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Repulsive double many-body expansion potential energy surface for the reactions $N(^4S) + H_2 \rightleftharpoons NH(X\,^3\Sigma^-) + H$ from accurate *ab initio* calculations

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Table 1: Numerical values of linear parameters in three-body EHF energy [Eq. (11)]

Monomial[a)]	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$	$P^{(4)}$	$P^{(5)} + P^{(6)}$
1	−1.05178744	−1.28631580	37.18142283	−0.36996706	−0.00028873
Q_1	0.24297418	0.03529024	−9.52870187	0.59566597	−0.00052680
Q_3	0.09997771	−4.00515202	10.77084293	−0.73171800	0.00073558
Q_1^2	−0.34468440	−0.41988830	8.19635500	−0.26319608	−0.00119021
S_{2a}^2	−0.21282735	0.11821915	4.39845323	−0.55472055	−0.00150357
Q_1Q_3	−0.02247595	0.24427013	−11.36109339	0.71732588	0.00261679
S_{2b}^2	0.01482181	−0.72030626	−1.67107981	0.17332326	0.00197284
Q_1^3	0.07220708	−0.04850940	−2.23938524	0.69383297	
$Q_1S_{2a}^2$	0.05292190	1.55023506	−4.97684545	1.46306626	
S_3^3	−0.02642770	0.53428223	1.23385500	0.12909653	
$Q_1^2Q_3$	−0.00247296	−1.90412100	6.13705769	−1.69759656	
$Q_1S_{2b}^2$	0.01671696	−1.18615220	3.93340670	−0.19983955	
$Q_3S_{2a}^2$	0.04116850	−1.48771633	3.67760509	−0.93810278	
Q_1^4	−0.03838601	0.00571499	0.49395874	−0.00640085	
$Q_1^2S_{2a}^2$	−0.02354100	0.73768833	1.03845518	0.42536278	
S_{2a}^4	−0.01776613	0.24998135	0.86110270	−0.07269609	
$Q_1S_3^3$	0.00347241	0.11559547	−1.63392487	0.36422847	
$Q_1^3Q_3$	−0.01454571	−0.24422230	−1.14450028	0.14580878	
$Q_1^2S_{2b}^2$	0.02517522	−0.10991995	−1.84885114	0.82279545	
$Q_1Q_3S_{2a}^2$	−0.01541134	−0.98518996	−2.89770159	0.09241726	
$Q_3S_3^3$	0.00309870	−0.18348663	0.84393923	0.03998637	
$S_{2a}^2S_{2b}^2$	−0.00863339	−0.18787207	0.05322814	0.30692547	
Q_1^5	0.00467027	−0.01479406	0.01363897	0.19427432	
$Q_1^3S_{2a}^2$	0.00305180	0.38670452	0.17650072	0.70168290	
$Q_1S_{2a}^4$	0.00563664	0.08641209	−0.52995149	0.40349765	
$Q_1^2S_3^3$	−0.00635590	−0.31232982	0.38257825	−0.47029746	

