

Supplementary Material

Phosphine interacting with argon: Potential energy surface and line widths of PH₃ perturbed by Ar

J. Salem, A. Badri, M. Salem, M. Mogren Al-Mogren, M. Hochlaf

Table S1: The radial coefficients, $V_{lm}(R)$, as defined in equation 2. $V_{lm}(R)$ coefficients are in cm^{-1} and R is in bohr.

l	m	R	V _{lm}
0	0	4.000	204226.8061400691221934
0	0	4.250	139542.6015718522248790
0	0	4.500	94911.5826682702754624
0	0	4.750	63951.1623252182398573
0	0	5.000	42517.5533050409430871
0	0	5.250	27797.5478407275295467
0	0	5.500	17807.2422010590416903
0	0	5.750	11122.3333387807706458
0	0	6.000	6720.0400599249142033
0	0	6.250	3872.6700551870458185
0	0	6.500	2069.1770601765388164
0	0	6.750	955.8931964422024521
0	0	7.000	291.6169164603278432
0	0	7.250	-85.8143865795348546
0	0	7.500	-283.8586533699855750
0	0	7.750	-372.6685181943375369
0	0	8.000	-397.3094329004502470
0	0	8.250	-386.1957379013471154
0	0	8.500	-356.8552269427608508
0	0	8.750	-319.8013250711665592
0	0	9.000	-281.0869461276070069
0	0	9.250	-244.0085493074909380
0	0	9.500	-210.1809084422540934
0	0	9.750	-180.2132961840821395
0	0	10.000	-154.1628972168836356
0	0	10.250	-131.8045246516860232
0	0	10.500	-112.7675161982308794
0	0	10.750	-96.6276266228373828
0	0	11.000	-82.9602756505372980
0	0	11.250	-71.4216761309435526
0	0	11.500	-61.7007066472268164
0	0	11.750	-53.4819362157730325
0	0	12.000	-46.5005380091472560
0	0	12.250	-40.5398901362305821
0	0	12.500	-35.4550982301879998
0	0	12.750	-31.1180208918486052
0	0	13.000	-27.4005109502116788
0	0	13.250	-24.1859938745616248
0	0	13.500	-21.4041672957143092
0	0	13.750	-18.9962941225402524
0	0	14.000	-16.9036364763432658
0	0	14.250	-15.0724608207481676
0	0	14.500	-13.4690493576209604
0	0	14.750	-12.0646880831350618
0	0	15.000	-10.8306632597914199
0	0	15.250	-9.7404951326309721
0	0	15.500	-8.7766386811984649
0	0	15.750	-7.9237824297290382
0	0	16.000	-7.1666151510127554
0	0	16.250	-6.4910584507822033
0	0	16.500	-5.8879638266520526
0	0	16.750	-5.3494150573957011
0	0	17.000	-4.8674958879991488
0	0	17.250	-4.4348221475793324
0	0	17.500	-4.0461377957914468
0	0	17.750	-3.6967188323482429
0	0	18.000	-3.3818413103637828
0	0	18.250	-3.0971159874647771
0	0	18.500	-2.8394923211398684
0	0	18.750	-2.6062544512971648
0	0	19.000	-2.3946866048760302
0	0	19.250	-2.2022557903236897
0	0	19.500	-2.0271599251992076
0	0	19.750	-1.8677796584703275
0	0	20.000	-1.7224957319853185
0	0	20.250	-1.589788944779450
0	0	20.500	-1.4685399614572481
0	0	20.750	-1.3577294108445790
0	0	21.000	-1.2563380037580403
0	0	21.250	-1.1634003609054449
0	0	21.500	-1.0781664432501097
0	0	21.750	-0.9999400358474591
0	0	22.000	-0.9280250296095148
0	0	22.250	-0.8617713560969015
0	0	22.500	-0.8007128951165995
0	0	22.750	-0.7444295311612305
0	0	23.000	-0.6925012435531457
0	0	23.250	-0.6445295364354928
0	0	23.500	-0.6002016164972079
0	0	23.750	-0.5592261077488904
0	0	24.000	-0.5213117147338464
0	0	24.250	-0.4861799750903723
0	0	24.500	-0.4536034858115348
0	0	24.750	-0.4233676590215222
0	0	25.000	-0.3952580358228685
0	0	25.250	-0.3690778166076948
0	0	25.500	-0.3447006035893430
0	0	25.750	-0.3220176720084536
0	0	26.000	-0.3009205300280023
0	0	26.250	-0.2812984991682391
0	0	26.500	-0.2630315007314339

0	0	26.750	-0.2459971543651383
0	0	27.000	-0.2300732897744850
0	0	27.250	-0.2151611066097932
0	0	27.500	-0.2012547415089030
0	0	27.750	-0.1883717054373213
0	0	28.000	-0.1765299255622218
0	0	28.250	-0.1656670745824798
0	0	28.500	-0.1553988318056094
0	0	28.750	-0.1452604818277258
0	0	29.000	-0.1347877857961212
0	0	29.250	-0.1238855624676121
0	0	29.500	-0.1139333360333052
0	0	29.750	-0.1066794083200693
0	0	30.000	-0.1038727066638911
1	0	4.000	-72947.0095132162387017
1	0	4.250	-48357.1546752302674577
1	0	4.500	-32550.4225833419950504
1	0	4.750	-22018.5010849302780116
1	0	5.000	-14840.6497943678277807
1	0	5.250	-9911.8303847122861043
1	0	5.500	-6538.1832943677245567
1	0	5.750	-4249.9728140316201461
1	0	6.000	-2716.4392497683056718
1	0	6.250	-1702.3311879628449788
1	0	6.500	-1041.3085365344052207
1	0	6.750	-617.1060981090283803
1	0	7.000	-349.6261113513395458
1	0	7.250	-184.4431872587769590
1	0	7.500	-85.0654682766031840
1	0	7.750	-27.3379853798831256
1	0	8.000	4.5257629618297051
1	0	8.250	20.6898485653485480
1	0	8.500	27.6002890923147532
1	0	8.750	29.2666377960485100
1	0	9.000	28.1407826002354966
1	0	9.250	25.6714574496998296
1	0	9.500	22.6849155526153083
1	0	9.750	19.6489090686726087
1	0	10.000	16.8010289329469273
1	0	10.250	14.2459394481691088
1	0	10.500	12.0200362755169667
1	0	10.750	10.1201408958293975
1	0	11.000	8.5264590919530647
1	0	11.250	7.1780907394400630
1	0	11.500	6.0313085494362477
1	0	11.750	5.0796102651296682
1	0	12.000	4.3144294832289507
1	0	12.250	3.6736107124345856
1	0	12.500	3.1314844058904927
1	0	12.750	2.6757985426286233
1	0	13.000	2.2942972415323899
1	0	13.250	1.9752594584509042
1	0	13.500	1.7090929851256931
1	0	13.750	1.4867361756686754
1	0	14.000	1.2991269126711802
1	0	14.250	1.1382053491874777
1	0	14.500	0.9999196775302077
1	0	14.750	0.8812200568958730
1	0	15.000	0.7790568083831398
1	0	15.250	0.6906129930322410
1	0	15.500	0.6140018553027943
1	0	15.750	0.5475691036765219
1	0	16.000	0.4896605834974287
1	0	16.250	0.4387705304998206
1	0	16.500	0.3939856744490692
1	0	16.750	0.3545407333798980
1	0	17.000	0.3196703883672818
1	0	17.250	0.2886781564022498
1	0	17.500	0.2611428583525724
1	0	17.750	0.2367121501146636
1	0	18.000	0.2150336991771344
1	0	18.250	0.1957708027828892
1	0	18.500	0.1786491381825301
1	0	18.750	0.1634099688932717
1	0	19.000	0.1497945745642689
1	0	19.250	0.1375624850215597
1	0	19.500	0.1265462603293717
1	0	19.750	0.1165967381835790
1	0	20.000	0.1075647952305490
1	0	20.250	0.0993176250497887
1	0	20.500	0.0917874968095703
1	0	20.750	0.0849229399199877
1	0	21.000	0.0786725199909898
1	0	21.250	0.0729853088581381
1	0	21.500	0.0678122444563763
1	0	21.750	0.0631046993784601
1	0	22.000	0.0588140413656759
1	0	22.250	0.0548954672697159
1	0	22.500	0.0513195044735408
1	0	22.750	0.0480605194545122
1	0	23.000	0.0450928862098445
1	0	23.250	0.0423889822201783
1	0	23.500	0.0399131822679981
1	0	23.750	0.0376278625337104

