 1.00	.1146000000D+00	.1000000000D+01
	D 1 1.00	.7500000000D+00	.1000000000D+01
N	S 6 1.00	.5909440000D+04	.2004000000D-02
		.8874510000D+03	.1531000000D-02
		.2047900000D+03	.7429300000D-01
		.5983760000D+02	.2533640000D+00
		.1999810000D+02	.6005760000D+00
		.2686000000D+01	.2451110000D+00
	S 1 1.00	.7192700000D+01	.1000000000D+01
	S 1 1.00	.7000000000D+00	.1000000000D+01
	S 1 1.00	.2133000000D+00	.1000000000D+01

atom	shell	exponent	coefficient
N	P 4 1.00	.2678600000D+02	.1825700000D-01
		.5956400000D+01	.1164070000D+00
		.1707400000D+01	.3901110000D+00
		.5314000000D+00	.6372210000D+00
	P 1 1.00	.1654000000D+00	.1000000000D+01
	D 1 1.00	.8000000000D+00	.1000000000D+01
O	S 6 1.00	.7816540000D+04	.2031000000D-02
		.1175820000D+04	.1543600000D-01
		.2731880000D+03	.7377100000D-01
		.8116960000D+02	.2476060000D+00
		.2718360000D+02	.6118320000D+00
		.3413600000D+01	.2412050000D+00
	S 1 1.00	.9532000000D+01	.1000000000D+01
	S 1 1.00	.9398000000D+00	.1000000000D+01
	S 1 1.00	.2846000000D+00	.1000000000D+01
	P 4 1.00	.3518320000D+02	.1958000000D-01
		.7904000000D+01	.1241890000D+00
		.2305100000D+01	.3947270000D+00
		.7171000000D+00	.6273750000D+00
	P 1 1.00	.2137000000D+00	.1000000000D+01
	D 1 1.00	.8500000000D+00	.1000000000D+01

Appendix II

Optimized coefficients in the analytical pair potential functions:

---

a) The MCY potential for water-water interactions (28) (ΔE in kcal/mol, r in Angstroms) is

$$\Delta E = \frac{Q^2}{4\pi\varepsilon_o}[(\frac{1}{r_{13}}+\frac{1}{r_{23}}+\frac{1}{r_{14}}+\frac{1}{r_{24}})+\frac{4}{r_{78}}-2(\frac{1}{r_{28}}+\frac{1}{r_{18}}+\frac{1}{r_{37}}+\frac{1}{r_{47}})]$$
$$+a_1\exp(-b_1r_{56})+a_2[\exp(-b_2r_{13})+\exp(-b_2r_{14})$$
$$+\exp(-b_2r_{23})+\exp(-b_2r_{24})]+a_3[\exp(-b_3r_{16})+\exp(-b_3r_{26})$$
$$+\exp(-b_3r_{35})+\exp(-b_3r_{45})]-a_4[\exp(-b_4r_{16})+\exp(-b_4r_{26})$$
$$+\exp(-b_4r_{35})+\exp(-b_4r_{45})]$$

where the constants are equivalent to those of equation [4.5].

parameter	coefficient	parameter	coefficient
$Q_2/4\pi\varepsilon_o$	170.9389	b1	5.152712
a1	1088213.2	b2	2.760844
a2	666.3373	b3	2.961895
a3	1455.427	b4	2.233264
a4	273.5954		

b) The HISH potential for ammonia-ammonia interaction (29) (ΔE in kcal/mol, r in Angstroms) is

$$\Delta E_{NN}(r) = \frac{q_Nq_N}{r}+\frac{A}{r^{12}}-\frac{B}{r^6}$$

$$\Delta E_{NH}(r) = -\frac{q_Nq_H}{r}+C\{\exp[-2D(r-E)]-2\exp[-D(r-E)]\}$$

$$\Delta E_{HH}(r) = \frac{q_Hq_H}{r}+F\exp(-Gr)$$

$$\Delta E = \Delta E_{NN}(r)+\Delta E_{NH}(r)+\Delta E_{HH}(r)$$

atom pair	coefficient	
N-N	q_Nq_N	213.5507633
	A	801444.3445
	B	195.665123
N-H	q_Nq_H	71.18358777
	C	0.1499016936
	D	2.3
	E	2.4
H-H	q_Hq_H	23.72786259
	F	699.5406326
	G	3.7

