

## Electronic Supplementary Information (ESI)

### “A New Potential Energy Surface of OH<sub>2</sub><sup>+</sup> System and State-to-State Quantum Dynamics Studies of the O<sup>+</sup>(<sup>4</sup>S) + H<sub>2</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) → OH<sup>+</sup>(X<sup>3</sup>Σ<sup>-</sup>) + H(<sup>2</sup>S) Reaction”

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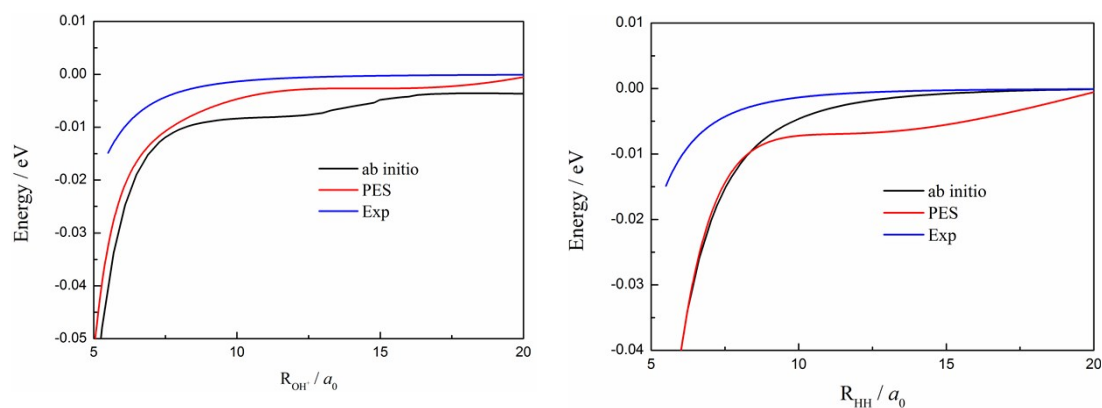
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### Long range interatomic potential energy figures



The left panel refers to the O<sup>+</sup> ion approach to the H<sub>2</sub> molecule and the right panel corresponds to the H atom close to the OH<sup>+</sup> ion.

### Total and vibrational integral cross section

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<b>Energy</b>	<b>Total</b>	<b>v'=0</b>	<b>v'=1</b>	<b>v'=2</b>	<b>v'=3</b>
0.040	93.40953591	63.54635548	29.83580396	--	--
0.041	93.30195467	63.58440225	29.68699406	--	--
0.042	92.74917932	63.28661392	29.43219814	--	--
0.043	92.20773677	63.09004385	29.08812896	--	--
0.044	92.11819220	63.32864822	28.76103894	--	--
0.045	91.13849436	62.78666855	28.32567717	--	--
0.046	90.33968950	62.34933628	27.96575577	--	--
0.047	89.46493205	61.86390727	27.57705356	--	--
0.048	88.42466267	61.23319426	27.16826886	--	--
0.049	87.26586898	60.48717745	26.75573888	--	--
0.050	86.18116054	59.77445792	26.38340017	--	--
0.051	84.99891698	58.96073636	26.01416736	--	--
0.052	83.88600887	58.17631759	25.68517605	--	--
0.053	82.80631407	57.40830700	25.37361873	--	--
0.054	81.83179608	56.70148707	25.10661050	--	--
0.055	80.99024130	56.07055328	24.89711478	--	--
0.056	80.26097066	55.52751553	24.71220232	--	--
0.057	79.62556063	55.06330434	24.54230965	--	--
0.058	79.05858400	54.65790432	24.38178860	--	--
0.059	78.53400690	54.28996704	24.22584476	--	--
0.060	78.01009836	53.92496178	24.06715673	--	--
0.061	77.45595521	53.53697199	23.90079411	--	--
0.062	76.84172538	53.10025021	23.72276338	--	--
0.063	76.14892598	52.59819113	23.53135593	--	--