1	0	24.000	0.0354953898324899
1	0	24.250	0.0334860346531944
1	0	24.500	0.0316016216730795
1	0	24.750	0.0298518657912126
1	0	25.000	0.0282464871649711
1	0	25.250	0.0267895277991112
1	0	25.500	0.0254622434888379
1	0	25.750	0.0242401645337594
1	0	26.000	0.0230987957121845
1	0	26.250	0.0220168465614923
1	0	26.500	0.0209858705398802
1	0	26.750	0.0200005879714508
1	0	27.000	0.0190556595845634
1	0	27.250	0.0181496817755286
1	0	27.500	0.0172968198969249
1	0	27.750	0.0165149888689202
1	0	28.000	0.0158217970720748
1	0	28.250	0.0152237118885602
1	0	28.500	0.0146835040783794
1	0	28.750	0.0141531114231506
1	0	29.000	0.0135843388934672
1	0	29.250	0.0129566728541925
1	0	29.500	0.0123611198212103
1	0	29.750	0.0119166236551557
1	0	30.000	0.0117420515876692
2	0	4.000	-10188.8636393931665225
2	0	4.250	-5918.0571977044965024
2	0	4.500	-3499.6204955525245168
2	0	4.750	-2054.9920989040801942
2	0	5.000	-1163.0163061869679950
2	0	5.250	-610.4791898923103872
2	0	5.500	-276.4887302013830777
2	0	5.750	-84.4144859173247823
2	0	6.000	17.2676608741403470
2	0	6.250	63.5497815917176467
2	0	6.500	77.8331579580476500
2	0	6.750	75.1025085981432312
2	0	7.000	64.5970245422515177
2	0	7.250	51.6420281331762681
2	0	7.500	39.0718650486093964
2	0	7.750	28.1881261670636718
2	0	8.000	19.4124322350324121
2	0	8.250	12.6991871143336539
2	0	8.500	7.7820982773159386
2	0	8.750	4.3217764029951269
2	0	9.000	1.9851983984331412
2	0	9.250	0.4770650724901486
2	0	9.500	-0.4436893428055697
2	0	9.750	-0.9597401687044709
2	0	10.000	-1.2149836356196531
2	0	10.250	-1.3007239714126371
2	0	10.500	-1.2837178943255694
2	0	10.750	-1.2133785900667959
2	0	11.000	-1.1155612147851457
2	0	11.250	-0.9930519237823070
2	0	11.500	-0.8787240874197089
2	0	11.750	-0.7642683962306904
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2	0	12.750	-0.4408631534623932
2	0	13.000	-0.3802547481498255
2	0	13.250	-0.3283834080253367
2	0	13.500	-0.2842688268085727
2	0	13.750	-0.2465933800975009
2	0	14.000	-0.2140399138658404
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2	0	14.500	-0.1604992451452327
2	0	14.750	-0.1388977539521457
2	0	15.000	-0.1204552371506695
2	0	15.250	-0.1049118092449932
2	0	15.500	-0.0918287125586166
2	0	15.750	-0.0807224407952454
2	0	16.000	-0.0711095497615868
2	0	16.250	-0.0625761253716544
2	0	16.500	-0.0549860321297717
2	0	16.750	-0.0482725427258694
2	0	17.000	-0.0423689310862314
2	0	17.250	-0.0372060681093576
2	0	17.500	-0.0327050922328123
2	0	17.750	-0.0287846866667716
2	0	18.000	-0.0253635261000358
2	0	18.250	-0.0223663170593021
2	0	18.500	-0.0197418630112213
2	0	18.750	-0.0174450046905276
2	0	19.000	-0.0154305892722005
2	0	19.250	-0.0136571905713642
2	0	19.500	-0.0120982751204857
2	0	19.750	-0.0107310524307489
2	0	20.000	-0.0095327751727074
2	0	20.250	-0.0084810984588669
2	0	20.500	-0.0075551829232927
2	0	20.750	-0.0067345398525177
2	0	21.000	-0.0059986988454273

2	0	21.250	-0.0053301289315968
2	0	21.500	-0.0047229903374358
2	0	21.750	-0.0041743368309702
2	0	22.000	-0.0036812124641628
2	0	22.250	-0.0032407300421715
2	0	22.500	-0.0028503396612959
2	0	22.750	-0.0025075685286178
2	0	23.000	-0.0022099430887193
2	0	23.250	-0.0019527713589503
2	0	23.500	-0.0017225896346039
2	0	23.750	-0.0015037657818363
2	0	24.000	-0.0012806886566522
2	0	24.250	-0.0010431960751103
2	0	24.500	-0.0008029071455497
2	0	24.750	-0.0005769077738448
2	0	25.000	-0.0003823620851153
2	0	25.250	-0.0002325726899785
2	0	25.500	-0.0001252740722845
2	0	25.750	-0.0000543228754012
2	0	26.000	-0.0000136432871910
2	0	26.250	0.0000052090291979
2	0	26.500	0.0000202905392888
2	0	26.750	0.0000519909135829
2	0	27.000	0.0001205457564464
2	0	27.250	0.0002372880966017
2	0	27.500	0.0003783340160175
2	0	27.750	0.0005109581460870
2	0	28.000	0.0006022362326987
2	0	28.250	0.0006289129775345
2	0	28.500	0.0006071102313077
2	0	28.750	0.0005628403016752
2	0	29.000	0.0005220021734683
2	0	29.250	0.0005042607271185
2	0	29.500	0.0005049284697776
2	0	29.750	0.0005132582745238
2	0	30.000	0.0005184421055757
3	0	4.000	55084.1420532262127381
3	0	4.250	35822.6578407431661617
3	0	4.500	24065.1113817728837603
3	0	4.750	16427.9474315561128606
3	0	5.000	11243.4379776391633641
3	0	5.250	7651.0067926708888990
3	0	5.500	5154.0544588369648409
3	0	5.750	3429.6313744095687071
3	0	6.000	2251.4167871421664131
3	0	6.250	1456.3043770917124675
3	0	6.500	926.6798788495639201
3	0	6.750	578.6315233204326205
3	0	7.000	353.0761356768074393
3	0	7.250	209.1110079676159330
3	0	7.500	118.7779379034079739
3	0	7.750	63.2338052968172661
3	0	8.000	29.9257777289314042
3	0	8.250	10.6035376529339196
3	0	8.500	-0.0803524173097658
3	0	8.750	-5.5474974379344770
3	0	9.000	-7.9492213244403302
3	0	9.250	-8.6167562595916927
3	0	9.500	-8.3485938910854784
3	0	9.750	-7.6252302622507671
3	0	10.000	-6.7276314557685364
3	0	10.250	-5.8040372553138733
3	0	10.500	-4.9348060431714300
3	0	10.750	-4.1617796360939217
3	0	11.000	-3.4903275667678022
3	0	11.250	-2.9171576637451926
3	0	11.500	-2.4234372468142595
3	0	11.750	-2.0051999095897552
3	0	12.000	-1.6768327072917986
3	0	12.250	-1.4048616377372061
3	0	12.500	-1.1755273279347920
3	0	12.750	-0.9840370085665409
3	0	13.000	-0.8255957299229683
3	0	13.250	-0.6954852526889006
3	0	13.500	-0.5892875152653179
3	0	13.750	-0.5026584700355338
3	0	14.000	-0.4312538052921829
3	0	14.250	-0.3712076069120782
3	0	14.500	-0.3205667790766769
3	0	14.750	-0.2778563289757338
3	0	15.000	-0.2416012769447453
3	0	15.250	-0.2104776682887900
3	0	15.500	-0.1837653319480428
3	0	15.750	-0.1608950148961961
3	0	16.000	-0.1412974576704609
3	0	16.250	-0.1244385713518003
3	0	16.500	-0.1099247944659179
3	0	16.750	-0.0973976793362303
3	0	17.000	-0.0864987363763551
3	0	17.250	-0.0769086699743680
3	0	17.500	-0.0684649960124951
3	0	17.750	-0.0610444614105414
3	0	18.000	-0.0545238167155505
3	0	18.250	-0.0487866353089994

