

## **Accurate global potential energy surface for ground state of CH+ 2by extrapolation to the complete basis set limit**

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**Table 1.** Fitted parameters of two-body energy term in Eq. (8) and (9), the root-mean square derivations ( $\Delta E_{RMSD}$ ) are in kcal/mol.

	CH <sup>+</sup> ( $X^1\Sigma^+$ )	H <sub>2</sub> ( $X^1\Sigma^+ g$ )
$a_0$	$0.68749081 \times 10^3$	$0.10524396 \times 10^1$
$a_1$	$-0.39969300 \times 10^1$	$-0.58820524 \times 10^{-1}$
$a_2$	$0.57825124 \times 10^2$	$-0.98926851 \times 10^1$
$a_3$	$-0.84050850 \times 10^3$	$0.76642439 \times 10^2$
$a_4$	$0.95974671 \times 10^4$	$0.39114853 \times 10^3$
$a_5$	$-0.70346709 \times 10^5$	$0.13715868 \times 10^4$
$a_6$	$0.32377985 \times 10^6$	$-0.32031792 \times 10^4$
$a_7$	$-0.83941570 \times 10^6$	$0.44814936 \times 10^4$
$a_8$	$0.95845581 \times 10^6$	$-0.28282256 \times 10^4$
$\beta_1$	9.1180	2.2730
$\beta_2$	1.4160	1.1280
$\Delta E_{RMSD}$	0.049444	0.0046165

**Table 2.** Parameters and reference geometries in the three-body energy term of Eq. (10) for ground state  $\text{CH}_2^+$  PES.

Coefficients	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$
$\gamma(j)1/a_0^{-1}$	0.4	1.4	1.4
$\gamma(j)2/a_0^{-1}$	1.0	0.5	0.5
$\gamma(j)3/a_0^{-1}$	1.0	0.6	0.6
$R(j)1_{\text{ref}}/a_0$	1.5	4.0	4.0
$R(j)2_{\text{ref}}/a_0$	2.5	3.0	3.0
$R(j)3_{\text{ref}}/a_0$	3.5	3.5	3.5

**Table 3.**Linear coefficients in the three-body energy term which used in Eq. (10).

Coefficients	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$
$C_1/a_0^0$	3.0414614822	0.4875449048	-0.1459518090
$C_2/a_0^{-1}$	1.5884754507	1.6796021351	-2.3131550256
$C_3/a_0^{-1}$	0.7829609099	0.2054445499	0.2123848344
$C_4/a_0^{-2}$	-0.0246501521	-0.4914758788	0.1145048312
$C_5/a_0^{-2}$	-0.2024395298	0.1924919711	0.0408065987
$C_6/a_0^{-2}$	0.2108929703	-0.2683057446	-0.5846008578
$C_7/a_0^{-2}$	-0.7103998370	0.0602930567	0.2476510112
$C_8/a_0^{-3}$	0.3094103241	0.0244719271	-0.0268377039
$C_9/a_0^{-3}$	0.0109815694	-0.0844730123	-0.0063074906
$C_{10}/a_0^{-3}$	-0.0788051045	-0.1326368487	-0.0208125604
$C_{11}/a_0^{-3}$	0.0416220187	0.0441455708	-0.0138245702
$C_{12}/a_0^{-3}$	0.0068967088	0.0003386145	0.0035484502
$C_{13}/a_0^{-3}$	-0.0038626275	-0.0112047593	-0.0018380159
$C_{14}/a_0^{-4}$	0.0039340281	-0.0016742396	-0.0042785057
$C_{15}/a_0^{-4}$	-0.0075607514	0.0033283700	0.0003176933
$C_{16}/a_0^{-4}$	-0.0060301500	0.0005363062	-0.0043942503
$C_{17}/a_0^{-4}$	0.0052856716	0.0061124842	-14.1532406443
$C_{18}/a_0^{-4}$	5.0763090893	-1.4381877721	-3.0263766302
$C_{19}/a_0^{-4}$	-1.9182964917	-0.0399935171	3.0822769058
$C_{20}/a_0^{-4}$	0.4921191941	0.9046797875	-0.4342600437
$C_{21}/a_0^{-4}$	1.5730246304	-1.0249359646	-0.3629080478
$C_{22}/a_0^{-4}$	-0.1786355977	0.9235218936	0.0778153262
$C_{23}/a_0^{-5}$	0.2044899335	0.2890371718	-0.6998826527
$C_{24}/a_0^{-5}$	1.0547501187	-0.1902059608	0.1539080720
$C_{25}/a_0^{-5}$	-0.0226814080	0.0349281254	0.1023863743
$C_{26}/a_0^{-5}$	0.0645015955	-0.0570632072	-0.0822206224
$C_{27}/a_0^{-5}$	-0.0485249582	0.3144496160	-0.0586076591
$C_{28}/a_0^{-5}$	-0.1386100557	0.0057042405	0.0468758646
$C_{29}/a_0^{-5}$	-0.0028928535	-0.0037712097	0.0395711107
$C_{30}/a_0^{-5}$	0.0034986458	0.0038618764	0.0078831520
$C_{31}/a_0^{-5}$	-0.0010079582	-0.0084766494	0.0109183990
$C_{32}/a_0^{-5}$	0.0102753355	0.0183766933	-0.0139180265
$C_{33}/a_0^{-5}$	0.0514820122	-0.0035346667	-0.0120342665
$C_{34}/a_0^{-5}$	-0.0124267789	-1.8744679178	0.4400172916
$C_{35}/a_0^{-6}$	-3.4596202229	0.0087416310	-0.7549804994
$C_{36}/a_0^{-6}$	-1.0681863361	0.4955391941	0.0770823719

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$C_{37}/a_0^{-6}$	-0.5476732009	-0.2020269535	-0.4277248710
$C_{38}/a_0^{-6}$	0.6432499961	-0.9956212552	0.0470613833
$C_{39}/a_0^{-6}$	-0.0930917343	-0.1228740323	-0.0853562138
$C_{40}/a_0^{-6}$	0.0404700067	0.0455836525	-0.3144261128
$C_{41}/a_0^{-6}$	-0.0424467672	0.0709904072	0.0076602305
$C_{42}/a_0^{-6}$	0.0016992660	-0.0432866548	-0.0135017811
$C_{43}/a_0^{-6}$	-0.0180500284	-0.0013874189	0.0238691012
$C_{44}/a_0^{-6}$	-0.0382553716	0.0053250063	0.0454531895
$C_{45}/a_0^{-6}$	-0.0539613489	-0.0019129031	0.0015443974
$C_{46}/a_0^{-6}$	-0.0046509249	-0.0136196496	-0.0017237226
$C_{47}/a_0^{-6}$	-0.0040444248	-0.0061137839	-0.0002850657
$C_{48}/a_0^{-6}$	0.0008934090	0.0005727100	-0.0107846696
$C_{49}/a_0^{-6}$	-0.0065497196	0.0029050872	-0.0203324375
$C_{50}/a_0^{-6}$	0.0061373270	-0.0014896807	0.0056284355

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