0.064	75.37507340	52.02640927	23.32861657	--	--
0.065	74.52742686	51.38853934	23.11832061	--	--
0.066	73.62425909	50.69836163	22.90501470	--	--
0.067	72.69164576	49.97679958	22.69390044	--	--
0.068	71.75869737	49.24899481	22.48897904	--	--
0.069	70.85211504	48.53916098	22.29263465	--	--
0.070	69.99584956	47.87040744	22.10564519	--	--
0.071	69.20652691	47.26073737	21.92659373	--	--
0.072	68.49172655	46.72074056	21.75234183	--	--
0.073	67.85266324	46.25530868	21.57915087	--	--
0.074	67.28243011	45.86120060	21.40328597	--	--
0.075	66.76815253	45.52899719	21.22126055	--	--
0.076	66.29562868	45.24584129	21.03178266	--	--
0.077	65.84930749	44.99599842	20.83508860	--	--
0.078	65.42111856	44.76903886	20.63361061	--	--
0.079	64.99796643	44.54783417	20.43143907	--	--
0.080	64.56780736	44.31522380	20.23373855	--	--
0.081	64.12594171	44.06135145	20.04568834	--	--
0.082	63.67233361	43.78200137	19.87147360	--	--
0.083	63.21100819	43.47876513	19.71351237	--	--
0.084	62.74760824	43.15737299	19.57168843	--	--
0.085	62.28838975	42.82694634	19.44309849	--	--
0.086	61.83841517	42.49766870	19.32259032	--	--
0.087	61.39998620	42.17895432	19.20302991	--	--
0.088	60.97325706	41.87867429	19.07669535	--	--

0.089	60.55505364	41.60083832	18.93640110	--	--
0.090	60.14005041	41.34583393	18.77644655	--	--
0.091	59.72178654	41.11013990	18.59391041	--	--
0.092	59.29348746	40.88676807	18.38902290	--	--
0.093	58.85010073	40.66725264	18.16521355	--	--
0.094	58.38915266	40.44283876	17.92876006	--	--
0.095	57.91149960	40.20636649	17.68765775	--	--
0.096	57.43324094	39.95362733	17.46218901	--	--
0.097	56.96324930	39.68395653	17.26185009	--	--
0.098	56.50287391	39.40055474	17.08475890	--	--
0.099	56.05991851	39.10970547	16.93241458	--	--
0.100	55.63966357	38.81919318	16.80231430	--	--
0.101	55.24499289	38.53707409	16.68931911	--	--
0.102	54.87605223	38.26985265	16.58712604	--	--
0.103	54.53026173	38.02122753	16.48953087	--	--
0.104	54.20255481	37.79182719	16.39091281	--	--
0.105	53.88585764	37.57870929	16.28720985	--	--
0.106	53.57311288	37.37692021	16.17636410	--	--
0.107	53.25793972	37.18012960	16.05834240	--	--
0.108	52.93659868	36.98225216	15.93547913	--	--
0.109	52.60892954	36.77893166	15.81192744	--	--
0.110	52.27827523	36.56808301	15.69305094	--	--
0.111	51.95059755	36.35007639	15.58435756	--	--
0.112	51.63361009	36.12774549	15.49064079	--	--
0.113	51.33452233	35.90504340	15.41506917	--	--

0.114	51.05856479	35.68614061	15.35862607	--	--
0.115	50.80746258	35.47427400	15.31974223	--	--
0.116	50.57843605	35.27078814	15.29426568	--	--
0.117	50.36474079	35.07467158	15.27647192	--	--
0.118	50.15581880	34.88282524	15.25894457	--	--
0.119	49.93988137	34.69075868	15.23446523	--	--
0.120	49.70504648	34.49315276	15.19657572	--	--
0.121	49.44147409	34.28521954	15.14034306	--	--
0.122	49.14403422	34.06431494	15.06339448	--	--
0.123	48.81205300	33.82950861	14.96607878	--	--
0.124	48.45076308	33.58312932	14.85135220	--	--
0.125	48.06981625	33.32979667	14.72424986	--	--
0.126	47.68339967	33.07708064	14.59133753	--	--
0.127	47.30741153	32.83371366	14.45968362	--	--
0.128	46.95804373	32.60929749	14.33574670	--	--
0.129	46.64941106	32.41286629	14.22446428	--	--
0.130	46.39202112	32.25170462	14.12893051	--	--
0.131	46.19069340	32.13019087	14.04948987	--	--
0.132	46.04416426	32.04902609	13.98413236	--	--
0.133	45.94425912	32.00400707	13.92889683	--	--
0.134	45.87667106	31.98641711	13.87825850	--	--
0.135	45.82175287	31.98275355	13.82617671	--	--
0.136	45.75720215	31.97639138	13.76710254	--	--
0.137	45.65995013	31.94901195	13.69641395	--	--
0.138	45.50939071	31.88291955	13.61131171	--	--