3	0	18.500	-0.0437437567866092
3	0	18.750	-0.0393128402700342
3	0	19.000	-0.0354115538044966
3	0	19.250	-0.0319636493965197
3	0	19.500	-0.0289171951496233
3	0	19.750	-0.0262263315604047
3	0	20.000	-0.0238452277916181
3	0	20.250	-0.0217290648145310
3	0	20.500	-0.0198370370027531
3	0	20.750	-0.0181293168265887
3	0	21.000	-0.0165660651683420
3	0	21.250	-0.0151147893160641
3	0	21.500	-0.0137723617143990
3	0	21.750	-0.0125429689948927
3	0	22.000	-0.0114307674733440
3	0	22.250	-0.0104375020329741
3	0	22.500	-0.0095553532152779
3	0	22.750	-0.0087741200559621
3	0	23.000	-0.0080835611758394
3	0	23.250	-0.0074714980380654
3	0	23.500	-0.0069182039433327
3	0	23.750	-0.0064020923401357
3	0	24.000	-0.0059015835057578
3	0	24.250	-0.0054029436249152
3	0	24.500	-0.0049237903027351
3	0	24.750	-0.0044895868162432
3	0	25.000	-0.0041258195154856
3	0	25.250	-0.0038488865248472
3	0	25.500	-0.0036388326541746
3	0	25.750	-0.0034666448335699
3	0	26.000	-0.0033033324217809
3	0	26.250	-0.0031254377190627
3	0	26.500	-0.0029315379500951
3	0	26.750	-0.0027257544266001
3	0	27.000	-0.0025122881677807
3	0	27.250	-0.0022963807532053
3	0	27.500	-0.0020871407555567
3	0	27.750	-0.0018946012383912
3	0	28.000	-0.0017287950928234
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18	3	9.250	0.0014846661222347
18	3	9.500	0.0005374662522418
18	3	9.750	0.0005470742817738
18	3	10.000	-0.0009792997924605
18	3	10.250	0.0004468199564229
18	3	10.500	0.0008493295471209
18	3	10.750	0.0013769528683436
18	3	11.000	-0.0105911011261210
18	3	11.250	0.0044444930098935
18	3	11.500	0.0008813844070311
18	3	11.750	0.0055100351057663
18	3	12.000	0.0001215842911638
18	3	12.250	-0.0044756564596901
18	3	12.500	-0.0047629179717253
18	3	12.750	-0.0026766868922453
18	3	13.000	-0.0001769079999667
18	3	13.250	0.0011598303619796
18	3	13.500	0.0013669871058329
18	3	13.750	0.0008875258085993

18	3	14.000	0.0001692436379956
18	3	14.250	-0.0004134767958339
18	3	14.500	-0.0007910490544346
18	3	14.750	-0.0009712112437395
18	3	15.000	-0.0009628013724462
18	3	15.250	-0.0007868197211239
18	3	15.500	-0.0005093204450102
18	3	15.750	-0.0002071840145653
18	3	16.000	0.0000430921645312
18	3	16.250	0.0001835368020244
18	3	16.500	0.0002295001605002
18	3	16.750	0.0002145020838971
18	3	17.000	0.0001719748264316
18	3	17.250	0.0001290127819382
18	3	17.500	0.0000878066099853
18	3	17.750	0.0000442968147514
18	3	18.000	-0.0000055814534867
18	3	18.250	-0.0000635066931559
18	3	18.500	-0.0001214889849705
18	3	18.750	-0.0001690285316002
18	3	19.000	-0.0001955540406051
18	3	19.250	-0.0001951708984294
18	3	19.500	-0.0001807177926011
18	3	19.750	-0.0001698183522646
18	3	20.000	-0.0001802172462401
18	3	20.250	-0.0002211826813113
18	3	20.500	-0.0002676757174467
18	3	20.750	-0.0002860062890467
18	3	21.000	-0.0002424407753271
18	3	21.250	-0.0001185012027280
18	3	21.500	0.0000432932963133
18	3	21.750	0.0001853997380268
18	3	22.000	0.0002505533324873
18	3	22.250	0.0002013401607766
18	3	22.500	0.0000793264443339
18	3	22.750	-0.0000542279858914
18	3	23.000	-0.0001378394019929
18	3	23.250	-0.0001291719897190
18	3	23.500	-0.0000632374331107
18	3	23.750	0.0000052971413265
18	3	24.000	0.0000215956254099
18	3	24.250	-0.0000504388516741
18	3	24.500	-0.0001718067721554
18	3	24.750	-0.0002842904321286
18	3	25.000	-0.0003291819305398
18	3	25.250	-0.0002669809733095
18	3	25.500	-0.0001367742301031
18	3	25.750	0.0000021411030721
18	3	26.000	0.0000897944654764
18	3	26.250	0.0000845965297153
18	3	26.500	0.0000219356930392
18	3	26.750	-0.0000424890855052
18	3	27.000	-0.0000510802489675
18	3	27.250	0.0000359724453417
18	3	27.500	0.0001783328126912
18	3	27.750	0.0003133353296043
18	3	28.000	0.0003753426443275
18	3	28.250	0.0003173923233838
18	3	28.500	0.0001772321995430
18	3	28.750	0.0000151492952100
18	3	29.000	-0.0001077030112555
18	3	29.250	-0.0001462347012301
18	3	29.500	-0.0001231394213324
18	3	29.750	-0.0000786872332818
18	3	30.000	-0.0000544506604505
18	6	4.000	-641.3667628062498807
18	6	4.250	-208.6052369512406131
18	6	4.500	-70.0830787319434876
18	6	4.750	-23.1728292381951064
18	6	5.000	-7.5066724168981409
18	6	5.250	-2.4005114269378254
18	6	5.500	-0.7813863010454511
18	6	5.750	-0.2516700155573321
18	6	6.000	-0.0802399971035799
18	6	6.250	-0.0021210043063711
18	6	6.500	-0.0207167560719768
18	6	6.750	0.0170665052079073
18	6	7.000	0.0017434780927807
18	6	7.250	0.0070959181370256
18	6	7.500	0.0058062391385079
18	6	7.750	0.0028337803270624
18	6	8.000	0.0023043129239544
18	6	8.250	0.0044834693016669
18	6	8.500	0.0017177293931776
18	6	8.750	-0.0036329165904845
18	6	9.000	0.0003520184692007
18	6	9.250	0.0079109021693462
18	6	9.500	-0.0020803674324343
18	6	9.750	0.0052107058733020
18	6	10.000	0.0032211540306408
18	6	10.250	0.0055065077305368
18	6	10.500	-0.0024941098549812
18	6	10.750	0.0000164464757156
18	6	11.000	-0.0077574679279852
18	6	11.250	-0.0091692741020227