c) The TR potential for ammonia-water interactions (ΔE in kcal/mol, r in Angstroms) (30) is

$$\Delta E = \sum_{i<j} \frac{q_i q_j}{r_{ij}} + \sum_{m<n} [A_{mn} \exp(-B_{mn} r_{mn}) - C_{mn} \exp(-D_{mn} r_{mn})]$$

where *i* and *j* refer to charges and *m* and *n* to atoms of the water and ammonia molecules, respectively.

atom pair	coefficient			
NH3/H2O	A	B	C	D
N-O	5805.2	1.2380	-	-
N-H	2552.1	1.3158	1209.1	1.0046
H-O	3488.4	1.4722	1520.8	1.1593
H-H	324.12	1.1622	-	-

$q_N = -1.386$, $q_H(NH_3) = 0.462$, $q_O = -1.04385$, $q_H(H_2O) = 0.52193$

Appendix III

Programme generates HONDO Input/Output and calculates stabilization energy and coordinate (FORTRAN).

```
C*****************************************************
C      SCF Accelerator Version 2.00
C*****************************************************
       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
       REAL  R,Zeta,Phi,Pue
       CHARACTER  DD*2,DENS*27
C
       DATA  Pi/3.14159265/
       OPEN(UNIT=11,FILE='Fitinp')
       READ(*,1) DD
    1  FORMAT(A2)
       DO WHILE (DD.NE.'99')
           OPEN(UNIT=7,FILE=DD)
           READ(7,*) Zeta,Phi,Pue
              WRITE(11,444) Phi,Zeta,Pue
  444  FORMAT('Phi=',F6.2,'   Zeta=',F6.2,'   Pue=',F6.2)
           READ(7,*) R
           DO WHILE (R.NE.-1.0)
              CALL  Geninput(R,Zeta,Phi,Pue)
              CALL  System('hondo < input > opt.o')
              OPEN(UNIT=9,FILE='opt.o')
    5  CONTINUE
              READ(9,'(A)') DENS
              IF (DENS.NE.'           DENSITY CONVERGED') GOTO 5
              READ(9,555) ENERGY
  555 FORMAT(//64X,F17.9)
              CLOSE(9)
              OPEN(UNIT=20,FILE='tran')
              READ(20,*) XO2,YO2,ZO2,XH12,YH12,ZH12,
     +                   XH22,YH22,ZH22
              CLOSE(20)
                 EGY= (ENERGY+600.7814029)*627.5
              WRITE(11,333) EGY,XO2,YO2,ZO2,R,XH12,YH12,ZH12,
     +                      XH22,YH22,ZH22
  333 FORMAT(F12.5,' ,',5X,3(F9.5,','),F5.2/19X,3(F9.5,',')/
     + 19X,3(F9.5,','))
              READ(7,*) R
           END DO
          WRITE(11,*)
          READ(*,1) DD
       END DO
C
        CALL  System('rm fort.*')
        CALL  System('rm opt.o tran coord input')
  999   STOP
       END
C-------------------------------------------------------
       SUBROUTINE  Geninput(R,Zeta,Phi,Pue)
       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
       REAL  R,Zeta,Phi,Pue,B,C
       CHARACTER   S1*19
       CHARACTER   S2*19
       CHARACTER   S3*19
C
       DATA  Pi/3.14159265/
         roh=0.9572
         B=Phi-Pue+180
         C=Phi-Pue+75.5
```

```
        XO=R*SIN(Pi*Phi/180)*COS(Pi*Zeta/180)
        YO=R*SIN(Pi*Phi/180)*SIN(Pi*Zeta/180)
        ZO=R*COS(Pi*Phi/180)
       XH1=roh*SIN(Pi*(B)/180)*COS(Pi*Zeta/180)+XO
       YH1=roh*SIN(Pi*(B)/180)*SIN(Pi*Zeta/180)+YO
       ZH1=roh*COS(Pi*(B)/180)+ZO
       XH2=roh*SIN(Pi*(C)/180)*COS(Pi*Zeta/180)+XO
       YH2=roh*SIN(Pi*(C)/180)*SIN(Pi*Zeta/180)+YO
       ZH2=roh*COS(Pi*(C)/180)+ZO
C
      CALL  System('cp part1  input')
      S1 = 'O            8.    '
      S2 = 'H1           1.    '
      S3 = 'H2           1.    '
          OPEN(UNIT=8,FILE= 'coord')
      WRITE(8,111) S1,XO,YO,ZO,S2,XH1,YH1,ZH1,
     + S3,XH2,YH2,ZH2
  111 FORMAT((A),F13.7,7X,F13.7,7X,F13.7/(A),F13.7,7X,F13.7,7X,F13.7/
     +(A),F13.7,7X,F13.7,7X,F13.7)
      CLOSE(8)
        XO2 = XO
        YO2 = YO
        ZO2 = ZO
        XH12 = XH1
        YH12 = YH1
        ZH12 = ZH1
        XH22 = XH2
        YH22 = YH2
        ZH22 = ZH2
      OPEN(UNIT=20,FILE='tran')
      WRITE(20,*) XO2,YO2,ZO2,XH12,YH12,ZH12,
     + XH22,YH22,ZH22
      CLOSE(20)
      Call System('cat coord part2 >> input')
      RETURN
      END
C-------------------------------------------------
```

