

# Electronic Supplementary Information for “A Ground State Potential Energy Surface for HONO based on a Neural Network with Exponential Fitting Functions”

Ekadashi Pradhan<sup>a</sup> and Alex Brown<sup>a\*</sup>

## S0 Fit to 1D Potential Energy Curves

To obtain the sum over 1D energies,  $V_{tot}^0(x_i)$ , the potentials for the bond distances were fit to Morse functional form:

$$V(r_i) = A_0[1 - e^{-A_1(r_i - A_2)}]^2. \quad (1)$$

The bond angles (in their cosine form) were fit to a 4th order polynomial, i.e.,

$$V(\cos \theta_i) = A_0 + A_1 \cos(\theta_i) + A_2(\cos \theta_i)^2 + A_3(\cos \theta_i)^3 + A_4(\cos \theta_i)^4. \quad (2)$$

The dihedral angle was fit to  $\cos(nx)$  form:

$$V(\phi) = A_0 + A_1 \cos(\phi) + A_2 \cos(2\phi) + A_3 \cos(3\phi) + A_4 \cos(4\phi). \quad (3)$$

The fitting parameters are presented in Tables S1 and S2. As discussed in the main text, the energy filtering was performed using only the 1D potential fits from the trans geometry; however, data for both the trans- and cis-isomers is presented here.

**Table S1** Fitting Parameters of bond lengths (in au) for trans- and cis-HONO

Fitting Parameter	A <sub>0</sub>	A <sub>1</sub>	A <sub>2</sub>
trans-HONO			
$R_{N=O}$	0.234724	1.3613	2.2109
$R_{ON}$	0.071236	1.21988	2.68149
$R_{OH}$	0.1772	1.2145	1.8254
cis-HONO			
$R_{N=O}$	0.22438	1.3443	2.2355
$R_{ON}$	0.07585	1.27968	2.6172
$R_{OH}$	0.156615	1.24114	1.84378

<sup>a</sup>Department of Chemistry, University of Alberta, Edmonton, Alberta T6G 2G2 Canada. Fax: 780-492-8231; Tel: 780-492-1854; E-mail: alex.brown@ualberta.ca

**Table S2** Fitting parameters for bond angles and dihedral angle of cis- and trans-HONO

Fitting Parameter	A <sub>0</sub>	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A <sub>4</sub>
trans-HONO					
cos $\theta_{ONO}$	0.0454297	0.289274	0.57919	0.445615	0.265011
cos $\theta_{HON}$	0.00483919	0.0470909	0.123341	0.0478834	0.0299907
$\phi$	0.0103183	0.00118698	-0.0096204	-0.000340861	-0.000142621
cis-HONO					
cos $\theta_{ONO}$	0.0675922	0.398938	0.786201	0.662467	0.357884
cos $\theta_{HON}$	0.0081536	0.062814	0.145385	0.0737161	0.045309
$\phi$	0.0111641	-0.000004713	-0.0104423	-0.00032032	0.000195262

**Table S3** Previous experimental and theoretical<sup>a</sup> values for the bond distances (Å) and angles (degrees), defining the equilibrium geometry for trans-HONO, cis-HONO and the transition state (TS<sub>trans↔cis</sub>).

Methods	R <sub>N=O</sub>	R <sub>ON</sub>	R <sub>OH</sub>	$\theta_{ONO}$	$\theta_{HON}$	$\phi$
trans-HONO						
CCSD(T)/cc-pVQZ(fc) <sup>1</sup>	1.1690	1.4178	0.9684	110.76	102.08	180.0
CCSD(T)/cc-pwCVQZ(ae) <sup>1</sup>	1.1693	1.4175	0.9644	110.75	102.12	180.0
CCSD(T)/cc-pVQZ(-g) (fc) <sup>2</sup>	1.170	1.426	0.964	110.70	101.90	180.00
CCSD(T)/TZ2P(fc) <sup>3</sup>	1.173	1.453	0.966	110.50	101.40	180.00
MP2/6-311++G(d,p)(ae) <sup>4</sup>	1.1786	1.4181	0.9677	111.04	101.93	180.0
MP4SDTQ/6-311+G(d,p) (fc) <sup>4</sup>	1.1817	1.4522	0.9698	110.97	101.52	180.0
B3LYP/6-311++G(d,p) <sup>5</sup>	1.166	1.433	0.969	111.20	102.90	180.00
B3LYP/6-311G(3df,3pd) <sup>6</sup>	1.163	1.430	0.966	111.0	102.5	180.0
Experiment <sup>1</sup>	1.1689(3)	1.4250(3)	0.9647(6)	110.69(8)	102.086(45)	180.0
Experiment <sup>7</sup>	1.173(2)	1.441(2)	0.947(3)	110.5(2)	102.1(2)	180.0
Experiment <sup>8,b</sup>	1.185	1.392	0.982	113.6	104.0	180.00
Experiment <sup>9</sup>	1.170	1.432	0.958	110.7	102.1	180.00
Experiment <sup>10</sup>	1.169	1.442	0.959	110.6	102.1	180.0
cis-HONO						
CCSD(T)/cc-pVQZ (fc) <sup>11</sup>	1.1841	1.3863	0.9750	113.22	104.52	0.00
CCSD(T)/cc-pVQZ(-g) (fc) <sup>2</sup>	1.183	1.390	0.974	113.20	104.40	0.00
CCSD(T)/TZ2P(fc) <sup>3</sup>	1.187	1.414	0.974	113.00	104.30	0.00
MP2/6-311++G(d,p)(ae) <sup>4</sup>	1.1921	1.3809	0.9780	113.44	105.34	0.0
MP4SDTQ/6-311+G(d,p) (fc) <sup>4</sup>	1.1976	1.4081	0.9793	113.35	104.86	0.0
B3LYP/6-311++G(d,p) <sup>5</sup>	1.180	1.392	0.980	113.9	106.8	0.0
B3LYP/6-311G(3df,3pd) <sup>6</sup>	1.176	1.387	0.978	113.7	105.8	0.0
Experiment <sup>11</sup>	1.1816(10)	1.3887(10)	0.9744(7)	113.18(1)	104.67(4)	0.00
Experiment <sup>7</sup>	1.190(5)	1.397(6)	0.973(3)	113.5(3)	104.4(4)	0.0
Experiment <sup>8,b</sup>	1.170	1.432	0.958	110.7	102.1	0.00
Experiment <sup>9</sup>	1.185	1.392	0.982	113.6	104.0	0.0
Experiment <sup>10</sup>	1.186	1.399	0.989	113.6	103.9	0.0
TS <sub>trans↔cis</sub>						
CCSD(T)/cc-pVQZ(-g) (fc) <sup>2</sup>	1.164	1.506	0.962	110.50	100.70	86.40
MP2/6-311++G(d,p)(ae) <sup>4</sup>	1.1652	1.5120	0.9690	111.43	102.54	85.53
B3LYP/6-311G(3df,3pd) <sup>6</sup>	1.153	1.500	0.967	111.5	104.4	87.8

<sup>a</sup> Several of the references contain equilibrium geometries computed with multiple methods and basis sets. Generally only the values determined using the highest level(s) of theory are reported here. <sup>b</sup> Provided as given in the original paper but when compared to other values, suggests that the trans- and cis- labels may have been inadvertently switched.

**Table S4** CCSD(T)-F12/cc-pVTZ-F12 (F12) optimized geometries including bond distances (Å) and angles (degrees), of HNO<sub>2</sub>, TS<sub>trans↔HNO<sub>2</sub></sub> and TS<sub>HONO↔1,3HONO</sub>. Also provided are experimental and previous theoretical results.

Methods	R <sub>N=O</sub>	R <sub>O-N</sub>	R <sub>O-H</sub>	θ <sub>O-N-O</sub>	θ <sub>H-O-N</sub>	φ
HNO <sub>2</sub>						
CCSD(T)-F12/cc-pVTZ-F12 <sup>a</sup>	1.217	1.217	1.911	128.00	29.09	180.00
CCSD(T)/TZ2P(fc) <sup>12</sup>	1.225	1.225	1.917	128.20	28.97	180.00
B3LYP/6-311G(3df,3pd) <sup>6</sup>	1.231	1.231	1.936	128.70	29.29	180.00
B3LYP/6-311++G(d,p) <sup>5</sup>	1.216	1.216	1.044 <sup>a</sup>	104.4	180.0	
TS <sub>trans↔HNO<sub>2</sub></sub>						
CCSD(T)-F12/cc-pVTZ-F12 <sup>a</sup>	1.189	1.319	1.301	53.57	123.23	180.00
CCSD(T)/aug-cc-pVTZ <sup>a</sup>	1.194	1.325	1.304	53.32	123.34	180.00
B3LYP/6-311G(3df,3pd) <sup>6</sup>	1.188	1.317	1.300	53.80	123.50	180.00
TS <sub>HONO↔1,3HONO</sub>						
CCSD(T)-F12/cc-pVTZ-F12 <sup>a</sup>	1.262	1.262	1.299	105.06	76.99	0.00
CCSD(T)/aug-cc-pVTZ <sup>a</sup>	1.268	1.268	1.298	104.86	76.84	0.00
B3LYP/6-311G(3df,3pd) <sup>6</sup>	1.260	1.260	1.304	105.30	77.40	0.00
CCSD(T)/aug-cc-pVQZ(-g functions) <sup>2</sup>	1.265	1.265	1.298	105.10	76.90	0.00