0.139	45.29048184	31.76399346	13.51095462	--	--
0.140	44.99614002	31.58398837	13.39654103	--	--
0.141	44.63259186	31.34261189	13.27458668	--	--
0.142	44.22294107	31.04815276	13.15986435	--	--
0.143	43.77418557	30.71760127	13.04231245	--	--
0.144	43.31332340	30.37411393	12.92568565	--	--
0.145	42.87072442	30.04389963	12.81405112	--	--
0.146	42.47915408	29.75740626	12.70964044	--	--
0.147	42.15483306	29.53016351	12.61307382	--	--
0.148	41.90726268	29.37158342	12.52439192	--	--
0.149	41.73724128	29.28267349	12.44336351	--	--
0.150	41.63387611	29.25257909	12.36995735	--	--
0.151	41.57631069	29.26029294	12.30435546	--	--
0.152	41.53820087	29.27921485	12.24686695	--	--
0.153	41.49269835	29.28208487	12.19796940	--	--
0.154	41.41692662	29.24581259	12.15794952	--	--
0.155	41.29587696	29.15577526	12.12649040	--	--
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0.157	40.91295155	28.81306276	12.08581276	--	--
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0.159	40.42932584	28.35459432	12.06089811	--	--
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0.162	39.86314216	27.85089352	11.99970482	--	--
0.163	39.76260150	27.78895619	11.96158362	--	--

0.164	39.69865323	27.77480222	11.91221738	--	--
0.165	39.65417942	27.79087355	11.85201716	--	--
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0.167	39.53690339	27.81891752	11.70710389	--	--
0.168	39.42588624	27.78602073	11.62906725	--	--
0.169	39.26508041	27.70145808	11.55285946	--	--
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0.172	38.52352819	27.13596168	11.37687927	--	--
0.173	38.23755458	26.88062287	11.34631107	--	--
0.174	37.96218248	26.61939018	11.33225995	--	--
0.175	37.71229005	26.36754042	11.33431480	--	--
0.176	37.49730799	26.13648247	11.35047983	--	--
0.177	37.31996764	25.93209288	11.37759111	--	--
0.178	37.17767941	25.75620152	11.41121583	--	--
0.179	37.06412567	25.60762205	11.44621471	--	--
0.180	36.97166646	25.48418811	11.47711640	--	--
0.181	36.89347287	25.38440208	11.49859902	--	--
0.182	36.82537459	25.30872629	11.50604826	--	--
0.183	36.76581713	25.25900567	11.49608702	--	--
0.184	36.71582408	25.23802283	11.46698034	--	--
0.185	36.67700404	25.24729663	11.41883931	--	--
0.186	36.64998032	25.28534466	11.35378423	--	--
0.187	36.63242563	25.34623935	11.27542282	--	--
0.188	36.61780776	25.41863290	11.18856718	--	--