Appendix IV

HONDO input file

```
 $CNTRL  runflg=0 , iprint=0 , nosym = 1, $END
$MASS    amass*50
         6.0 1.0 1.0  47*0.0
$GUESS   nguess  norb uhfflg
         3       48   0
$INTGRL  nkfil
         1
$WFN     wfnflg
         0
$SCF     nco  nseto  no     maxit  uhfflg acurcy
         53   0      10*0   90     0      0.001
 $BASIS
  cyclen
    0    0   15    1  STO  ...
C1
O           8.          0.1498558          -0.1483634          -2.352121
H           1.          0.5856424           0.5114275          -1.813035
H           1.         -0.3799119          -0.6512179          -1.733792
N1          7.         -1.34168            -1.34168            -0.39390
N2          7.          1.34167            -1.34168             0.39390
N3          7.          1.34168             1.34167            -0.39390
N4          7.         -1.34166             1.34168             0.39390
C1          6.         -0.72621            -2.50763             0.25518
C2          6.          0.72623            -2.50763            -0.25518
C3          6.          2.50762            -0.72624            -0.25518
C4          6.          2.50763             0.72622             0.25518
C5          6.          0.72624             2.50762             0.25518
C6          6.         -0.72621             2.50762            -0.25519
C7          6.         -2.50762             0.72624            -0.25518
C8          6.         -2.50763            -0.72621             0.25518
H1          1.         -1.21458            -3.44214            -0.03509
H2          1.          1.21461            -3.44214             0.03510
H3          1.          3.44213            -1.21462             0.03509
H4          1.          3.44214             1.21459            -0.03510
H5          1.          1.21463             3.44212            -0.03510
H6          1.         -1.21459             3.44214             0.03509
H7          1.         -3.44212             1.21462             0.03509
H8          1.         -3.44214            -1.21458            -0.03509
H9          1.         -0.72960            -2.41776             1.34513
H10         1.          0.72961            -2.41776            -1.34513
H11         1.          2.41776            -0.72962            -1.34514
H12         1.          2.41777             0.72961             1.34513
H13         1.          0.72963             2.41776             1.34513
H14         1.         -0.72960             2.41776            -1.34514
H15         1.         -2.41775             0.72962            -1.34514
H16         1.         -2.41776            -0.72960             1.34514
H17         1.          1.66177            -1.60058             1.32010
H18         1.          1.60058             1.66208            -1.32011
H19         1.         -1.66208             1.60058             1.32010
H20         1.         -1.60059            -1.66209            -1.32010
 $END
```

CURRICULUM VITAE

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1969	Born April, 3rd in Lampang, Thailand Father : Mr. Sitthisak Udomsub Mother : Mrs. Rossukonth Udomsub
1975-1981	Elementary School
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