<sup>a</sup> Present Work; <sup>b</sup> R<sub>NH</sub>**Table S5** T<sub>1</sub> diagnostic<sup>13</sup> from the CCSD of the CCSD(T)-F12/cc-pVTZ-F12 computations at the corresponding optimized geometries

	T <sub>1</sub>
trans-HONO	0.0210
TS <sub>cis↔trans</sub>	0.0191
cis-HONO	0.0209
HNO <sub>2</sub>	0.0200
TS <sub>trans↔HNO<sub>2</sub></sub>	0.0266
TS <sub>HONO↔1,3HONO</sub>	0.0246

**Table S6** Harmonic vibrational frequencies and zero point energies (ZPE) (both in cm<sup>-1</sup>) for the trans-HONO, cis-HONO, HNO<sub>2</sub>, TS\_ct (transition state of cis-trans isomerization), TS\_12(transition state of trans-HONO tautomerization to H-NO<sub>2</sub>) and TS\_13 (transition state of 1,3-H migration of Hydrogen). All results determined at the CCSD(T)-F12/cc-pVTZ-F12 level of theory.

Frequencies	trans	cis	HNO <sub>2</sub>	TS_ct	TS_12	TS_13	OH+NO
	577.0	649.0	788.0	593.0(i)	2125.5(i)	1962.3(i)	
	636.0	679.0	1040.3	555.7	465.2	1019.3	
	836.0	899.0	1385.5	788.4	692.0	1238.4	
	1320.0	1350.0	1511.5	1121.2	1293.4	1283.2	
	1732.0	1677.0	1649.4	1730.7	1584.2	1366.2	1916.7
	3780.0	3623.0	3265.8	3773.3	2496.3	2135.2	3741.9
ZPE	4440.5	4438.5	4820.3	3984.7	3265.6	3521.1	2829.3

**Table S7** Harmonic frequencies (in  $\text{cm}^{-1}$ ) of the fundamental modes for trans-HONO. The intensities (in  $\text{km/mol}$ ) are provided when determined.

Mode	MP2/AVTZ <sup>a</sup>	CCSD(T)			F12 <sup>b</sup>	Expt. <sup>c</sup>
		AVTZ <sup>a</sup>	AVQZ	AV5Z 5		
OH	3754.8 (90.4)	3760.0 (72.9)	3779.3	3782	3780.0	3590.7
N=O	1659.9 (108.6)	1715.4 (133.2)	1728.3	1729.6	1732.0	1699.8
HON	1283.4 (174.5)	1306.1 (170.1)	1315.7	1317.0	1320.0	1263.1
O-N	805.3 (159.4)	815.9 (145.6)	830.0	833.7	836.0	790.1
ONO	602.5 (196.0)	617.4 (121.8)	630.4	634.0	636.0	595.6
Torsion	586.5 (99.3)	565.1 (97.2)	575.7	576.0	577.0	543.8
RMSE	71.9	72.6	84.6	86.4	86.5	-

<sup>a</sup> Harmonic frequencies and intensities from CFOUR software<sup>14</sup><sup>b</sup> CCSD(T)-F12/cc-pVTZ-F12 level of theory<sup>c</sup> (Torsion, ONO bend) from Ref. 15; (ON stretching, HON bend) from Ref. 16; N=O stretching from Ref. 17; and OH stretching from Ref. 18**Table S8** Harmonic vibrational frequencies (in  $\text{cm}^{-1}$ ) of the fundamental modes of cis-HONO. The intensities (in  $\text{km/mol}$ ) are provided when determined.

Mode	MP2/AVTZ <sup>a</sup>	CCSD(T)			F12 <sup>b</sup>	Expt. <sup>c</sup>
		AVTZ <sup>a</sup>	AVQZ	AV5Z		
OH	3591.2 (37.6)	3608.4 (29.3)	3622.7	3625.6	3623.0	3426.2
N=O	1610.7 (141.7)	1658.3 (166.5)	1670.4	1674.0	1677.0	1640.5
HON	1320.2 (7.0)	1337.4 (9.6)	1348.0	1351.2	1350.0	1302.0
O-N	884.2 (359.4)	876.4 (298.5)	895.0	898.3	899.0	851.0
ONO	634.0 (36.3)	631.9 (26.2)	645.4	648.7	649.0	609.0
Torsion	693.7 (97.7)	667.5 (97.3)	681.4	685.0	679.0	638.5
RMSE	74.0	78.1	88.3	90.6	89.4	-

<sup>a</sup> Harmonic frequencies and intensities from CFOUR software<sup>14</sup>; <sup>b</sup> CCSD(T)-F12/cc-pVTZ-F12 level of theory; <sup>c</sup> From Ref. 8**Table S9** The energy difference (in  $\text{cm}^{-1}$ ) between trans-HONO and cis-HONO without ZPE correction ( $\Delta E$ ) and with ZPE correction ( $\Delta E_{ZPE}$ ) as determined using various levels of theory.

Method	$\Delta E(\text{cm}^{-1})$	$\Delta E_{ZPE}(\text{cm}^{-1})$
MP2 /aug-cc-pVTZ	179.5	198.9
CCSD(T)/aug-cc-pVTZ	167.9	171.4
CCSD(T)/aug-cc-pVQZ	136.0	137.7
CCSD(T)/aug-cc-pV5Z	122.4	127.7
CCSD(T)-F12A/cc-pVTZ-F12	122.0	120.0
CCSD(T)-F12B/cc-pVTZ-F12	124.0	122.0
CCSD(T)-F12A/cc-pVTZ-F12/PES <sup>a</sup>	—	125.1
CCSD(T)/CBS/PES <sup>a</sup>	—	122.0

<sup>a</sup> As determined from MCTDH computations of the ZPE on the corresponding PESs fit with 90 NN.

**Table S10** trans-HONO 2D grid. Bond lengths are in a.u. and bond angles are in degrees.

Coordinates	Grid points
$R_1^{N=O}$	[1.99,2.05,2.1,2.15,2.21,2.246,2.28,2.32,2.4,2.5]
$R_2^{O-N}$	[2.33,2.45,2.53,2.61,2.681,2.765,2.845,2.96,3.14,3.32]
$R_3^{O-H}$	[1.56,1.67,1.72,1.77,1.825,1.874,1.91,1.99,2.09,2.24]
$\Theta_1^{ONO}$	[98,101,104,107,109,110.69,112.5,114.8,119,123,130]
$\Theta_2^{HON}$	[80,89,94,97,100,102.26,104.5,108,112,117,125]
Torsion ( $\phi$ )	[90,120,140,155,165,170,174,177,179,180]

**Table S11** cis-HONO 2D grid. Bond lengths are in a.u. and bond angles are in degrees.

Coordinates	Grid points
$R_1^{N=O}$	[1.99,2.05,2.1,2.15,2.2515,2.246,2.28,2.32,2.4,2.5]
$R_2^{O-N}$	[2.33,2.45,2.53,2.61,2.62194,2.765,2.845,2.96,3.14,3.32]
$R_3^{O-H}$	[1.56,1.67,1.72,1.77,1.85268,1.874,1.91,1.99,2.09,2.24]
$\Theta_1^{ONO}$	[98,101,104,107,109,113.3026,112.5,114.8,119,123,130]
$\Theta_2^{HON}$	[80,89,94,98,101,104.6118,106,108,112,117,125]
Torsion ( $\phi$ )	[70,60,45,35,25,15,9,6,3,0]

**Table S12**  $TS_{trans \leftrightarrow cis}$ -HONO 2D grid. Bond lengths are in a.u. and bond angles are in degrees.

Coordinates	Grid points
$R_1^{N=O}$	[1.99,2.06,2.12,2.16,2.194,2.23,2.29,2.34,2.45,2.57]
$R_2^{O-N}$	[2.35,2.5,2.6,2.71,2.819,2.93,3.06,3.19,3.47,3.9]
$R_3^{O-H}$	[1.57,1.65,1.73,1.76,1.827,1.875,1.94,2.0,2.13,2.3]
$\Theta_1^{ONO}$	[99,102,105,107.5,109.5,111.19,113,115,119,122,125]
$\Theta_2^{HON}$	[81,88,93,97.5,101,103.439,106,109,112.5,119,127]
Torsion ( $\phi$ )	[37,54,65,74,82,86.91,90.5,97,106,117,137]

**Table S13** RMSE vs NN of HONO

Number of Neurons (NN)	RMSE (in $\text{cm}^{-1}$ )			
	F12		CBS	
	Testset	Trainset	Testset	Trainset
20	96.9	101.9	104.4	91.0
30	49.1	46.9	51.3	41.3
40	31.6	30.8	32.3	24.2
50	22.6	21.1	20.3	14.0
60	19.8	18.0	15.1	9.9
70	15.1	13.8	12.8	8.4
80	11.0	7.8	13.0	9.3
90	10.2	8.5	10.4	6.8
100	12.2	10.4	10.5	7.0

**Table S14** Refitting previous PES<sup>2</sup> with NN-expnn; MCTDH vibrational states of trans-HONO and cis-HONO Number of neurons is 80 here. 5k, 7k, 8k, 9k, and 10k represent 5000, 700, 8000, 9000, and 10000 cm<sup>-1</sup> cut-off energy PES, respectively.

