Supplemental Material for: Adaptive vibrational configuration interaction (A-VCI): a posteriori error estimation to efficiently compute anharmonic IR spectra

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I. FORMALDEHYDE PES

TABLE I: Formaldehyde fourth order polynomial PES developed by Le Bris *et al.*[1] at the CCSD(T)/aug-cc-pVTZ level of theory (in cm^{-1})

Monomial exponents $(q_1, q_2, q_3, q_4, q_5, q_6)$	Coefficients (cm^{-1})
0 0 0 0 0 0	−25095381.0271
2 0 0 0 0 0	590.4173
0 2 0 0 0 0	631.1236
0 0 2 0 0 0	764.9452
0 0 0 2 0 0	882.0383
0 0 0 0 2 0	1465.8897
0 0 0 0 0 2	1500.2295
3 0 0 0 0 0	0.0960
2 1 0 0 0 0	0.2163
2 0 1 0 0 0	31.5260
2 0 0 1 0 0	−26.6070
2 0 0 0 1 0	170.6625
2 0 0 0 0 1	−0.0308
1 2 0 0 0 0	−0.0713
1 1 1 0 0 0	−0.0727
1 1 0 1 0 0	−0.4423
1 1 0 0 1 0	−0.6008
1 1 0 0 0 1	−0.5357
1 0 2 0 0 0	−0.0141
1 0 1 1 0 0	−0.3371
1 0 1 0 1 0	0.0372
1 0 1 0 0 1	0.2260
1 0 0 2 0 0	0.1359
1 0 0 1 1 0	−0.4127
1 0 0 1 0 1	−0.4464
1 0 0 0 2 0	0.8783
1 0 0 0 1 1	−0.1933
1 0 0 0 0 2	0.2418
0 3 0 0 0 0	0.1683
0 2 1 0 0 0	−54.5444
0 2 0 1 0 0	−10.8760
0 2 0 0 1 0	117.6384
0 2 0 0 0 1	−0.2017
0 1 2 0 0 0	−0.4279
0 1 1 1 0 0	0.5589
0 1 1 0 1 0	0.3850

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0 1 1 0 0 1	187.8915
0 1 0 2 0 0	−0.2309
0 1 0 1 1 0	−0.5135
0 1 0 1 0 1	−147.3953
0 1 0 0 2 0	−0.5134
0 1 0 0 1 1	−1.8219
0 1 0 0 0 2	−0.2431
0 0 3 0 0 0	5.9677
0 0 2 1 0 0	−64.8397
0 0 2 0 1 0	36.8717
0 0 2 0 0 1	0.3727
0 0 1 2 0 0	−64.7982
0 0 1 1 1 0	−55.9036
0 0 1 1 0 1	0.5401
0 0 1 0 2 0	0.1357
0 0 1 0 1 1	−0.2987
0 0 1 0 0 2	−64.3420
0 0 0 3 0 0	−92.4035
0 0 0 2 1 0	34.7107
0 0 0 2 0 1	−0.1535
0 0 0 1 2 0	9.8691
0 0 0 1 1 1	0.3385
0 0 0 1 0 2	62.9563
0 0 0 0 3 0	−224.8190
0 0 0 0 2 1	−2.0776
0 0 0 0 1 2	−710.7658
0 0 0 0 0 3	1.9657
4 0 0 0 0 0	7.0976
3 1 0 0 0 0	1.2443
3 0 1 0 0 0	−0.7370
3 0 0 1 0 0	−1.8929
3 0 0 0 1 0	−0.0052
3 0 0 0 0 1	−0.4747
2 2 0 0 0 0	11.1693
2 1 1 0 0 0	3.1438
2 1 0 1 0 0	2.1096
2 1 0 0 1 0	−2.9285
2 1 0 0 0 1	2.0135
2 0 2 0 0 0	2.8755
2 0 1 1 0 0	−7.3575
2 0 1 0 1 0	−6.8512
2 0 1 0 0 1	2.7369
2 0 0 2 0 0	0.9635
2 0 0 1 1 0	13.4172
2 0 0 1 0 1	−4.8209
2 0 0 0 2 0	−70.7691
2 0 0 0 1 1	−3.0371
2 0 0 0 0 2	−86.9005
1 3 0 0 0 0	−0.9631
1 2 1 0 0 0	−7.5276
1 2 0 1 0 0	1.2793
1 2 0 0 1 0	−1.8662
1 2 0 0 0 1	2.1237
1 1 2 0 0 0	4.6140
1 1 1 1 0 0	0.7736
1 1 1 0 1 0	−7.5303
1 1 1 0 0 1	−8.7534
1 1 0 2 0 0	1.6068
1 1 0 1 1 0	−6.0885
1 1 0 1 0 1	5.9404
1 1 0 0 2 0	−6.1629
1 1 0 0 1 1	3.5500
1 1 0 0 0 2	−2.1949
1 0 3 0 0 0	−0.3039