18	6	11.500	-0.0107518740569115
18	6	11.750	0.0001670658343886
18	6	12.000	-0.0004010856285989
18	6	12.250	-0.0025306675274690
18	6	12.500	-0.0023758776957820
18	6	12.750	-0.0010126398183603
18	6	13.000	0.0004915013225051
18	6	13.250	0.0012975881795503
18	6	13.500	0.0014272591108672
18	6	13.750	0.0011106677863436
18	6	14.000	0.0005736046685503
18	6	14.250	0.0000139693641108
18	6	14.500	-0.0004709695096096
18	6	14.750	-0.0008070843205244
18	6	15.000	-0.0009182120901520
18	6	15.250	-0.0007612760511691
18	6	15.500	-0.0004325165879671
18	6	15.750	-0.0000647078145711
18	6	16.000	0.0002073247596870
18	6	16.250	0.0002822760662313
18	6	16.500	0.0002002678672366
18	6	16.750	0.0000375857717342
18	6	17.000	-0.0001288832985923
18	6	17.250	-0.0002357377623773
18	6	17.500	-0.0002745594481735
18	6	17.750	-0.0002503367745293
18	6	18.000	-0.0001676125579379
18	6	18.250	-0.0000366721487992
18	6	18.500	0.0001078060971497
18	6	18.750	0.0002247711950467
18	6	19.000	0.0002732149596021
18	6	19.250	0.0002255168272176
18	6	19.500	0.0001067663367286
18	6	19.750	-0.0000446898406748
18	6	20.000	-0.0001903187765229
18	6	20.250	-0.0002988263433669
18	6	20.500	-0.0003682442125854
18	6	20.750	-0.0004039551599610
18	6	21.000	-0.0004111801022427
18	6	21.250	-0.0003973620765617
18	6	21.500	-0.0003786450084700
18	6	21.750	-0.0003731189995536
18	6	22.000	-0.0003983568749573
18	6	22.250	-0.0004629309086433
18	6	22.500	-0.0005413771478541
18	6	22.750	-0.0006000546088098
18	6	23.000	-0.0006054025061540
18	6	23.250	-0.0005363869113060
18	6	23.500	-0.0004217569194397
18	6	23.750	-0.0003026103020638
18	6	24.000	-0.0002197799998197
18	6	24.250	-0.0002022942461814
18	6	24.500	-0.0002332612776257
18	6	24.750	-0.0002843767391071
18	6	25.000	-0.0003275692012511
18	6	25.250	-0.0003409922995334
18	6	25.500	-0.0003276976161407
18	6	25.750	-0.0002969390668496
18	6	26.000	-0.0002579078789920
18	6	26.250	-0.0002170377979282
18	6	26.500	-0.0001701193826296
18	6	26.750	-0.0001101609815761
18	6	27.000	-0.0000303332514708
18	6	27.250	0.0000698078104916
18	6	27.500	0.0001654396464991
18	6	27.750	0.0002254146581575
18	6	28.000	0.0002184272017709
18	6	28.250	0.0001275436872134
18	6	28.500	-0.0000058940185130
18	6	28.750	-0.0001257992565864
18	6	29.000	-0.0001756803222295
18	6	29.250	-0.0001187771005010
18	6	29.500	0.0000010792709993
18	6	29.750	0.0001198483304696
18	6	30.000	0.0001736213380801
18	9	4.000	747.0197268914447477
18	9	4.250	251.7689575816636705
18	9	4.500	84.8083955055502798
18	9	4.750	27.7300664902407661
18	9	5.000	8.7805325719387781
18	9	5.250	2.7669529465759695
18	9	5.500	0.9313005925987028
18	9	5.750	0.2564866663822585
18	9	6.000	0.0585087775007196
18	9	6.250	0.1165400712585694
18	9	6.500	0.0169311215468184
18	9	6.750	-0.0262583178505338
18	9	7.000	-0.0048091527082370
18	9	7.250	-0.0243821240693904
18	9	7.500	-0.0217141957233480
18	9	7.750	-0.0313883628575695
18	9	8.000	-0.0155428236079871
18	9	8.250	-0.0050000278850015
18	9	8.500	0.0019976981901215
18	9	8.750	-0.0010780766869129

18	9	9.000	-0.0028702496735245
18	9	9.250	0.0046379953646901
18	9	9.500	-0.0093745294145343
18	9	9.750	-0.0011747700045248
18	9	10.000	0.0036081948478448
18	9	10.250	-0.0003191819395534
18	9	10.500	-0.0070998060986171
18	9	10.750	0.0204653549963889
18	9	11.000	0.0154502479589649
18	9	11.250	0.0082823585085245
18	9	11.500	-0.0035087652947721
18	9	11.750	0.0141891227190646
18	9	12.000	0.0000283549339270
18	9	12.250	-0.0123972347645999
18	9	12.500	-0.0132151641799211
18	9	12.750	-0.0077917609488903
18	9	13.000	-0.0015833841776588
18	9	13.250	0.0010539582621417
18	9	13.500	0.0006797126027067
18	9	13.750	-0.0008610524881542
18	9	14.000	-0.0016879505702327
18	9	14.250	-0.0004325456292316
18	9	14.500	0.0021542987543960
18	9	14.750	0.0047796785628859
18	9	15.000	0.0061370556767164
18	9	15.250	0.0053101254631173
18	9	15.500	0.0029844969221255
18	9	15.750	0.0002527945792410
18	9	16.000	-0.0017907779584682
18	9	16.250	-0.0023454290861348
18	9	16.500	-0.0017748201926804
18	9	16.750	-0.0007315876715226
18	9	17.000	0.0001324736506912
18	9	17.250	0.0003265908355199
18	9	17.500	0.0000058717603302
18	9	17.750	-0.0005151155068002
18	9	18.000	-0.0009241960075660
18	9	18.250	-0.0009885369191060
18	9	18.500	-0.0007853478459080
18	9	18.750	-0.0004671465680731
18	9	19.000	-0.0001851490575246
18	9	19.250	-0.0000556435543738
18	9	19.500	-0.0000598112968208
18	9	19.750	-0.0001467269901335
18	9	20.000	-0.0002675497653794
18	9	20.250	-0.0003849924351148
18	9	20.500	-0.0005015439856722
18	9	20.750	-0.0006288256251925
18	9	21.000	-0.0007785286451533
18	9	21.250	-0.0009586723591630
18	9	21.500	-0.0011606260864359
18	9	21.750	-0.0013718898672320
18	9	22.000	-0.0015805386281053
18	9	22.250	-0.0017757444717571
18	9	22.500	-0.0019479307489948
18	9	22.750	-0.0020869805559130
18	9	23.000	-0.0021825569252912
18	9	23.250	-0.0022228561557905
18	9	23.500	-0.0021887606541048
18	9	23.750	-0.0020598066013075
18	9	24.000	-0.0018155162386241
18	9	24.250	-0.0014576292956009
18	9	24.500	-0.0010753592581082
18	9	24.750	-0.0007792837272463
18	9	25.000	-0.0006789100985881
18	9	25.250	-0.0008352502369330
18	9	25.500	-0.0011181525659594
18	9	25.750	-0.0013508594486008
18	9	26.000	-0.0013574664924348
18	9	26.250	-0.0010312256109205
18	9	26.500	-0.0005405177113159
18	9	26.750	-0.0001222467325040
18	9	27.000	-0.0000141077324877
18	9	27.250	-0.0003642445640784
18	9	27.500	-0.0009631980375874
18	9	27.750	-0.0015129288109615
18	9	28.000	-0.0017179744650141
18	9	28.250	-0.0013896059955967
18	9	28.500	-0.0007585440027888
18	9	28.750	-0.0001592135292855
18	9	29.000	0.0000748468092922
18	9	29.250	-0.0002719953190375
18	9	29.500	-0.0009532853690285
18	9	29.750	-0.0016139252757784
18	9	30.000	-0.0019097231379688
18	12	4.000	-536.7062375170701216
18	12	4.250	-187.6573360907395340
18	12	4.500	-64.1210868951223176
18	12	4.750	-20.8851311631359806
18	12	5.000	-6.5132326804986178
18	12	5.250	-2.0010535534637484
18	12	5.500	-0.5432884693237554
18	12	5.750	-0.1469260933979513
18	12	6.000	-0.0236954226239021
18	12	6.250	-0.0890492805731355