	Torsion	ONO bend	ON str	HON bend	N=O str	OH str	ZPE
trans-HONO							
Ref [2]	538.0	601.0	796.0	1267.0	1698.0	3590.0	4367.6
5k	538.4	601.1	796.1	1267.5	1690.0	3587.0	4364.2
7k	538.0	601.0	795.0	1268.0	1690.0	3589.0	4365.4
8k	539.2	600.7	795.6	1268.2	1689.4	3586.0	4364.6
9k	537.5	600.5	794.4	1267.5	1689.0	3586.7	4366.8
10K	534.5	601.0	796.0	1268.6	1685.0	3587.5	4371.6
cis-HONO							
'Ref [2]	632.0	617.0	850.0	1312.0	1637.0	3436.0	4461.5
5k	632.2	617.2	850.1	1311.4	1632.8	3432.5	4457.7
7k	631.3	617.0	850.5	1311.0	1632.4	3436.0	4457.1
8k	629.2	616.3	850.3	1310.0	1634.0	3432.0	4458.5
9k	629.1	616.0	850.0	1310.0	1631.6	3434.3	4458.3
10k	632.0	616.0	848.5	1307.6	1633.6	3437.4	4458.7

**Table S15** Vibrational frequencies of selected overtones and combination modes (in cm<sup>-1</sup>) of trans-HONO for the CBS\_345 90 NN fit PES.

(v <sub>1</sub> v <sub>2</sub> v <sub>3</sub> v <sub>4</sub> v <sub>5</sub> v <sub>6</sub> ) <sup>a</sup>	This work		Previous Expt.	Guilmot <i>et al.</i> <sup>17</sup>	Richter <i>et al.</i> <sup>2</sup>
	F12	CBS			
020000	3402.1	3374.5	3372.1 <sup>b</sup>	3372.1	3367.4
101000	4220.2	4384.2	4379.0 <sup>c</sup>	4378.3	
100100	4853.7	4830.1	4829.0 <sup>c</sup>	4829.6	
100200	6078.8	6052.4		6045.8	
200000	7190.6	7012.1	7017.0 <sup>c</sup>	7016.8	
300000	10301.0	10297.0	10279.0 <sup>c</sup>	10280.5	
400000	13489.0	13507.0	13385.0 <sup>c</sup>		

<sup>a</sup> v<sub>1</sub>: CH stretch. (A'), v<sub>2</sub>: N=O stretch. (A'), v<sub>3</sub>: ON stretch. (A'), v<sub>4</sub>: HON bend. (A'), v<sub>5</sub>:ONO bend. (A') and v<sub>6</sub>: out-of-plane bend. (A''); <sup>b</sup> From Ref. 19; <sup>c</sup> From Ref. 20

**Table S16** Vibrational frequencies of selected overtones and combination modes (in cm<sup>-1</sup>) of cis-HONO for the CBS\_345 90 NN fit PES.

(v <sub>1</sub> v <sub>2</sub> v <sub>3</sub> v <sub>4</sub> v <sub>5</sub> v <sub>6</sub> ) <sup>a</sup>	This work		Previous Expt.	Guilmot <i>et al.</i> <sup>21</sup>	Richter <i>et al.</i> <sup>2</sup>
	F12	CBS			
011000	2531.9	2515.9	2493.0 <sup>b</sup>	2492.9	2476.7
020000	3292.2	3264.7	3257.9 <sup>c</sup>	3257.9	3253.6
101000	4317.1	4297.8	4281.0 <sup>d</sup>	4281.0	
200000	6876.0	6676.7	6665.0 <sup>d</sup>	6664.4	

<sup>a</sup> v<sub>1</sub>: CH stretch. (A'), v<sub>2</sub>: N=O stretch. (A'), v<sub>3</sub>: ON stretch. (A'), v<sub>4</sub>: HON bend. (A'), v<sub>5</sub>:ONO bend. (A') and v<sub>6</sub>: out-of-plane bend. (A''); <sup>b</sup> From Ref. 22; <sup>c</sup> From Ref. 15; <sup>d</sup> From Ref. 20

## S0 CBS\_345 Extrapolated PES of HONO using 90 NN: Operator file

OP.DEFINE-SECTION

title

HONO r1 = OH, r2 = N=O, r3 = ON, th1 = HON, th2 = ONO, p1 = torsion

This operator file is for cos-DVR for p.1 defined on [0,pi].

end-title

end-op\_define-section

PARAMETER-SECTION

q20 = 2.696732586, q30 = 1.822912197, q10 = 2.21332641, q11 = 1.8653, th20 = 1.777642018, th10 = 1.9315017, mh = 1.0, H-mass, mc = 12.0,AMU, mo = 15.9949,AMU, mn = 13.9939,AMU, M11 = 1.0/mo+1.0/mh, M22 = 1.0/mo+1.0/mn, M33 = M22, M13 = 1.0/mo, M23 = -1.0/mn, p1 = PI/2.0, p2 = 3.0\*PI/2.0  
, r0 = -0.0989292117084, w0u0 = -0.853200541447781, w0u1 = -0.242988044034525, w0u2 = 0.032555967181883, w0u3 = -3.167126278444403, w0u4 = 1.023820200338571, w0u5 = -0.577240957387413, r1 = -1508.01439595, w1u0 = -1.116352239758439, w1u1 = -1.220201517521363, w1u2 = -0.082661674734828, w1u3 = 2.947379294597612, w1u4 = 1.462903126335998, w1u5 = -0.634283038194566, r2 = -0.128339800865, w2u0 = -1.385927636257777, w2u1 = 0.219465874494011, w2u2 = 0.177429964888646, w2u3 = -2.425039201771836, w2u4 = -0.833476901989908, w2u5 = 0.025621397776061, r3 = 0.0013726184638, w3u0 = 1.172164241523227, w3u1 = -0.046358169379889, w3u2 = -0.510518623086877, w3u3 = -0.902072221830776, w3u4 = 0.810623163825699, w3u5 = 0.247067857977654, r4 = -26.831252236, w4u0 = -0.830803569743358, w4u1 = -1.254738392767832, w4u2 = -0.052145281280020, w4u3 = 2.433613560792109, w4u4 = 0.788339918473749, w4u5 = 0.287896108863929, r5 = 2.06716395215, w5u0 = -1.139502618837195, w5u1 = -0.745780602007849, w5u2 = -0.144726792484251, w5u3 = 2.521648506611887, w5u4 = -0.628725231599676, w5u5 = 0.830876257902396, r6 = -1780.7073866, w6u0 = -0.174941901862294, w6u1 = -1.552455925722280, w6u2 = 0.528321481092629, w6u3 = 0.870364481774773, w6u4 = 0.930407607983181, w6u5 = -2.549588002817600, r7 = -6.38328173171, w7u0 = -0.913923338264948, w7u1 = -0.008661645227680, w7u2 = -0.985703331513715, w7u3 = 0.416036304537306, w7u4 = 0.110828177799288, w7u5 = -0.029286582009631, r8 = -5.81956169623, w8u0 = -0.135284485884308, w8u1 = -0.756002099321000, w8u2 = 0.011881233056163, w8u3 = 0.209568220113634, w8u4 = -0.331784935201660, w8u5 = -0.140061782546228, r9 = 27.9797440321, w9u0 = -0.083882765867326, w9u1 = -0.003920098550541, w9u2 = -3.291668678940854, w9u3 = 0.040412533788156, w9u4 = -0.000834420720384, w9u5 = -0.002462237001581, r10 = -0.0253279567409, w10u0 = -0.001170018143470, w10u1 = 0.196830207136118, w10u2 = -0.054412522758295, w10u3 = -1.945917804810354, w10u4 = -0.709593222350115, w10u5 = -0.089766870498877, r11 = 98.4626718188, w11u0 = -3.262419556847753, w11u1 = -0.110957884054188, w11u2 = 0.177158207998086, w11u3 = 0.154254582503147, w11u4 = 0.070920532770424, w11u5 = 0.014359565042413, r12 = 12.681082388, w12u0 = -0.441581732986989, w12u1 = -2.085985476420360, w12u2 = 1.593200968323242, w12u3 = 4.239052477949012, w12u4 = 1.912412741392200, w12u5 = -0.410189143178070, r13 = 60.7842797092, w13u0 = -0.007757010932104, w13u1 = -1.849278243352667, w13u2 = 0.316486564320230, w13u3 = 0.002283216008185, w13u4 = 1.065513138556361, w13u5 = 0.740150097599871, r14 = 302.88029365, w14u0 = 0.042851034679758, w14u1 = -1.683351419041932, w14u2 = 0.284225602714214, w14u3 = -0.213896900552025, w14u4 = 0.299100130731710, w14u5 = -1.349385144150157, r15 = -4.48807896894d-06, w15u0 = 0.607708924306238, w15u1 = 0.426576944920903, w15u2 = 1.712110145997201, w15u3 = -1.411032256844647, w15u4 = -0.552983689791342, w15u5 = 0.228822602002352, r16 = 0.0216293358866, w16u0 = -2.131474531082708, w16u1 = 1.311118087753804, w16u2 = 0.368320618243550, w16u3 = -1.344277324684069, w16u4 = -0.808790548757823, w16u5 = -0.002424788885103, r17 = 0.00158638367554, w17u0 = -0.784269168971525, w17u1 = 0.333758298135627, w17u2 = 0.352940486491789, w17u3 = -1.227408509846475, w17u4 = -0.148142379584223, w17u5 = 0.652270253883597, r18 = 0.000227158475832, w18u0 = 0.758572710520038, w18u1 = 0.417239790748004, w18u2 = 0.114856949700676, w18u3 = 1.501277180953857, w18u4 = 2.682662326012086, w18u5 = -0.554418157956709, r19 = 0.000139366976479, w19u0 = 1.143215612528171, w19u1 = -0.290214640082409, w19u2 = 0.518999082645808, w19u3 = 1.702906874775170, w19u4 = -1.329319112341047, w19u5 = 0.266271389891513, r20 = -101.19900991, w20u0 = -0.476776755992009, w20u1 = -0.976681652891100, w20u2 = 0.180554624366756, w20u3 = 1.387920647609959, w20u4 = -0.588509397942507, w20u5 = -1.144615710998483, r21 = -2.23384787572, w21u0 = -0.048995644555810, w21u1 = -1.570467878270445, w21u2 = -0.471327235755910, w21u3 = 0.887074121265057, w21u4 = -2.313439432967188, w21u5 = 0.451814747021784, r22 = -22.0913040748, w22u0 = -0.305088924550694, w22u1 = -1.548481227852525, w22u2 = -0.176945143494662, w22u3 = 1.275086376167996, w22u4 = -1.560524658481483, w22u5 = 0.365415909969871, r23 = -574.969181043, w23u0 = 0.048244606725621, w23u1 = -1.738542745787764, w23u2 = 0.290286663994938, w23u3 = -0.205220464482039, w23u4 = 0.581857557864165, w23u5 = -0.604455373831783, r24 = 3.38195755122, w24u0 = -0.181860523296136, w24u1 = -1.367671219069719, w24u2 = -0.200237326825643, w24u3 = 0.246814670149435, w24u4 = -1.814169510762366, w24u5 = -0.321163641280683, r25 = 5.56916957922, w25u0 = -1.211123452136019, w25u1 = -0.925633687152736, w25u2 = 0.376581147047806, w25u3 = 1.592679628065842, w25u4 = 3.036450254631379, w25u5 = -0.603234808841615, r26 = -3.60255222952d-05, w26u0 = 0.946857763941655, w26u1 = 0.895864786558203, w26u2 = 0.709734683038783, w26u3 = 1.379115858238740, w26u4 = 1.570465761487129, w26u5 = -0.014818140556473, r27 = -0.0529327316423, w27u0 = -0.552611745806075, w27u1 = -0.237250987650281, w27u2 = 0.092855747811619, w27u3 = -2.222441791074366, w27u4 = -0.911055094237467, w27u5 = 0.459298832167413, r28 = -0.00208806646172, w28u0 = -2.597222595695893, w28u1 = 2.171083226033266, w28u2 = 0.394856290811928, w28u3 = -0.448033984839479,