1 0 2 1 0 0	−3.6662
1 0 2 0 1 0	−0.6088
1 0 2 0 0 1	−0.2453
1 0 1 2 0 0	0.5377
1 0 1 1 1 0	−1.2736
1 0 1 1 0 1	3.0460
1 0 1 0 2 0	−1.9110
1 0 1 0 1 1	2.0588
1 0 1 0 0 2	−3.2470
1 0 0 3 0 0	1.2174
1 0 0 2 1 0	2.6591
1 0 0 2 0 1	−0.5310
1 0 0 1 2 0	−3.1549
1 0 0 1 1 1	−5.3151
1 0 0 1 0 2	2.0494
1 0 0 0 3 0	−3.6534
1 0 0 0 2 1	1.7796
1 0 0 0 1 2	−0.6587
1 0 0 0 0 3	0.8342
0 4 0 0 0 0	4.9769
0 3 1 0 0 0	−0.8667
0 3 0 1 0 0	−1.0767
0 3 0 0 1 0	1.5363
0 3 0 0 0 1	4.7744
0 2 2 0 0 0	10.9300
0 2 1 1 0 0	−8.7411
0 2 1 0 1 0	17.0454
0 2 1 0 0 1	6.4141
0 2 0 2 0 0	0.1232
0 2 0 1 1 0	3.5783
0 2 0 1 0 1	−6.3267
0 2 0 0 2 0	−57.6547
0 2 0 0 1 1	−3.7096
0 2 0 0 0 2	−58.3779
0 1 3 0 0 0	0.3842
0 1 2 1 0 0	5.5105
0 1 2 0 1 0	−3.0359
0 1 2 0 0 1	−5.6438
0 1 1 2 0 0	−1.0278
0 1 1 1 1 0	5.4113
0 1 1 1 0 1	26.0237
0 1 1 0 2 0	−1.5006
0 1 1 0 1 1	−184.4163
0 1 1 0 0 2	−3.5752
0 1 0 3 0 0	−0.4104
0 1 0 2 1 0	0.5347
0 1 0 2 0 1	−3.3344
0 1 0 1 2 0	2.9891
0 1 0 1 1 1	100.7258
0 1 0 1 0 2	−6.6891
0 1 0 0 3 0	−0.5885
0 1 0 0 2 1	−1.4034
0 1 0 0 1 2	−3.6509
0 1 0 0 0 3	8.9864
0 0 4 0 0 0	0.4244
0 0 3 1 0 0	0.2988
0 0 3 0 1 0	−1.1190
0 0 3 0 0 1	1.8101
0 0 2 2 0 0	6.0833
0 0 2 1 1 0	9.4266
0 0 2 1 0 1	−0.5527
0 0 2 0 2 0	−32.1911
0 0 2 0 1 1	−2.3498
0 0 2 0 0 2	−46.9982

0 0 1 3 0 0	8.0683
0 0 1 2 1 0	−7.3651
0 0 1 2 0 1	6.5107
0 0 1 1 2 0	37.0572
0 0 1 1 1 1	−6.0258
0 0 1 1 0 2	49.8780
0 0 1 0 3 0	−0.1957
0 0 1 0 2 1	−0.2232
0 0 1 0 1 2	21.8095
0 0 1 0 0 3	−2.1886
0 0 0 4 0 0	7.8772
0 0 0 3 1 0	−0.4879
0 0 0 3 0 1	−3.5763
0 0 0 2 2 0	−8.7286
0 0 0 2 1 1	−3.3250
0 0 0 2 0 2	−14.3540
0 0 0 1 3 0	0.3174
0 0 0 1 2 1	0.7772
0 0 0 1 1 2	−16.1218
0 0 0 1 0 3	0.2744
0 0 0 0 4 0	22.0414
0 0 0 0 3 1	3.6410
0 0 0 0 2 2	142.6646
0 0 0 0 1 3	−0.1402
0 0 0 0 0 4	23.7096

[1]V. Le Bris, M. Odunlami, R. Garnier, D. Bégué, O. Coulaud, and I. Baraille, J. Chem. Theory Comput. **submitted** (2016).