0.189	36.59554109	25.48667163	11.09847199	--	--
0.190	36.55570807	25.53173038	11.01260939	0.00121583	--
0.191	36.48773101	25.53511714	10.93803899	0.00467729	--
0.192	36.36900400	25.48104893	10.87131465	0.00698339	--
0.193	36.19004571	25.35987469	10.81252897	0.00819009	--
0.194	35.94853219	25.16985046	10.76018754	0.00919579	--
0.195	35.65012348	24.91827270	10.71149219	0.01115439	--
0.196	35.30629097	24.62065202	10.66326110	0.01320709	--
0.197	34.93578358	24.29880713	10.61271830	0.01506432	--
0.198	34.56171507	23.97783683	10.55793252	0.01668157	--
0.199	34.20863357	23.68281127	10.49837138	0.01807917	--
0.200	33.89927296	23.43533601	10.43514626	0.01928419	--
0.201	33.65209865	23.25093516	10.37099704	0.02050716	--
0.202	33.48089385	23.13723872	10.31001042	0.02382211	--
0.203	33.38838977	23.09372363	10.25682111	0.02785526	--
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0.205	33.41639265	23.17911116	10.19077602	0.03619116	--
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0.207	33.63127268	23.38493761	10.19159549	0.04415356	--
0.208	33.75939200	23.48671624	10.21408313	0.04790499	--
0.209	33.87367649	23.56597374	10.24546854	0.05147368	--
0.210	33.95604047	23.61072236	10.27967195	0.05484472	--
0.211	33.99228334	23.61321804	10.31025600	0.05800272	--
0.212	33.97271117	23.56990969	10.33110035	0.06092678	--
0.213	33.89539832	23.48117982	10.33756078	0.06595560	--



0.214	33.75876127	23.35056692	10.32674128	0.07086532	--
0.215	33.56730696	23.18385807	10.29777091	0.07524839	--
0.216	33.33002186	22.98875384	10.25189384	0.07914642	--
0.217	33.05893782	22.77421295	10.19207518	0.08266447	--
0.218	32.76901487	22.55095481	10.12241329	0.08593843	--
0.219	32.47328118	22.32706280	10.04768363	0.08912536	--
0.220	32.18528927	22.11100710	9.97278522	0.09239220	--
0.221	31.91786289	21.91083437	9.90232536	0.09588808	--
0.222	31.68232504	21.73384345	9.84019224	0.09972622	--
0.223	31.48772316	21.58592648	9.78945086	0.10397767	--
0.224	31.33984277	21.47058604	9.75234101	0.10867171	--
0.225	31.24075261	21.38867614	9.73007824	0.11380310	--
0.226	31.18872557	21.33811093	9.72305915	0.11933888	--
0.227	31.17844845	21.31427363	9.73064124	0.12524066	--
0.228	31.20143241	21.31007471	9.75118256	0.13177300	--
0.229	31.24615175	21.31663327	9.78216059	0.13883950	--
0.230	31.29930388	21.32429455	9.82014483	0.14624756	--
0.231	31.34699808	21.32351954	9.86081838	0.15398139	--
0.232	31.37625125	21.30590335	9.89953896	0.16211741	--
0.233	31.37643246	21.26549926	9.93155735	0.17072365	--
0.234	31.34015981	21.19928777	9.95248467	0.17982389	--
0.235	31.26446119	21.10762636	9.95901332	0.18938679	--
0.236	31.15064929	20.99400324	9.94904009	0.19932936	--
0.237	31.00447319	20.86458561	9.92226353	0.20952347	--
0.238	30.83435197	20.72667328	9.87996130	0.21980107	--

0.239	30.65044071	20.58758906	9.82513758	0.22998286	--
0.240	30.46297550	20.45364404	9.76189734	0.23988440	--
0.241	30.28035878	20.32863962	9.69499810	0.24934641	--
0.242	30.10856399	20.21372900	9.62938466	0.25824363	--
0.243	29.95327115	20.10741923	9.57230243	0.26650196	--
0.244	29.81191145	20.00618421	9.52472109	0.27410690	--
0.245	29.68095411	19.90576182	9.48732651	0.28110063	--
0.246	29.55771418	19.80244320	9.45934459	0.28927568	--
0.247	29.43857388	19.69425047	9.43888117	0.29887946	--
0.248	29.31933612	19.58192581	9.42315906	0.30774378	--
0.249	29.20036404	19.46898106	9.40889008	0.31600099	--
0.250	29.08451430	19.36123384	9.39283966	0.32392040	--
0.251	28.97657887	19.26602286	9.37218792	0.33177213	--
0.252	28.88163303	19.19023016	9.34486777	0.33981930	--
0.253	28.80389676	19.13910553	9.30961737	0.34829950	--
0.254	28.74545407	19.11486718	9.26609444	0.35743085	--
0.255	28.70524009	19.11565513	9.21492694	0.36739360	--
0.256	28.67895356	19.13569705	9.15746532	0.37832411	--
0.257	28.65954395	19.16587683	9.09571648	0.39029568	--
0.258	28.63833143	19.19506337	9.03214337	0.40331011	--
0.259	28.60654586	19.21182831	8.96952742	0.41725462	--
0.260	28.55663180	19.20608968	8.91061847	0.43191111	--
0.261	28.48385787	19.17084966	8.85803257	0.44693035	--
0.262	28.38690018	19.10299821	8.81398716	0.46187670	--
0.263	28.26821210	19.00385118	8.78010339	0.47625755	--