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Table 1: Continue

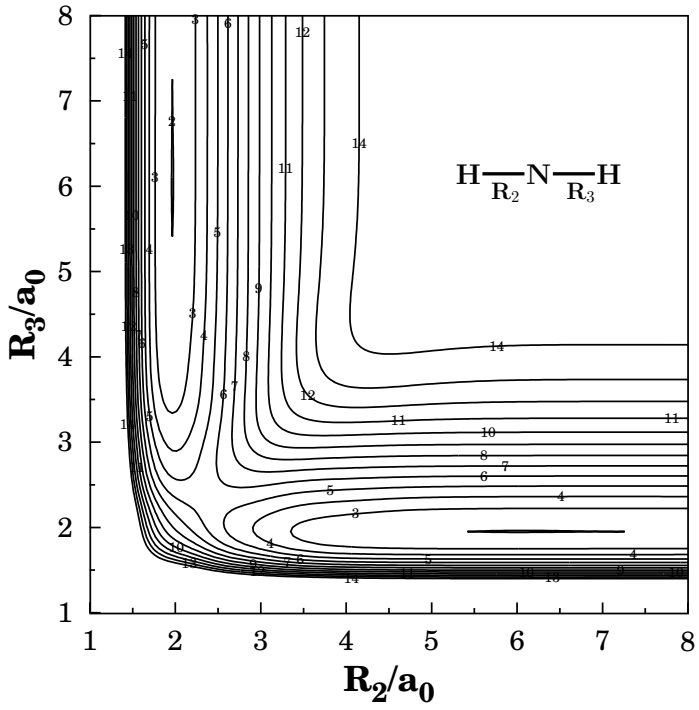
$S_{2a}^2 S_3^3$	0.00093067	0.03717180	0.06406620	0.16517591
$Q_1^4 Q_3$	−0.00191289	−0.20524932	−0.14914096	−0.82459620
$Q_1^3 S_{2b}^2$	−0.00028851	−0.26653852	0.13247676	−0.69926553
$Q_1^2 Q_3 S_{2a}^2$	−0.00055169	−0.36831991	0.45992621	−0.62439125
$Q_1 Q_3 S_3^3$	−0.00855949	0.42015452	−0.46087700	0.54237803
$Q_1 S_{2a}^2 S_{2b}^2$	−0.00142487	0.19015713	0.31461667	0.56930997
$Q_3 S_{2b}^4$	−0.00014422	0.02758644	0.28767150	−0.08102447
$S_{2b}^2 S_3^3$	−0.00458444	0.12336714	−0.06927595	0.17307234
Q_1^6	−0.00060270	0.00526833	0.01483105	0.00295053
$Q_1^4 S_{2a}^2$	0.00102479	0.07492846	−0.06260909	0.02187464
$Q_1^2 S_{2a}^4$	0.00087590	0.06539543	0.08008578	0.00914510
$Q_1^3 S_3^3$	0.00016780	−0.12824595	−0.07001586	0.11881671
$Q_1 S_{2a}^2 S_3^3$	0.00088514	−0.05562035	−0.02230554	0.11426900
S_{2a}^6	−0.00124979	−0.00965497	0.02972053	0.04872057
S_3^6	0.00056795	0.01339990	0.00410558	−0.02759933
$Q_1^5 Q_3$	−0.00055137	−0.05727853	−0.01465181	−0.01776944
$Q_1^4 S_{2b}^2$	0.00124398	−0.12068992	−0.04002109	0.08408040
$Q_1^3 Q_3 S_{2a}^2$	0.00183727	−0.18574568	0.04578215	0.12831533
$Q_1^2 Q_3 S_3^3$	0.00519425	0.20430378	0.12184588	−0.17614952
$Q_1^2 S_{2a}^2 S_{2b}^2$	0.00466357	0.02339944	0.01431361	0.10604234
$Q_1 Q_3 S_{2a}^4$	−0.00253519	0.03520933	−0.13895356	−0.05121423
$Q_1 S_{2b}^2 S_3^3$	−0.00108523	0.07406005	0.02868872	−0.05760229
$Q_3 S_{2a}^2 S_3^3$	0.00044764	0.01897105	−0.02283982	0.03013954
$S_{2a}^4 S_{2b}^2$	−0.00059907	0.00683649	−0.06159597	0.07370483

[a)] The variables are defined as follows: $S_{2a}^2 = Q_2^2 + Q_3^2$, $S_{2b}^2 = Q_2^2 - Q_3^2$, $S_3^3 = Q_3^3 - 3Q_2^2 Q_3$.

Table 2: Range-determining parameters and reference geometries in Eq. (11)

Polynomial	$\gamma_1^{(j)}$	$\gamma_2^{(j)}$	$\gamma_3^{(j)}$	$R_1^{(j),ref}$	$R_2^{(j),ref}$	$R_3^{(j),ref}$
$P^{(1)}$	0.6	0.7	0.7	1.5	4.0	4.0
$P^{(2)}$	0.35	1.35	1.35	2.5	3.0	3.0
$P^{(3)}$	0.45	0.8	0.8	3.5	2.0	2.0
$P^{(4)}$	0.75	2.1	2.1	5.0	2.5	2.5
$P^{(5)}$	0.81	1.87	1.03	4.8	1.965	6.765
$P^{(6)}$	0.81	1.03	1.87	4.8	6.765	1.965

Figure 1: Contour plot for symmetric stretching of collinear $\mathrm{H}-\mathrm{N}-\mathrm{H}$. Contours are equally speced by $0.01\,\mathrm{E_h}$, starting at $-0.1303\,\mathrm{E_h}$.


H—N—H
R2
R3
R3/a0
R2/a0
1
2
3
4
5
6
7
8