18	12	6.500	0.0053433943199366
18	12	6.750	0.0211045483843582
18	12	7.000	-0.0141738302645766
18	12	7.250	0.0324750262001032
18	12	7.500	0.0236170904455868
18	12	7.750	0.0255964637019765
18	12	8.000	0.0213075159509444
18	12	8.250	0.0065350685774612
18	12	8.500	-0.0017040216969648
18	12	8.750	-0.0026488642072826
18	12	9.000	0.0057125606574857
18	12	9.250	0.0079089814378193
18	12	9.500	0.0073275339454287
18	12	9.750	0.0071927473676305
18	12	10.000	-0.0023397085436614
18	12	10.250	0.0031967033943259
18	12	10.500	0.0076392296560749
18	12	10.750	0.0166231418256125
18	12	11.000	0.0222387806929740
18	12	11.250	-0.0308381979652043
18	12	11.500	0.0100144129397945
18	12	11.750	-0.0005616724352001
18	12	12.000	-0.0006666985694183
18	12	12.250	0.0030870695273518
18	12	12.500	0.0032813539429643
18	12	12.750	0.0021436545430030
18	12	13.000	0.0015524273807508
18	12	13.250	0.0026336310260525
18	12	13.500	0.0044783528177645
18	12	13.750	0.0057549704186061
18	12	14.000	0.0052091694553321
18	12	14.250	0.0021169610240846
18	12	14.500	-0.0023636766444092
18	12	14.750	-0.0066278482908872
18	12	15.000	-0.0090862345948363
18	12	15.250	-0.0086332747288508
18	12	15.500	-0.0060599060720069
18	12	15.750	-0.0026261724870067
18	12	16.000	0.0004163670895011
18	12	16.250	0.0020899276570548
18	12	16.500	0.0024770398950130
18	12	16.750	0.0019213620414366
18	12	17.000	0.0007652235071465
18	12	17.250	-0.0006614712155016
18	12	17.500	-0.0020790883474388
18	12	17.750	-0.0032212374855166
18	12	18.000	-0.0038221625030175
18	12	18.250	-0.0037059175050700
18	12	18.500	-0.0030551656501038
18	12	18.750	-0.0021416432453341
18	12	19.000	-0.0012367273511159
18	12	19.250	-0.0005586417282784
18	12	19.500	-0.0001119079503077
18	12	19.750	0.0001526834936329
18	12	20.000	0.0002849042337800
18	12	20.250	0.0003305403869604
18	12	20.500	0.0003186694547053
18	12	20.750	0.0002743786849267
18	12	21.000	0.0002243993256871
18	12	21.250	0.0001947375494503
18	12	21.500	0.0002019140648522
18	12	21.750	0.0002586407656295
18	12	22.000	0.0003767245618200
18	12	22.250	0.0005517776778532
18	12	22.500	0.0007197666611980
18	12	22.750	0.0008021947954702
18	12	23.000	0.0007212819392660
18	12	23.250	0.0004419000381551
18	12	23.500	0.0000969981909349
18	12	23.750	-0.0001387784643780
18	12	24.000	-0.0000912377452628
18	12	24.250	0.0003422568151488
18	12	24.500	0.0009805904307805
18	12	24.750	0.0015717603545724
18	12	25.000	0.0018639190602141
18	12	25.250	0.0016788956027720
18	12	25.500	0.0011326903511169
18	12	25.750	0.0004153195367614
18	12	26.000	-0.0002824651127850
18	12	26.250	-0.0007993386960812
18	12	26.500	-0.0010914558710155
18	12	26.750	-0.0011438147886227
18	12	27.000	-0.0009402134563905
18	12	27.250	-0.0004934596106030
18	12	27.500	0.0000641866720991
18	12	27.750	0.0005708339478653
18	12	28.000	0.0008652230750910
18	12	28.250	0.0008350829754905
18	12	28.500	0.0005640887294273
18	12	28.750	0.0001877670429982
18	12	29.000	-0.0001525830786422
18	12	29.250	-0.0003428147800022
18	12	29.500	-0.0004021214252977
18	12	29.750	-0.0003896999104045
18	12	30.000	-0.0003707839369273

The distances R (in bohr) are converted in Angstrom (Å) such as:
1 bohr = 0.529177249 Å.

Table S2: The $C_{lm}^{(n)}$ 3D- PES's fitted parameters according to Eq (3).

l	m	$n = 12$	11	10	9	8	7	6
0	0	-2.67226E11	5.757E11	-4.96938E11	2.17085E11	-4.98597E10	5.69501E9	-2.56615E8
1	0	1.06834E11	-2.26632E11	1.9285E11	-8.33746E10	1.90753E10	-2.18473E9	9.83668E7
2	0	1.85693E10	-4.31203E10	4.02389E10	-1.91978E10	4.88919E9	-6.24772E8	3.11451E7
3	0	-9.38464E10	1.95924E11	-1.63863E11	6.96367E10	-1.56884E10	1.77369E9	-7.89045E7
3	3	8.73717E10	-1.82076E11	1.52023E11	-6.45336E10	1.45366E10	-1.64487E9	7.32872E7
4	0	4.24644E10	-8.67746E10	7.09642E10	-2.9543E10	6.54901E9	-7.32251E8	3.23488E7
4	3	-9.71189E10	2.00119E11	-1.65139E11	6.93958E10	-1.55284E10	1.75208E9	-7.80607E7
5	0	7.40735E9	-1.5398E10	1.28239E10	-5.4548E9	1.24153E9	-1.43045E8	6.51883E6
5	3	3.97815E10	-8.13571E10	6.66302E10	-2.78403E10	6.21625E9	-7.0257E8	3.14522E7