w28u4 = -0.695564980839464, w28u5 = -0.006606432251146, r29 = 5230.44961875, w29u0 = -0.208532879423894, w29u1 = -1.522020968063148, w29u2 = 0.538824605293654, w29u3 = 0.965430484869679, w29u4 = 1.095851879665458, w29u5 = -2.373631280783556, r30 = -3.21227572404, w30u0 = -0.884542704955197, w30u1 = -0.896737022464103, w30u2 = -0.394222102962516, w30u3 = 2.233039582570567, w30u4 = -1.636133128361070, w30u5 = 0.697587078088605, r31 = -6.35164830561, w31u0 = -0.052937709043642, w31u1 = -1.954013858263051, w31u2 = 0.363741581766958, w31u3 = 0.161431540826286, w31u4 = 1.400830260036604, w31u5 = 1.323780704237094, r32 = -109.077881759, w32u0 = -0.585039102406441, w32u1 = -2.078217949582065, w32u2 = -0.007409299594651, w32u3 = -1.155802125734104, w32u4 = -0.393628889192751, w32u5 = 0.038064962722235, r33 = 1053.8582557, w33u0 = -0.267602627330121, w33u1 = -1.431376491521275, w33u2 = 0.503371601217953, w33u3 = 1.067634993014797, w33u4 = 1.352712750267209, w33u5 = -1.936652294363815, r34 = 2.79631198739, w34u0 = -0.918900165139691, w34u1 = -1.057722380525383, w34u2 = 0.228113235201292, w34u3 = -3.021541435174714, w34u4 = 0.639675749337384, w34u5 = -0.403032721435919, r35 = 575.430310193, w35u0 = 0.033424232613503, w35u1 = -1.747279572303321, w35u2 = 0.279656984126069, w35u3 = -0.13505586827669, w35u4 = 0.682189038559053, w35u5 = -0.131162586021134, r36 = 0.221496310598, w36u0 = -0.379433266696707, w36u1 = -0.933378015959205, w36u2 = -0.103703587364877, w36u3 = -0.462422980873508, w36u4 = 1.558378531837801, w36u5 = 0.960775931934566, r37 = 1225.4654584, w37u0 = -1.264020557323582, w37u1 = -1.081251242133842, w37u2 = -0.097543709225388, w37u3 = 2.916697966487550, w37u4 = 1.384330203445063, w37u5 = -1.055142598143193, r38 = 61.078809273, w38u0 = -0.897347372506697, w38u1 = -1.260995879578610, w38u2 = 0.048505647756097, w38u3 = 3.641794019756450, w38u4 = 0.822505434555556, w38u5 = -0.176919383794468, r39 = -0.625443964648, w39u0 = -0.190266449096388, w39u1 = -0.770490969723237, w39u2 = -0.023482707308682, w39u3 = -0.336736459632039, w39u4 = 0.987560609610161, w39u5 = 0.531758122229973, r40 = -59.407002278, w40u0 = 0.101214982556129, w40u1 = -1.729413561918831, w40u2 = 0.337413239482047, w40u3 = -0.433940354834691, w40u4 = 0.621133121753826, w40u5 = -1.743321582919458, r41 = 277.396650513, w41u0 = -0.381492688528870, w41u1 = -2.726704556918439, w41u2 = -0.006400992688819, w41u3 = -0.894972531473500, w41u4 = -0.183496909350533, w41u5 = 0.007795157446639, r42 = -44.2859262806, w42u0 = -0.422722654548365, w42u1 = -1.090583834033585, w42u2 = 0.249907769350965, w42u3 = 1.132228901801507, w42u4 = 1.603180065644242, w42u5 = -0.979617410003878, r43 = -19.6124451693, w43u0 = -0.389983349897434, w43u1 = -2.223063549427904, w43u2 = 1.473181471142833, w43u3 = 4.278620420924543, w43u4 = 2.273988166419923, w43u5 = -0.552897232750255, r44 = 181.424316715, w44u0 = -0.043412569150406, w44u1 = -1.622572492810102, w44u2 = 0.365526920710989, w44u3 = 0.252545649182365, w44u4 = 0.214467625921422, w44u5 = -2.642456206447654, r45 = 4.25602381683, w45u0 = -1.686431874230609, w45u1 = -0.748120098063037, w45u2 = 0.736674047787979, w45u3 = 3.356277881527543, w45u4 = 0.727048177960433, w45u5 = -0.537570612793289, r46 = 93.1882305967, w46u0 = -2.846768115677090, w46u1 = -0.235158142655243, w46u2 = -0.313631352999750, w46u3 = -0.091787744040771, w46u4 = -0.207983718116708, w46u5 = -0.008442499858882, r47 = -593.626309794, w47u0 = -1.377215013960184, w47u1 = -1.065705784176306, w47u2 = -0.072209929543213, w47u3 = 2.989465037729329, w47u4 = 1.428535582592924, w47u5 = -1.404041727480120, r48 = 0.125687375803, w48u0 = 0.123282795599564, w48u1 = 0.015229251412603, w48u2 = 0.268107687972553, w48u3 = -0.510112707986040, w48u4 = -0.439426859721460, w48u5 = -0.018049192950398, r49 = 674.485672065, w49u0 = -0.976222860755648, w49u1 = -1.487068810451600, w49u2 = 0.079282666146500, w49u3 = 3.175035561581900, w49u4 = 1.784825395491587, w49u5 = -0.590322608622887, r50 = -0.000361435319442, w50u0 = 0.555175175615836, w50u1 = -0.473300016128945, w50u2 = 1.907919244892818, w50u3 = 1.446672943806077, w50u4 = 0.84668237016211, w50u5 = -0.036336083315722, r51 = -0.911959825282, w51u0 = -0.422815203234790, w51u1 = -0.800658261790613, w51u2 = -0.558546530740072, w51u3 = -0.562989580817477, w51u4 = 2.157705297390107, w51u5 = 0.353618133800870, r52 = -0.00193843512306, w52u0 = 0.065466276243004, w52u1 = 0.400908991238494, w52u2 = 0.573662373066993, w52u3 = 0.728485987200476, w52u4 = -1.207985962482644, w52u5 = -0.051180908647078, r53 = 0.680696692143, w53u0 = -0.087237459061078, w53u1 = -2.046249404573328, w53u2 = 0.404738487390972, w53u3 = 0.327649613801521, w53u4 = 1.629352151511890, w53u5 = 1.731054751161620, r54 = -4562.22979995, w54u0 = -0.231889083735443, w54u1 = -1.493507774086708, w54u2 = 0.534632526298388, w54u3 = 1.017060959587281, w54u4 = 1.202604755798767, w54u5 = -2.220734108774852, r55 = -0.0853555934593, w55u0 = -0.331101426021603, w55u1 = -0.416618238188913, w55u2 = 0.481797863825400, w55u3 = -1.522373726019507, w55u4 = -1.414328234707931, w55u5 = -0.367940662422277, r56 = -0.131660740837, w56u0 = -1.00048599118995, w56u1 = 0.005004485839668, w56u2 = -0.035310021685393, w56u3 = -0.552490896406840, w56u4 = -2.393235242892378, w56u5 = -0.001034305992917, r57 = 50.496012763, w57u0 = -0.447644799218347, w57u1 = -2.235578085887514, w57u2 = 0.038984524343030, w57u3 = 2.248166797902178, w57u4 = -0.252321966638586, w57u5 = 0.046673029006847, r58 = 226.102788325, w58u0 = -1.266574242520516, w58u1 = -0.882399864468584, w58u2 = -0.162486493344137, w58u3 = 2.270452437053196, w58u4 = 1.128341862119909, w58u5 = -0.174725135867112, r59 = 0.189617787097, w59u0 = 0.217939463304283, w59u1 = -0.407462851713085, w59u2 = 0.068815755975560, w59u3 = 0.857681040888670, w59u4 = -0.107851092852573, w59u5 = -0.479890040699518, r60 = 0.0065851328342, w60u0 = 0.543891969469446, w60u1 = 0.267535203389521, w60u2 = 0.483376146094136, w60u3 = 0.602888065420696, w60u4 = 0.736576748500787, w60u5 = 0.041887904288526, r61 = 0.00196145819997, w61u0 = 0.128706401000954, w61u1 = 0.452536634303965, w61u2 = -0.194494772548922, w61u3 = -3.000288590391380, w61u4 = -0.135940362677618, w61u5 = -0.393835531797970, r62 = 81.9552259081, w62u0 = 0.097870478857965, w62u1 = -1.822733467319629, w62u2 = 0.366206691436438, w62u3 = -0.384037460748237, w62u4 = 0.986649036962584, w62u5 = -0.911250749027846, r63 = -2.73782172547, w63u0 = -0.926211410273082, w63u1 = -0.557977509853844, w63u2 = -0.211788744931458, w63u3 = 2.414091010216209, w63u4 = -2.203513719217510, w63u5 = -0.183753981836098, r64 = 7.9684689004, w64u0 = -0.999424259535155, w64u1 = -0.920594756485300, w64u2 = 0.132165427921620, w64u3 = -1.176508103650211, w64u4 = -0.649727851306425, w64u5 = 0.063532190963042, r65 = 6.18655197699, w65u0 = -0.763517986230063, w65u1 = -1.005905916856115, w65u2



