

**An accurate many-body expansion potential energy surface for AlH_2 ($2^2\text{A}'$) and quantum
dynamics in Al (^3P) + H_2 ($\nu_0 = 0 - 3, j_0 = 0, 2, 4, 6$) collisions**

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Table. M1 (a) 150 linear coefficients for three-body energy term AlH_2 ($2^2A'$) PES.

Coefficients	$\mathbf{P}^{(1)}$	$\mathbf{P}^{(2)}$	$\mathbf{P}^{(3)}$
$\mathbf{C}_1/\mathbf{a}_0^0$	-5.2645723402	0.9364090238	0.2439914253
$\mathbf{C}_2/\mathbf{a}_0^{-1}$	-1.3370882184	-0.7156072220	-1.0863184069
$\mathbf{C}_3/\mathbf{a}_0^{-1}$	0.6412507234	0.1618946726	0.0604060532
$\mathbf{C}_4/\mathbf{a}_0^{-2}$	-0.0337136603	0.1515072546	-0.2227947715
$\mathbf{C}_5/\mathbf{a}_0^{-2}$	-0.0952725699	-0.1105396447	-0.0001123129
$\mathbf{C}_6/\mathbf{a}_0^{-2}$	-0.0283436316	0.0308378600	-0.1658105677
$\mathbf{C}_7/\mathbf{a}_0^{-2}$	0.0435446779	-0.0271183872	-0.0155561607
$\mathbf{C}_8/\mathbf{a}_0^{-3}$	0.0895531777	0.0060441410	-0.0407458297
$\mathbf{C}_9/\mathbf{a}_0^{-3}$	-0.0253911762	-0.0114689183	-0.0207636792
$\mathbf{C}_{10}/\mathbf{a}_0^{-3}$	-0.0108160030	0.0160696241	-0.0748393861
$\mathbf{C}_{11}/\mathbf{a}_0^{-3}$	-0.0069740701	0.0470902522	-0.0188551504
$\mathbf{C}_{12}/\mathbf{a}_0^{-3}$	0.0049518140	-0.0030179218	0.0022793686
$\mathbf{C}_{13}/\mathbf{a}_0^{-3}$	-0.0074783335	-0.0048765991	-0.0119744073
$\mathbf{C}_{14}/\mathbf{a}_0^{-4}$	-0.0049903525	-0.0001394047	-0.0071054690
$\mathbf{C}_{15}/\mathbf{a}_0^{-4}$	0.0059354085	-0.0001022154	-0.0040033383
$\mathbf{C}_{16}/\mathbf{a}_0^{-4}$	0.0118020604	-0.0176414006	-0.0004958594
$\mathbf{C}_{17}/\mathbf{a}_0^{-4}$	-0.0069338635	-0.0002935665	-10.5376362706
$\mathbf{C}_{18}/\mathbf{a}_0^{-4}$	-4.9620434398	9.9386943120	-2.4316536635
$\mathbf{C}_{19}/\mathbf{a}_0^{-4}$	-3.3775975274	4.1108827767	-1.1230160163
$\mathbf{C}_{20}/\mathbf{a}_0^{-4}$	-1.1158194738	-2.7932817124	-0.5684039907

C_{21}/a_0^{-4}	3.7880003091	1.0091888013	1.6993788273
C_{22}/a_0^{-4}	-0.1529055633	-0.4075010816	-0.2758018836
C_{23}/a_0^{-5}	0.1556542270	0.6218044898	0.5275078435
C_{24}/a_0^{-5}	0.5584539412	-0.1390809611	-0.3110956121
C_{25}/a_0^{-5}	-0.0621968649	-0.2029408786	-0.0866024329
C_{26}/a_0^{-5}	0.2585968231	-0.0484810643	0.3024095903
C_{27}/a_0^{-5}	0.3458067625	0.2284141817	-0.2112172026
C_{28}/a_0^{-5}	-0.1005444439	0.0248774135	-0.0612319874
C_{29}/a_0^{-5}	-0.0019752620	-0.0337639598	-0.0112001726
C_{30}/a_0^{-5}	0.0290968845	0.0089509289	-0.0125815940
C_{31}/a_0^{-5}	0.0001225161	0.0215221063	0.0275089938
C_{32}/a_0^{-5}	0.0670397818	-0.0345626010	0.0380262612
C_{33}/a_0^{-5}	0.0153560511	-0.0065621008	-0.0031318827
C_{34}/a_0^{-5}	-0.0011493839	5.2082825659	6.4976287278
C_{35}/a_0^{-6}	-15.2722963015	-0.5954521635	-1.6336044389
C_{36}/a_0^{-6}	6.0328029987	3.0986407143	0.4230809217
C_{37}/a_0^{-6}	0.0832506323	-0.4553710188	-1.4134350013
C_{38}/a_0^{-6}	0.1455419822	-1.7655674053	-0.0543620285
C_{39}/a_0^{-6}	-0.0445696010	-0.0949352476	-0.1533874043
C_{40}/a_0^{-6}	0.3682739829	-0.0662530223	-0.0191551165
C_{41}/a_0^{-6}	-0.0324927008	0.0837293315	-0.0023001210
C_{42}/a_0^{-6}	0.0018161648	-0.0342828494	0.0053389801

C_{43}/a_0^{-6}	-0.0230925274	-0.0589959472	0.0210750080
C_{44}/a_0^{-6}	-0.0383818977	-0.0321331589	0.0175220226
C_{45}/a_0^{-6}	0.0059346246	0.0031292433	0.0001678583
C_{46}/a_0^{-6}	-0.0003957156	-0.0060117449	-0.0046556677
C_{47}/a_0^{-6}	0.0014267498	0.0021360740	0.0002271803
C_{48}/a_0^{-6}	0.0024156870	0.0010734350	-0.0040984993
C_{49}/a_0^{-6}	-0.0028454595	0.0038099546	-0.0077787999
C_{50}/a_0^{-6}	0.0026740970	-0.0005597149	-0.0002453801

Table. M1 (b) 9 nonlinear parameters and 9 reference geometric distances

	$\mathbf{P}^{(1)}$	$\mathbf{P}^{(2)}$	$\mathbf{P}^{(3)}$
$\gamma_1^{(j)}/\alpha_0^{-1}$	0.9	0.5	0.5
$\gamma_2^{(j)}/\alpha_0^{-1}$	0.2	0.9	0.9
$\gamma_3^{(j)}/\alpha_0^{-1}$	0.5	0.5	0.5
$R_{1,\text{ref}}^{(j)}/\alpha_0$	2.0	4.0	4.0
$R_{2,\text{ref}}^{(j)}/\alpha_0$	3.0	3.0	3.0
$R_{3,\text{ref}}^{(j)}/\alpha_0$	4.0	2.5	2.5