Code to generate the 3D-PES of PH₃ – Ar as given by equation (2)

The main program test calls the routine Vpot_init (once to read and initialize the data) and the function Vl(r,theta,phi) returns the energy value at this point. The compilation is done as follows:

gfortran -o test.x vpot.f90. It needs the radial coefficients, $V_{lm}(R)$, in the format given at the end of this file (and not that in the format of Table S1).

```
Vpot.f90 ( program test + subroutine Vpot_init )
*****
Subroutines of the 3D-PES of PH3-Ar system
*****

module mod_pot
  implicit real(kind=8) (a-h,o-z)
  integer, parameter :: dp = 8
  integer :: nmax,lamax
  real(kind=dp),allocatable, dimension(:) :: ri,hh,vv1
  real(kind=dp),allocatable, dimension(:,:) :: fi,fs
  integer, allocatable, dimension(:) :: l1,m1
  real(kind=dp) :: r
contains
end module mod_pot

program test
  implicit real(kind=8) (a-h,o-z)
  call Vpot_init

  read(*,*)r , theta, phi
  E=Vl(r,theta,phi)
  write(*,*)r,theta,phi,E
end program test

subroutine Vpot_init
  use mod_pot

  implicit real(kind=8) (a-h,o-z)
  real(kind=dp), parameter :: pi=3.141592653589793d0
  ipot=10
  !*****
  !
  ! lecture des Vlambdas
  !
  !*****
  open(unit=ipot,file='Vl.pot',status='OLD')
  read(ipot,*)
  read(ipot,*) lamax,nmax,rmin1,deltar
  write(*,*) lamax,nmax,rmin1,deltar
  allocate(ri(0:nmax),hh(0:nmax))
  allocate(fi(0:nmax,0:lamax),fs(0:nmax,0:lamax))
  allocate(l1(0:lamax),m1(0:lamax))
  allocate(vv1(0:lamax))

  irf=1
  select case (irf)
  case (1)

  ri(0)=rmin1!/0.529177d0
  deltar=deltar!/0.529177d0
  do i=1,nmax
    ri(i)=ri(0)+dfloat(i)*deltar
  enddo
  case (2)
  read(ipot,*) ri
  ! write(output,*) ri
  ! ri=ri/0.529177d0
  end select

  do i=0,nmax-1
    hh(i)=ri(i+1)-ri(i)
  enddo
  do il=0,lamax
    read(ipot,*) l1(il),m1(il)
    ! write(*,*) l1(il),m1(il)
    ! READ(ipot,*) fi(0:nmax,il)
    ! write(*,*) fi(0:nmax,il)
  enddo
  !*****
  !
  ! conversion des Vlambdas (cm-1 -----> ua)
  !
  !*****
  ! fi=fi*(2.d0*mu)/uacmm1
```

```

!*****
!
!   calcul des dÃ©rivÃ©es seconde des Vlambda
!
!*****
do il=0,lamax
  call splinel(ri,fi(:,il),fs(:,il),nmax)
enddo

end subroutine Vpot_init

real*8 function Vl(rl,thetal,phil)
  use mod_pot

  implicit real(kind=8) (a-h,o-z)
  real(kind=dp), parameter :: pi=3.141592653589793d0

  theta=thetal*pi/180.d00
  phi=phil*pi/180.d00
  r=rl
  E=0.d00
call pot
  do il=0,lamax
    som=plm(l1(il),m1(il),dcos(theta))*dcos(dfloat(m1(il))*phi)
    if(m1(il)==0) som=som/2.d0
    E=E+som*vvl(il)
  enddo
  E=E*dsqrt(2.d0/pi)
!write(*,*)r,theta*180.d0/pi,phi*180.d0/pi,E
Vl=E
return
end function Vl

subroutine pot
!implicit real(kind=8) (a-h,o-z)
use mod_pot
implicit real(kind=dp) (a-h,o-z)
real(kind=dp), parameter :: eps=0.0000001d0
real(kind=dp) :: Ai,Bi,Ao,Bo,z
integer :: n
integer :: i,k,il
n=nmax
k=0
if((r>=ri(0)-eps).and.(r<=ri(n)+eps)) then
  do i=0,n-1
    if(r>=ri(i)) k=i
  enddo
else
! print *, 'pot : reervoir x !!!',i,x(i),k
  if(r>=ri(n)+eps) then
!$OMP PARALLEL DO PRIVATE (il, Bo,Ao,z)
    do il=0,lamax
      Bo=dlog(dabs(fi(n-1,il)/fi(n,il)))/dlog(dabs(ri(n)/ri(n-1)))
      Ao=fi(n,il)*ri(n)**Bo
      z=Ao/(r**Bo)
      if(fi(n-1,il)*fi(n,il)<=0.d0.or.fi(n-1,il)/fi(n,il)<=1.0d0.or.Bo>8.0d1.or.Bo<=2.d0) then
        z=0.d0
!write(2,*)r,il,z,Ao,Bo
      endif
      vvl(il)=z
! z=z/100.d0
! z=0.d0
!write(2,*)xp,z,Ao,Bo
    enddo
!$OMP END PARALLEL DO
  else
!$OMP PARALLEL DO PRIVATE (il, Bi,Ai,z)
    do il=0,lamax
      if(fi(0,il)*fi(1,il)>0.d0) then
        Bi=dlog(fi(0,il)/fi(1,il))/(ri(1)-ri(0))
        Ai=fi(0,il)*dexp(Bi*ri(0))
        z=Ai*dexp(-Bi*r)
      else
        z=0.d0
      endif
      vvl(il)=z
! z=f(0)
!write(2,*)z,Ai,Bi
    enddo
!$OMP END PARALLEL DO
  endif
! z=0.d0
  return
! stop
endif
if((r>=ri(0)-eps).and.(r<=ri(n)+eps)) then
!$OMP PARALLEL DO PRIVATE (il,z)
  do il=0,lamax
    z=fs(k,il)*(((ri(k+1)-r)**3)/(6.d0*hh(k)))-((hh(k)/6.d0)*(ri(k+1)-r))
    z=z+fs(k+1,il)*(((r-ri(k))**3)/(6.d0*hh(k)))-((hh(k)/6.d0)*(r-ri(k)))
    z=z+(fi(k,il)/hh(k))*ri(k+1)-r
    z=z+(fi(k+1,il)/hh(k))*(r-ri(k))
    vvl(il)=z
  enddo
!$OMP END PARALLEL DO
endif