= -0.429867628690347 , w65u3 = 2.220634201402487 , w65u4 = -2.257201589168911 , w65u5 = 0.361375759999538 , r66 = -0.341978030449 , w66u0 = -0.784142352746678 ,  
w66u1 = -0.054523436584693 , w66u2 = 0.071387616551653 , w66u3 = 0.454536024102477 , w66u4 = -2.143024795890079 , w66u5 = -0.476333856582223 , r67 = -1.6707158833d-  
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0.034883165324201 , r68 = 0.147663494229 , w68u0 = -0.544923303363188 , w68u1 = -0.224360832524084 , w68u2 = 0.041570984350497 , w68u3 = -2.508904657211773 , w68u4  
= -0.849775638006786 , w68u5 = 0.239066081824531 , r69 = 15.2323310682 , w69u0 = -0.189983711105008 , w69u1 = -1.588756355584520 , w69u2 = -0.213873765953048 , w69u3  
= 1.007957408418801 , w69u4 = -1.601979254521126 , w69u5 = 0.600206354545307 , r70 = -49.8831281127 , w70u0 = -1.655543416717991 , w70u1 = -0.712853480766423 , w70u2  
= 0.122190582046248 , w70u3 = 2.295407348923297 , w70u4 = 1.652406134347526 , w70u5 = -0.144378329693445 , r71 = 0.0870370244542 , w71u0 = -0.541406770781474 ,  
w71u1 = -0.327636083751474 , w71u2 = 0.308053033164774 , w71u3 = -1.439136062385166 , w71u4 = -1.899194449363643 , w71u5 = -0.755097456006860 , r72 = 100.524935445  
 , w72u0 = -0.357024736108426 , w72u1 = -1.167059199296991 , w72u2 = 0.220816918904788 , w72u3 = 1.134737190631993 , w72u4 = -0.401877160883981 , w72u5 = -  
1.474621392140092 , r73 = -203.720774031 , w73u0 = -0.023856811511239 , w73u1 = -1.614848639592133 , w73u2 = 0.285638867312887 , w73u3 = 0.057609205669916 , w73u4  
= 0.002573330168387 , w73u5 = -2.113751429780027 , r74 = -5.87605049756 , w74u0 = -1.026241840785672 , w74u1 = -1.628336027553843 , w74u2 = 0.401381269683886 ,  
w74u3 = -2.978011789556087 , w74u4 = 0.623249014018689 , w74u5 = -0.465518157446707 , r75 = 27.4126157644 , w75u0 = -0.656353537918256 , w75u1 = -0.664191441448378  
 , w75u2 = 0.106481301362692 , w75u3 = 1.582176871694944 , w75u4 = -1.018782191987313 , w75u5 = -0.668815465280137 , r76 = -12.927468165 , w76u0 = -0.045209861455305  
 , w76u1 = -1.585862665944186 , w76u2 = 0.168865611040203 , w76u3 = -0.275611465280897 , w76u4 = 2.249194348340661 , w76u5 = -0.253986320655227 , r77 = 12.496975294  
 , w77u0 = -0.194367695372616 , w77u1 = -1.126078377919176 , w77u2 = -0.213469825153766 , w77u3 = -0.182548682434478 , w77u4 = 2.428232979837427 , w77u5 = -  
0.186778136734243 , r78 = -291.733476682 , w78u0 = 0.017441228154574 , w78u1 = -1.789464719566123 , w78u2 = 0.290848490594049 , w78u3 = -0.082550124047248 , w78u4 =  
0.827006650855694 , w78u5 = 0.266113971665171 , r79 = -0.0123568749458 , w79u0 = 1.093157278117163 , w79u1 = -0.354522112867225 , w79u2 = -0.084186224381153 , w79u3  
= -0.350857088318056 , w79u4 = 0.512649263692106 , w79u5 = -0.019582478201197 , r80 = 0.0468485146234 , w80u0 = -0.597187446533896 , w80u1 = 0.182448374811714 ,  
w80u2 = 0.007499731372618 , w80u3 = -0.193699033262930 , w80u4 = -2.646771277959585 , w80u5 = -0.120831772080295 , r81 = 0.08250396022 , w81u0 = -2.387280457568731 ,  
w81u1 = 1.275128807334748 , w81u2 = 0.353931986674469 , w81u3 = 1.709004017608853 , w81u4 = -0.499425055528652 , w81u5 = -0.042603634930531 , r82 = -3.41343381676  
 , w82u0 = -0.378748052464797 , w82u1 = -0.860100980120145 , w82u2 = -0.651492531568689 , w82u3 = -0.158627662888725 , w82u4 = 3.080812474154300 , w82u5 = -  
0.356363573965471 , r83 = -1.86983043645 , w83u0 = -0.135059536508859 , w83u1 = -1.660306997280813 , w83u2 = -0.173508657991779 , w83u3 = 0.929178005647870 , w83u4 =  
-1.514467259825964 , w83u5 = 0.919236312738092 , r84 = -3.49671817501 , w84u0 = -1.465387484271082 , w84u1 = 0.209201459078548 , w84u2 = 0.083466744329406 , w84u3 =  
-0.358582680143965 , w84u4 = -0.088303057178119 , w84u5 = 0.028397343901877 , r85 = -13.7986625711 , w85u0 = -0.875230690981353 , w85u1 = -1.655258203236874 , w85u2  
= 1.137750415813348 , w85u3 = 3.966978248351146 , w85u4 = 1.169760945877422 , w85u5 = -0.088961687331179 , r86 = -1.7419666959 , w86u0 = -1.893799075323081 , w86u1  
= -0.578109751875194 , w86u2 = 0.566512770615569 , w86u3 = 3.388694189613314 , w86u4 = 0.522269618956901 , w86u5 = 0.830023084172927 , r87 = 1.9440733751 , w87u0 =  
-2.206351009389263 , w87u1 = 0.612150779781037 , w87u2 = -0.073053573472707 , w87u3 = -0.286373241387269 , w87u4 = 0.103607841677780 , w87u5 = 0.003729659405271 ,  
r88 = -5.19267553629 , w88u0 = -1.877925392282306 , w88u1 = 0.158362507414769 , w88u2 = 0.247477318533934 , w88u3 = 2.103789216903190 , w88u4 = -0.159263225339767 ,  
w88u5 = -0.149474375023733 , r89 = 9.39902361112 , w89u0 = -1.119588902850321 , w89u1 = -0.804257372341186 , w89u2 = 0.604351028154454 , w89u3 = 2.151255306147235  
 , w89u4 = 0.771871330394636 , w89u5 = -0.607304936238123