```

```

!$OMP END PARALLEL DO
endif
!print *, 'l intervalle est:',k
!print *, 'pi(x)=' ,z
end subroutine pot

subroutine spline1(x,f,fs,n)
  implicit real(kind=8) (a-h,o-z)
  integer, parameter :: dp = 8
  real(kind=dp) , allocatable, dimension(:,:) :: a
  real(kind=dp) , intent(in), dimension(0:n) :: x, f
  real(kind=dp) , intent(out), dimension(0:n) :: fs
  real(kind=dp) , allocatable, dimension(:) :: b, h
  integer , intent(in) :: n
  integer :: i,j,k
  real(kind=dp) :: z, xp
  allocate(a(0:n,1:3))
  allocate(b(0:n))
  allocate(h(0:n))
  a(:,1)=0.d0
  do i=0,n-1
    h(i)=x(i+1)-x(i)
  enddo
  do i=1,n-1
    a(i,2)=2.d0*(h(i)+h(i-1))
  enddo
  a(0,2)=2.d0*h(0)
  a(n,2)=2.d0*h(n-1)
  do i=0,n-1
    a(i+1,1)=h(i)
  enddo
  !a(n,1)=0.d0
  do i=1,n
    a(i-1,3)=h(i-1)
  enddo
  !a(0,3)=0.d0
  do i=1,n-1
    b(i)=6.d0*((f(i+1)-f(i))/h(i)-(f(i)-f(i-1))/h(i-1))
  enddo
  b(0)=6.d0*((f(1)-f(0))/h(0)-((f(i)-f(i-1))/h(i-1)+(f(1)-f(0))/h(0)-(f(2)-f(1))/h(1))))
  b(n)=6.d0*((f(n)-f(n-1))/h(n-1))

  if (f(n-1)*f(n)<=0.d0.or.f(n-1)/f(n)<=1.0d0.or.dabs(f(n))<1.d-2)b(n)=0.d0
! write(9,*)b(0),b(n)
!b(0)=0.d0
!b(n)=0.d0
do i=1,n
  a(i,1)=a(i,1)/a(i-1,2)
  a(i,2)=a(i,2)-a(i,1)*a(i-1,3)
enddo
do i=1,n
  b(i)=b(i)-a(i,1)*b(i-1)
enddo
fs(n)=b(n)/a(n,2)
do i=n-1,0,-1
  fs(i)=(b(i)-a(i,3)*fs(i+1))/a(i,2)
enddo
end subroutine spline1

! COMPUTES NORMALIZED ASSOC. LEGENDRE POLYNOMIALS BY RECURSION.
! THE VALUES RETURNED ARE NORMALIZED FOR INTEGRATION OVER X
! (I.E. INTEGRATION OVER COS THETA BUT NOT PHI).
! NOTE THAT THE NORMALIZATION GIVES
! PLM(L,0,1)=SQRT(L+0.5)
! PLM(L,0,X)=SQRT(L+0.5) P(L,X)
! FOR M.NE.0, THE VALUE RETURNED DIFFERS FROM THE USUAL
! DEFINITION OF THE ASSOCIATED LEGENDRE POLYNOMIAL
! (E.G. EDMONDS PAGES 23-24)
! BY A FACTOR OF (-1)**M*SQRT(L+0.5)*SQRT((L-M)!/(L+M)!)
! THUS THE SPHERICAL HARMONICS ARE
! CLM = PLM * EXP(I*M*PHI) / SQRT(L+0.5)
! YLM = PLM * EXP(I*M*PHI) / SQRT(2*PI)
! THIS ROUTINE ALWAYS RETURNS THE VALUE FOR ABS(MIN) NOTE THAT
! FOR MIN.LT.0 THIS VALUE SHOULD BE MULTIPLIED BY PARITY(MIN)
!
! FUNCTION PM1(LIN,MIN,COSTH)
! This routine appears to be much more stable for large l, m than
! the routine from Nerf/ modified according to R.T Pack
! It was obtained:
! From: Marie-Lise Dubernet <ml@dipp-garching.mpg.de>
! Date: Mon, 19 Jun 1995 12:48:11 +0200 (MET DST)
! Some mods 27-28 June 95 by SG for speed and to accord w/ MOLSCAT
! Bugs fixed 21 Sept 95 (SG)
!*****
double precision FUNCTION PLM(LIN,MINa,COSTH)
  IMPLICIT real*8 (a-h,o-z)
  if (ABS(COSTH).GT.1.0d00)THEN
    WRITE(6,*)'***ILLEGAL ARGEMENT TO PLM X=',COSTH
    STOP
  ENDIF
! SAVE IN LOCAL VARIABLES
  L=LIN
  M=IABS(MINa)
  X=COSTH
!

```

```

IF(M.GT.L) THEN
PLM=0.0d00
return
ENDIF
LMAX=L
IF (M.GT.0) GO TO 5
!
PLM=1.0d0
PM2=0.d0
XL=0.d0
DO 2 L=1,LMAX
XL=XL+1.0d0
PP=(2.d0*XL-1.d0)*X*PLM-(XL-1.d0)*PM2/XL
PM2=PLM
2 PLM=PP
GO TO 9000
!
5 IMAX=2*M
RAT=1.d0
AI=0.d0
DO 6 I=2,IMAX,2
AI=AI+2.d0
6 RAT=RAT*((AI-1)/AI)
! Y=SIN(THETA)
Y=SQRT(1.0d0-X*X)
PLM=SQRT(RAT)*(Y**M)
PM2=0.d0
LOW=M+1
XL=LOW-1
DO 10 L=LOW,LMAX
XL=XL+1.0d0
AL=DBLE((L+1)*(L-1))
AL=1.d0/AL
AL2=DBLE((L+M-1)*(L-M-1))*AL
AL=SQRT(AL)
AL2=SQRT(AL2)
PP=(2.d0*XL-1.D0)*X*PLM*AL-PM2*AL2
10 PM2=PLM
PLM=PP
PLM=PLM*AAPARITY(MINa)
9000 PLM=PLM*SQRT(XL+0.5d0)
!9000 PLM=PLM
RETURN
END
!.....

double precision FUNCTION AAPARITY(I)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
AAPARITY=1.d0
IF ((I/2)*2.NE.I) AAPARITY=-1.d0
RETURN
END
!.....

```

The radial coefficients, $V_{l,m}(R)$, to be used in the potential subroutines

The coefficients are in cm-1 and Each block contains the coefficients corresponding to the distances with a regular increasing order (step 0,25) going from [4 ---30] Bohr.

64: number of couples l,m

105: number of distance values used from 4 to 30 by step of 0.25

```
Vl.pot
 64 105 4.0 0.25
 0 0
 0.2042268061400691E+06 0.1395426015718522E+06 0.9491158266827028E+05 0.639511166232521824E+05 0.42517553305040094E+05 0.2779754784072753E+05
 0.1780724220105904E+05 0.111223333878077E+05 0.6720040059924914E+04 0.3872670055187046E+04 0.2069177060176539E+04 0.9558931964422025E+03
 0.2916169164603278E+03 -0.8581438657953485E+02 -0.283858653699856E+03 -0.3726685181943375E+03 -0.3973094329004502E+03 -0.3861957379013471E+03 -
 0.3568552269427609E+03 -0.3198013250711666E+03 -0.2810869461276070E+03 -0.2440085493074909E+03 -0.2101809084422541E+03 -0.1802132961840821E+03 -
 0.1541628972168836E+03 -0.1318045246516860E+03 -0.1127675161982309E+03 -0.9662762662283738E+02 -0.8296027565053730E+02 -0.7142167613094355E+02 -
 0.6170070664722682E+02 -0.5348193621577303E+02 -0.4650053800914726E+02 -0.4053989013623058E+02 -0.3545509823018800E+02 -0.3111802089184861E+02 -
 0.2740051095021168E+02 -0.2418599387456162E+02 -0.2140416729571431E+02 -0.1899629412254025E+02 -0.1690363647634327E+02 -0.1507246082074817E+02 -
 0.1346904935762096E+02 -0.1206468808313506E+02 -0.1083066325979142E+02 -0.9740495132630972E+01 -0.8776638681198465E+01 -0.7923782429729038E+01 -
 0.7166615151012755E+01 -0.6491058450782203E+01 -0.5887963826652053E+01 -0.5349415057395701E+01 -0.4867495887999149E+01 -0.4434822147579332E+01 -
 0.4046137795791447E+01 -0.3696718832348243E+01 -0.3381841310363783E+01 -0.3097115987464777E+01 -0.2839492321139868E+01 -0.2606254451297165E+01 -
 0.2394686604876030E+01 -0.2202255790323690E+01 -0.2027159925199208E+01 -0.1867779658470327E+01 -0.1722495731985318E+01 -0.1589788944777945E+01 -
 0.1468539961457248E+01 -0.1357729410844579E+01 -0.1256338003758040E+01 -0.1163400360905445E+01 -0.1078166443250110E+01 -0.9999400358474591E+00 -
 0.9280250296095148E+00 -0.8617713560969015E+00 -0.8007128951165995E+00 -0.7444295311612305E+00 -0.6925012435531457E+00 -0.6445295364354928E+00 -
 0.6002016164972079E+00 -0.5592261077488904E+00 -0.5213117147338464E+00 -0.4861799750903723E+00 -0.4536034858115348E+00 -0.4233676590215222E+00 -
 0.3952580358228685E+00 -0.3690778166076948E+00 -0.3447006035893430E+00 -0.3220176720084536E+00 -0.3009205300280023E+00 -0.2812984991682391E+00 -
 0.2630315007314339E+00 -0.2459971543651383E+00 -0.2300732897744850E+00 -0.21516110662097932E+00 -0.2012547415089030E+00 -0.1883717054373213E+00 -
 0.1765299255622218E+00 -0.1656670745824798E+00 -0.1553988318056094E+00 -0.1452604818277258E+00
 -0.134787857961212E+00 -0.1238855624676121E+00 -0.113933360333052E+00 -0.1066794083200693E+00 -0.1038727066638911E+00
 1 0
 -0.7294700951321624E+05 -0.4835715467523027E+05 -0.3255042258334200E+05 -0.2201850108493028E+05 -0.1484064979436783E+05 -0.9911830384712286E+04 -
 0.6538183294367725E+04 -0.4249972814031620E+04 -0.2716439249768306E+04 -0.1702331187962845E+04 -0.1041308536534405E+04 -0.6171060981090284E+03 -
 0.3496261113513395E+03 -0.1844431872587770E+03 -0.8506546827660318E+02 -0.2733798537988313E+02 0.4525762961829705E+01 0.2068984856534855E+02
 0.2760028909231475E+02 -0.2922663779604851E+02 -0.2814078260023550E+02 0.2567145744969983E+02 0.2268491555261531E+02 0.1964890906867261E+02
 0.1680102893294693E+02 0.1424593944816911E+02 0.1202003627551697E+02 0.1012014089582940E+02 0.8526459091953065E+01 0.7178090739440063E+01
 0.6031308549436248E+01 0.5079610265129668E+01 0.4314429483228951E+01 0.3673610712434586E+01 0.3131484405890493E+01 0.2675798542628623E+01
 0.2294297241532390E+01 0.1975259485450904E+01 0.1709092985125693E+01 0.1486736175668675E+01 0.1299126912671180E+01 0.1138205349187478E+01
 0.999196775302077E+00 0.88112200568958730E+00 0.7790568083831398E+00 0.6906129930322410E+00 0.6140018553027943E+00 0.5475691036765219E+00
 0.4896605834974287E+00 0.4387705304998206E+00 0.3939856744490692E+00 0.354540733798980E+00 0.3196703883672818E+00 0.2886781564022498E+00
 0.2611428583525724E+00 0.2367121501146636E+00 0.2150336991771344E+00 0.195778027828892E+00 0.1786491381825301E+00 0.163409988932717E+00
 0.1497945745642689E+00 0.1375624850215597E+00 0.1265462603293717E+00 0.1165967381835790E+00 0.1075647952305490E+00 0.9931762504978869E+01 0.9178749680957025E-
 01 0.8492293991998773E-01 0.7867251999098983E-01 0.7298530885813811E-01 0.6781224445637626E-01 0.6310469937846008E-01 0.588140413665788E-01 0.5489546726971585E-
 01 0.5131950447354079E-01 0.4806051945451217E-01 0.4509288620984454E-01 0.423889822017828E-01 0.3991318226799810E-01 0.3762786253371038E-01 0.3549538983248986E-
 01 0.3348603465319441E-01 0.3160162163709795E-01 0.2985186579121259E-01 0.2824648716497108E-01 0.2678952779911122E-01 0.2546224488883792E-01 0.2424016453375944E-
 01 0.2309879571218448E-01 0.2201684656149230E-01 0.2098587053988017E-01 0.2000558791450874E-01 0.1905565958456343E-01 0.1814968177552864E-01 0.172968189692487E-
 01 0.1651498886892024E-01 0.1582179707207477E-01 0.1522371188856015E-01 0.146835004793936E-01 0.1415311142315063E-01
 0.1358433889346723E-01 0.1295667285419253E-01 0.1236111982121026E-01 0.1191662365515565E-01 0.1174205158766922E-01
 2 0
 -0.1018886363939317E+05 -0.5918057197704497E+04 -0.3499620495552525E+04 -0.2054992098904080E+04 -0.1163016306186968E+04 -0.6104791898923104E+03 -
 0.2764887302013831E+03 -0.8441448591732478E+02 0.1726766087414035E+02 0.6354978159171765E+02 0.7783315795804765E+02 0.7510250859814323E+02
 0.6459702454225152E+02 0.5164202813317627E+02 0.3907186504860940E+02 0.2818812616706367E+02 0.1941243223503241E+02 0.1269918711433365E+02
 0.772098277315939E+01 0.4321776402995127E+01 0.1985198398433141E+01 0.4770650724901486E+01 -0.4436893428055697E+00 -0.9597401687044709E+00 -
 0.1214983635619653E+00 -0.1300723971412637E+01 -0.1283717894325569E+01 -0.1213378590066796E+01 -0.1115561214785146E+01 -0.9930519237823070E+00 -
 0.8787240874197080E+00 -0.7642683962306904E+00 -0.6700086058223444E+00 -0.58645465694419423E+00 -0.5098347210217327E+00 -0.4408631534623932E+00 -
 0.3802547481498255E+00 -0.3283834080253367E+00 -0.2842688268085727E+00 -0.2465933800975009E+00 -0.2140399138658404E+00 -0.185474880323224E+00 -
 0.1604992451452327E+00 -0.1388977539521457E+00 -0.1204552371506695E+00 -0.1049118092449932E+00 -0.9182871255861658E-01 -0.8072244079525438E-01 -0.7110954976158679E-
 01 -0.6257612537165436E-01 -0.5498603212977171E-01 -0.482725427586945E-01 -0.4236893108623141E-01 -0.3720606810935756E-01 -0.32705223281226E-01 -
 0.287848666667159E-01 -0.2536352610003578E-01 -0.2236631705930214E-01 -0.1974186301122127E-01 -0.1744500469052757E-01 -0.1543058927220053E-01 -0.1365719057136416E-01 -
 0.1209887512048576E-01 -0.1073105243074890E-01 -0.9532775172707397E-02 -0.8481098458866909E-02 -0.7555182923292658E-02 -0.6734539852517707E-02 -0.5998698845427253E-
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