c = 0.013478924

end-parameter-section

LABELS-SECTION

q1 = exp1[-0.70,q10]

q2 = exp1[-0.70,q20]

q3 = exp1[-0.70,q30]

t1 = acos[1.0 0.0 th20]

t2 = acos[1.0 0.0 th10]

qs1 = qs[1.0]

g1 = gauss[1.0,q10]

g2 = gauss[1.0/9.0,q20]

g3 = gauss[0.25,q30]

g4 = tgauss[0.25,th10]

g5 = tgauss[0.25,th20]

```

c1 = gauss[-4.0,q10]
c2 = gauss[-1.0,q20]
c3 = gauss[-4.0,q30]
c4 = tgauss[-4.0,th10]
c5 = tgauss[-4.0,th20]
g0pi = gauss[2.0,0.0]
g1pi = gauss[2.0,PI]
g2pi = gauss[2.0,2.0*PI]
cos2 = cos[2.0]
cos3 = cos[3.0]
cos4 = cos[4.0]
st1 = step[p1]
st2 = rstep[p2]
# General form of the labels are given in order to save space.
# qiuj = exp[wiuj, 0.0]
# Where i goes from 0 to 89 and j goes from 0 to 5.
# So, there will be 90x6 = 540 labels term in this operator file.
end-labels-section
HAMILTONIAN-SECTION

```

---

```

modes | r_2 | r_3 | r_1 | t_2 | t_1 | p_1

```

---

```

-M11/2.0 | 1 | 1 | dq2 | 1 | 1 | 1
-M22/2.0 | dq2 | 1 | 1 | 1 | 1 | 1
-M33/2.0 | 1 | dq2 | 1 | 1 | 1 | 1
-M13 | 1 | dq | dq | 1 | q | 1
M23 | dq | dq | 1 | q | 1 | 1
-M13 | 1 | q^1 | q^1 | 1 | q | 1
M23 | q^1 | q^1 | 1 | q | 1 | 1
-M13 | 1 | q^1 | dq | 1 | udq2 | 1
M13 | 1 | q^1 | dq | udq | qs1 | cos
-M23 | dq | q^1 | 1 | qs1 | udq | cos
M23 | dq | q^1 | 1 | udq2 | 1 | 1
-M13 | 1 | dq | q^1 | 1 | udq2 | 1
M23 | q^1 | dq | 1 | udq2 | 1 | 1
M13 | 1 | q^1 | dq | q*qs1^1 | qs1 | sdq
-M23 | dq | q^1 | 1 | qs1 | q*qs1^1 | sdq
-M11/2.0 | 1 | 1 | q^2 | 1 | dq*qs1^2*dq | 1
-M33/2.0 | 1 | q^2 | 1 | 1 | dq*qs1^2*dq | 1
M13 | 1 | q^1 | q^1 | 1 | dq*qs1^2*q*dq | 1
-M22/2.0 | q^2 | 1 | 1 | dq*qs1^2*dq | 1 | 1
-M33/2.0 | 1 | q^2 | 1 | dq*qs1^2*dq | 1 | 1
-M23 | q^1 | q^1 | 1 | dq*qs1^2*q*dq | 1 | 1
-M13/2.0 | 1 | q^1 | q^1 | qs1*dq | dq*q*qs1 | cos

```

-M13/2.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | dq\*qs1 | q\*qs1\*dq | cos  
M23/2.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | q\*qs1\*dq | dq\*qs1 | cos  
M23/2.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | dq\*q\*qs1 | qs1\*dq | cos  
M33/2.0 | 1 | q<sup>2</sup> | 1 | qs1\*dq | dq\*qs1 | cos  
M33/2.0 | 1 | q<sup>2</sup> | 1 | dq\*qs1 | qs1\*dq | cos  
-M13/2.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | dq\*q\*qs1 | sdq  
-M13/2.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | q\*qs1\*dq | sdq  
-M13/4.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | q<sup>2</sup>\*qs1<sup>1</sup> | cos  
M13/4.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | qs1 | cos  
M23 | q<sup>1</sup> | q<sup>1</sup> | 1 | qs1<sup>1</sup> | udq | sdq  
-0.25\*M23 | q<sup>1</sup> | q<sup>1</sup> | 1 | qs1<sup>1</sup> | q\*qs1<sup>1</sup> | cos  
M33 | 1 | q<sup>2</sup> | 1 | q\*qs1<sup>1</sup> | udq | sdq  
M23/2.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | dq\*q\*qs1 | q\*qs1<sup>1</sup> | sdq  
M23/2.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | q\*qs1\*dq | q\*qs1<sup>1</sup> | sdq  
M23/4.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | q<sup>2</sup>\*qs1<sup>1</sup> | q\*qs1<sup>1</sup> | cos  
-M23/4.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | qs1 | q\*qs1<sup>1</sup> | cos  
-M13 | 1 | q<sup>1</sup> | q<sup>1</sup> | udq | qs1<sup>1</sup> | sdq  
-M13/4.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | qs1<sup>1</sup> | cos  
M33 | 1 | q<sup>2</sup> | 1 | udq | q\*qs1<sup>1</sup> | sdq  
-M11/2.0 | 1 | 1 | q<sup>2</sup> | 1 | qs1<sup>2</sup> | dq<sup>2</sup>  
M13/2.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | qs1<sup>1</sup> | cos\*dq<sup>2</sup>  
M13/2.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | qs1<sup>1</sup> | dq<sup>2</sup>\*cos  
M13/2.0 | 1 | q<sup>1</sup> | q<sup>1</sup> | q\*qs1<sup>1</sup> | qs1<sup>1</sup> | cos  
M13 | 1 | q<sup>1</sup> | q<sup>1</sup> | 1 | q\*qs1<sup>2</sup> | dq<sup>2</sup>  
-M22/2.0 | q<sup>2</sup> | 1 | 1 | qs1<sup>2</sup> | 1 | dq<sup>2</sup>  
-M23/2.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | qs1<sup>1</sup> | q\*qs1<sup>1</sup> | dq<sup>2</sup>\*cos  
-M23/2.0 | q<sup>1</sup> | q<sup>1</sup> | 1 | qs1<sup>1</sup> | q\*qs1<sup>1</sup> | cos\*dq<sup>2</sup>  
-M23 | q<sup>1</sup> | q<sup>1</sup> | 1 | q\*qs1<sup>2</sup> | 1 | dq<sup>2</sup>  
-M33/2.0 | 1 | q<sup>2</sup> | 1 | 1 | q<sup>2</sup>\*qs1<sup>2</sup> | dq<sup>2</sup>  
-M33/2.0 | 1 | q<sup>2</sup> | 1 | q<sup>2</sup>\*qs1<sup>2</sup> | 1 | dq<sup>2</sup>  
-M33/2.0 | 1 | q<sup>2</sup> | 1 | q\*qs1<sup>1</sup> | q\*qs1<sup>1</sup> | dq<sup>2</sup>\*cos  
-M33/2.0 | 1 | q<sup>2</sup> | 1 | q\*qs1<sup>1</sup> | q\*qs1<sup>1</sup> | cos\*dq<sup>2</sup>

---

c | 1 | 1 | 1 | 1 | 1 | 1

# The following lines would have the following genral form

ri | qiu0 | qiu1 | qiu2 | qiu3 | qiu4 | qiu5

# So, total 90 lines will be there; i goes from 0 to 89

---

end-hamiltonian-section

HAMILTONIAN-SECTION.cis

usediag

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modes | r\_2 | r\_3 | r\_1 | t\_2 | t\_1 | p\_1

---

5.862318d-6 | q<sup>1</sup> | 1 | 1 | 1 | 1 | 1 | 1  
-3.674923d-5 | dq<sup>2</sup> | 1 | 1 | 1 | 1 | 1 | 1  
0.199815 | q1<sup>0</sup> | 1 | 1 | 1 | 1 | 1 | 1  
-0.1995720744 | g1 | 1 | 1 | 1 | 1 | 1 | 1  
-0.02919914 | g1\*q1 | 1 | 1 | 1 | 1 | 1 | 1  
0.4880250 | g1\*q1<sup>2</sup> | 1 | 1 | 1 | 1 | 1 | 1  
-1.303379 | g1\*q1<sup>3</sup> | 1 | 1 | 1 | 1 | 1 | 1  
0.9694112 | g1\*q1<sup>4</sup> | 1 | 1 | 1 | 1 | 1 | 1

---

1.152891d-5 | 1 | q<sup>1</sup> | 1 | 1 | 1 | 1 | 1  
-3.6749237d-5 | 1 | dq<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
0.199815 | 1 | q2<sup>0</sup> | 1 | 1 | 1 | 1 | 1  
-0.19939010 | 1 | g2 | 1 | 1 | 1 | 1 | 1  
0.017770776 | 1 | g2\*q2 | 1 | 1 | 1 | 1 | 1  
0.1326029 | 1 | g2\*q2<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
-0.19864533 | 1 | g2\*q2<sup>3</sup> | 1 | 1 | 1 | 1 | 1  
0.0963012354 | 1 | g2\*q2<sup>4</sup> | 1 | 1 | 1 | 1 | 1

---

3.243973d-6 | 1 | 1 | q<sup>1</sup> | 1 | 1 | 1 | 1  
-2.893093d-4 | 1 | 1 | dq<sup>2</sup> | 1 | 1 | 1 | 1  
0.199815 | 1 | 1 | q3<sup>0</sup> | 1 | 1 | 1 | 1  
-0.1997286 | 1 | 1 | g3 | 1 | 1 | 1 | 1  
-0.01330962 | 1 | 1 | g3\*q3<sup>1</sup> | 1 | 1 | 1 | 1  
0.41641177 | 1 | 1 | g3\*q3<sup>2</sup> | 1 | 1 | 1 | 1  
-0.50147370 | 1 | 1 | g3\*q3<sup>3</sup> | 1 | 1 | 1 | 1  
0.23521044 | 1 | 1 | g3\*q3<sup>4</sup> | 1 | 1 | 1 | 1  
-0.4574862 | 1 | 1 | g3\*q3<sup>5</sup> | 1 | 1 | 1 | 1  
0.8193689 | 1 | 1 | g3\*q3<sup>6</sup> | 1 | 1 | 1 | 1

---

-6.65897d-6 | 1 | 1 | 1 | q | 1 | 1 | 1  
-1.26493d-5 | 1 | 1 | 1 | dq\*qs1<sup>2</sup>\*dq | 1 | 1 | 1  
6.65897d-6 | 1 | 1 | 1 | dq\*q\*qs1<sup>2</sup>\*dq | 1 | 1 | 1  
0.199815 | 1 | 1 | 1 | t2<sup>0</sup> | 1 | 1 | 1  
-0.1992434 | 1 | 1 | 1 | g4 | 1 | 1 | 1  
-0.026653980 | 1 | 1 | 1 | g4\*t2 | 1 | 1 | 1  
0.27134390 | 1 | 1 | 1 | g4\*t2<sup>2</sup> | 1 | 1 | 1  
-0.26446122 | 1 | 1 | 1 | g4\*t2<sup>3</sup> | 1 | 1 | 1  
0.23762334 | 1 | 1 | 1 | g4\*t2<sup>4</sup> | 1 | 1 | 1

---

-7.07777d-6 | 1 | 1 | 1 | 1 | q | 1 | 1  
-9.06079d-5 | 1 | 1 | 1 | 1 | dq\*qs1<sup>2</sup>\*dq | 1 | 1 | 1  
7.07777d-6 | 1 | 1 | 1 | 1 | dq\*q\*qs1<sup>2</sup>\*dq | 1 | 1 | 1  
0.199815 | 1 | 1 | 1 | 1 | t1<sup>0</sup> | 1 | 1 | 1  
-0.1996101 | 1 | 1 | 1 | 1 | g5 | 1 | 1 | 1

-0.00931089145 | 1 | 1 | 1 | 1 | g5\*t1 | 1  
 0.058163918856 | 1 | 1 | 1 | 1 | g5\*t1<sup>2</sup> | 1  
 -0.05969423564 | 1 | 1 | 1 | 1 | g5\*t1<sup>3</sup> | 1  
 0.02626388225 | 1 | 1 | 1 | 1 | g5\*t1<sup>4</sup> | 1

---

-1.14605d-4 | 1 | 1 | 1 | 1 | dq<sup>2</sup>  
 -3.07824d-6 | 1 | 1 | 1 | 1 | dq<sup>2</sup>\*cos  
 -3.07824d-6 | 1 | 1 | 1 | 1 | cos\*dq<sup>2</sup>  
 -7.172084d-5 | 1 | 1 | 1 | 1 | cos  
 -0.0104828 | 1 | 1 | 1 | 1 | cos2  
 -0.000334943 | 1 | 1 | 1 | 1 | cos3  
 0.000171863 | 1 | 1 | 1 | 1 | cos4  
 0.006 | 1 | 1 | 1 | 1 | g1pi

---

end-hamiltonian-section  
 HAMILTONIAN-SECTION.trans  
 useddiag

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modes | r.2 | r.3 | r.1 | t.2 | t.1 | p.1

---

5.130465d-6 | q<sup>a</sup> | 1 | 1 | 1 | 1 | 1  
 -3.674923d-5 | dq<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
 0.200239252946 | q1<sup>0</sup> | 1 | 1 | 1 | 1 | 1  
 -0.200239252946 | g1 | 1 | 1 | 1 | 1 | 1  
 0.47224 | g1\*q1<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
 -1.28108 | g1\*q1<sup>3</sup> | 1 | 1 | 1 | 1 | 1  
 1.01278 | g1\*q1<sup>4</sup> | 1 | 1 | 1 | 1 | 1

---

1.0114998d-5 | q<sup>a</sup> | 1 | 1 | 1 | 1 | 1  
 -3.6749237d-5 | dq<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
 0.200239252946 | q2<sup>0</sup> | 1 | 1 | 1 | 1 | 1  
 -0.200239252946 | g2 | 1 | 1 | 1 | 1 | 1  
 0.148565 | g2\*q2<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
 -0.20644 | g2\*q2<sup>3</sup> | 1 | 1 | 1 | 1 | 1  
 0.1018 | g2\*q2<sup>4</sup> | 1 | 1 | 1 | 1 | 1

---

2.611952d-6 | q<sup>a</sup> | 1 | 1 | 1 | 1 | 1  
 -2.893093d-4 | dq<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
 0.2002393 | q3<sup>0</sup> | 1 | 1 | 1 | 1 | 1  
 -0.2002393 | g3 | 1 | 1 | 1 | 1 | 1  
 0.42615 | g3\*q3<sup>2</sup> | 1 | 1 | 1 | 1 | 1  
 -0.49848 | g3\*q3<sup>3</sup> | 1 | 1 | 1 | 1 | 1  
 0.29256 | g3\*q3<sup>4</sup> | 1 | 1 | 1 | 1 | 1  
 -0.36536 | g3\*q3<sup>5</sup> | 1 | 1 | 1 | 1 | 1

0.54825 | 1 | 1 | g3\*q3<sup>6</sup> | 1 | 1 | 1

-6.56776d-6 | 1 | 1 | 1 | q | 1 | 1

-1.25549d-5 | 1 | 1 | 1 | dq\*qs1<sup>2</sup>\*dq | 1 | 1

6.56776d-6 | 1 | 1 | 1 | dq\*q\*qs1<sup>2</sup>\*dq | 1 | 1

0.200239252946 | 1 | 1 | 1 | t2<sup>0</sup> | 1 | 1

-0.200239252946 | 1 | 1 | 1 | g4 | 1 | 1

0.28985 | 1 | 1 | 1 | g4\*t2<sup>2</sup> | 1 | 1

-0.173188 | 1 | 1 | 1 | g4\*t2<sup>3</sup> | 1 | 1

0.16913 | 1 | 1 | 1 | g4\*t2<sup>4</sup> | 1 | 1

-6.97676d-6 | 1 | 1 | 1 | 1 | q | 1 | 1

-9.21157d-5 | 1 | 1 | 1 | 1 | dq\*qs1<sup>2</sup>\*dq | 1 | 1

6.97676d-6 | 1 | 1 | 1 | 1 | dq\*q\*qs1<sup>2</sup>\*dq | 1 | 1

0.200239252946 | 1 | 1 | 1 | 1 | t1<sup>0</sup> | 1 | 1

-0.200239252946 | 1 | 1 | 1 | 1 | g5 | 1 | 1

0.0471315 | 1 | 1 | 1 | 1 | g5\*t1<sup>2</sup> | 1 | 1

-0.0446942 | 1 | 1 | 1 | 1 | g5\*t1<sup>3</sup> | 1 | 1

0.0120094 | 1 | 1 | 1 | 1 | g5\*t1<sup>4</sup> | 1 | 1

-1.131196d-4 | 1 | 1 | 1 | 1 | 1 | dq<sup>2</sup>

-2.481013d-6 | 1 | 1 | 1 | 1 | 1 | dq<sup>2</sup>\*cos

-2.481013d-6 | 1 | 1 | 1 | 1 | 1 | cos\*dq<sup>2</sup>

0.001091769 | 1 | 1 | 1 | 1 | 1 | cos

-0.00967354 | 1 | 1 | 1 | 1 | 1 | cos2

-0.358768d-3 | 1 | 1 | 1 | 1 | 1 | cos3

0.122464d-3 | 1 | 1 | 1 | 1 | 1 | cos4

0.005 | 1 | 1 | 1 | 1 | 1 | g0pi

0.005 | 1 | 1 | 1 | 1 | 1 | g2pi

end-hamiltonian-section

end-operator

## S0 CCSD(T)-F12 PES of HONO using 90 NN: Operator file

# Only the parameter section is provided here. The rest of the operator file is exactly same as the above PES

PARAMETER-SECTION

q20 = 2.696732586, q30 = 1.822912197, q10 = 2.21332641, q11 = 1.8653, th20 = 1.777642018, th10 = 1.9315017, mh = 1.0, H-mass, mc = 12.0,AMU, mo = 15.9949,AMU, mn = 13.9939,AMU, M11 = 1.0/mo+1.0/mh, M22 = 1.0/mo+1.0/mn, M33 = M22, M13 = 1.0/mo, M23 = -1.0/mn, p1 = PI/2.0, p2 = 3.0\*PI/2.0, r0 = 2.49062209164d-05, w0u0 = 0.990762672762274, w0u1 = 0.879399098300514, w0u2 = -0.998204926718832, w0u3 = -3.525116141524682, w0u4 = 0.564193127332052, w0u5 = -0.327202610773055, r1 = -2.05316402998, w1u0 = -0.395542270641128, w1u1 = -1.151186698851344, w1u2 = 0.219378454513705, w1u3 = -1.966509202272723, w1u4 = -1.030059216940918, w1u5 = -0.274367178332881, r2 = 0.0216475834271, w2u0 = 0.048679053214609, w2u1 = 0.122714516349700, w2u2 = -0.104010239795143, w2u3 = -0.016503270996388, w2u4 = -1.510131091491883, w2u5 = 0.005220679314363, r3 = 133.614802862, w3u0 = -0.054074894562940, w3u1 = -2.460543661361866, w3u2 = -0.084364690831152, w3u3 = -0.534886395276775, w3u4 = -0.653319356823815, w3u5 = -0.078208399814083, r4 = 10.3237242412, w4u0 = -0.347348858815260, w4u1 = -1.906616800776697, w4u2 = 0.370310069202191, w4u3 = 1.710668349976324, w4u4 = 1.102185002847695, w4u5 = 0.0972851164884847, r5 = 7.669040189, w5u0 = -0.402910337522161, w5u1 = -1.385915888252440, w5u2 = -0.404858103274222, w5u3 = -0.588840647914321, w5u4 = -3.069369689764649, w5u5 = 0.020375375402256, r6 = -5.91026514507, w6u0 = -0.804378870827043, w6u1 = -1.069084033353517, w6u2 = 0.103237338756679, w6u3 = -2.423900835193319, w6u4 = -0.357606996899715, w6u5 = -0.378433389205773, r7 = 24.7361354998, w7u0 = -0.329419372617922, w7u1 = -2.031018159125704, w7u2 = 1.412873846655821, w7u3 = 2.520780909301378, w7u4 = 3.049675854689634, w7u5 = -1.349648165642112, r8 = 0.0176305097524, w8u0 = 0.414279438834839, w8u1 = 0.413385314957824, w8u2 = 0.115766812989557, w8u3 = -0.313605789899979, w8u4 = -0.214954569647355, w8u5 = -0.078896036666991, r9 = -1112.29143858, w9u0 = -0.687344331337495, w9u1 = -1.907545521317971, w9u2 = 0.885639296553834, w9u3 = 2.599644035020769, w9u4 = 2.558669019832703, w9u5 = -1.512478901675200, r10 = 0.182975568461, w10u0 = -0.619865082327824, w10u1



= 0.597403172177595 , w74u5 = 0.929414143101435 , r75 = -0.64998006492 , w75u0 = 0.143637100216835 , w75u1 = -0.584116205048295 , w75u2 = -1.040855609256828 , w75u3 = 1.615763043760753 , w75u4 = 0.568869549198812 , w75u5 = -0.018595012791568 , r76 = 0.034629742118 , w76u0 = -0.692604044438775 , w76u1 = -0.351702435322966 , w76u2 = -0.037460329836420 , w76u3 = -3.670528747267317 , w76u4 = 0.021358018192332 , w76u5 = 0.294824368670593 , r77 = -16.5808390448 , w77u0 = -0.130166643101892 , w77u1 = -2.159867960215742 , w77u2 = 0.374170302518766 , w77u3 = -0.342264786795465 , w77u4 = 1.314601505645211 , w77u5 = 1.227997886655990 , r78 = -2041.39404382 , w78u0 = 0.011388817967271 , w78u1 = -1.903795397923566 , w78u2 = 0.164962450401440 , w78u3 = -0.577824494309113 , w78u4 = 0.342621843885036 , w78u5 = -0.675154616352694 , r79 = -14.6314113804 , w79u0 = -2.01252455932020 , w79u1 = 0.021418605417424 , w79u2 = 0.069822763866368 , w79u3 = 2.270396886264788 , w79u4 = -0.473086654453848 , w79u5 = 0.208108016853280 , r80 = 16.7969729663 , w80u0 = -0.575642256470214 , w80u1 = -0.505919522479461 , w80u2 = -0.090921417109244 , w80u3 = 1.415231650649504 , w80u4 = -0.502997497277590 , w80u5 = -0.252512888738305 , r81 = -5.65431196864 , w81u0 = -0.630769768243796 , w81u1 = 0.067125427397441 , w81u2 = -0.494430337938215 , w81u3 = 0.761563000898776 , w81u4 = -0.240464125726384 , w81u5 = -0.683052161110633 , r82 = 219.735353 , w82u0 = -0.565871906685466 , w82u1 = -1.615916967590171 , w82u2 = 0.366943301270937 , w82u3 = 2.165350364554112 , w82u4 = 1.559417550279331 , w82u5 = 0.040009101005226 , r83 = -0.323541806402 , w83u0 = -0.898282804454125 , w83u1 = -0.191011096900171 , w83u2 = -0.261616913382876 , w83u3 = -2.320657682273762 , w83u4 = 0.563653409811119 , w83u5 = -0.832740778852490 , r84 = 0.464811797795 , w84u0 = -0.902578052504099 , w84u1 = -1.007806643707185 , w84u2 = 0.292732861634498 , w84u3 = -3.208445735678016 , w84u4 = -0.433641679911096 , w84u5 = 0.043892421793918 , r85 = 0.827219022171 , w85u0 = -2.517357331051064 , w85u1 = 0.921597969753833 , w85u2 = -0.137251164255615 , w85u3 = 0.864113435785005 , w85u4 = -0.035859321762436 , w85u5 = -0.252004215826831 , r86 = -1.68819851241 , w86u0 = -0.666177909627336 , w86u1 = -1.308111815646731 , w86u2 = 0.128277257440241 , w86u3 = -2.220724117208560 , w86u4 = -0.240543066345113 , w86u5 = 0.468194664275139 , r87 = 6.26717323305 , w87u0 = -0.498322588399289 , w87u1 = -0.928990011242140 , w87u2 = 0.146651547828329 , w87u3 = -1.445277171265926 , w87u4 = -0.646909280849887 , w87u5 = 0.146439943503560 , r88 = -16.1457473468 , w88u0 = -0.390567216392888 , w88u1 = -0.801577528874908 , w88u2 = -0.078757833548664 , w88u3 = 1.198387538932790 , w88u4 = -0.365248523325655 , w88u5 = -0.715389713364273 , r89 = 0.00417235957961 , w89u0 = -1.228275636693260 , w89u1 = 1.489679611174510 , w89u2 = 0.064685858925743 , w89u3 = -1.921673031852332 , w89u4 = 0.450194447393512 , w89u5 = 0.048709445364414  
c = 0.065600224  
end-parameter-section

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