0.264	28.13300641	18.87842277	8.75708101	0.48956086	--
0.265	27.98885008	18.73495525	8.74467491	0.50134428	--
0.266	27.84398903	18.58335570	8.74155452	0.51126640	--
0.267	27.70585375	18.43362850	8.74530971	0.51915636	--
0.268	27.58039599	18.29484901	8.75260346	0.52522296	--
0.269	27.47131932	18.17397974	8.75952658	0.53011663	--
0.270	27.37882785	18.07524105	8.76195959	0.53394524	--
0.271	27.30113685	18.00017964	8.75602563	0.53725983	--
0.272	27.23436795	17.94760250	8.73851593	0.54059167	--
0.273	27.17390072	17.91434090	8.70744709	0.54447817	--
0.274	27.11512801	17.89592205	8.66216860	0.54943907	--
0.275	27.05402996	17.88699383	8.60363270	0.55585451	--
0.276	26.98776174	17.88219307	8.53415829	0.56391998	--
0.277	26.91479664	17.87638245	8.45734919	0.57363592	--
0.278	26.83483808	17.86509919	8.37756201	0.58480395	--
0.279	26.74857217	17.84471384	8.29945490	0.59707401	--
0.280	26.65710118	17.81230621	8.22751724	0.60997354	--
0.281	26.56176213	17.76597450	8.16550514	0.62298402	--
0.282	26.46365588	17.70458547	8.11614851	0.63561147	--
0.283	26.36368706	17.62797164	8.08095039	0.64743157	--
0.284	26.26253431	17.53688944	8.06012932	0.65815691	--
0.285	26.16080496	17.43294056	8.05280917	0.66767876	--
0.286	26.05943038	17.31878602	8.05723494	0.67603126	--
0.287	25.95979558	17.19787982	8.07112591	0.68343083	--
0.288	25.86399804	17.07457609	8.09189591	0.69020820	--

0.289	25.77472992	16.95363032	8.11709487	0.69674595	--
0.290	25.69507654	16.84005934	8.14435417	0.70347362	--
0.291	25.62809418	16.73856967	8.17164005	0.71076467	--
0.292	25.57688928	16.65389691	8.19703057	0.71890293	--
0.293	25.54224002	16.58841926	8.21874606	0.72806035	--
0.294	25.52320378	16.54242007	8.23483039	0.73896431	--
0.295	25.51762091	16.51488793	8.24327564	0.75247557	--
0.296	25.51850116	16.50281188	8.24190288	0.76679980	--
0.297	25.51823074	16.50153061	8.22861372	0.78109046	--
0.298	25.50949080	16.50525166	8.20232953	0.79490823	--
0.299	25.48576892	16.50782849	8.16295128	0.80799174	--
0.300	25.44005575	16.50345469	8.10945691	0.82016202	--
0.301	25.36855785	16.48746851	8.04284591	0.83128502	--
0.302	25.27048556	16.45666833	7.96564636	0.84123633	--
0.303	25.14826467	16.40967987	7.88171733	0.84994716	--
0.304	25.00707824	16.34670876	7.79605759	0.85738652	--
0.305	24.85423145	16.26932001	7.71434140	0.86361332	--
0.306	24.69774322	16.17989482	7.64208896	0.86874351	--
0.307	24.54510920	16.08111222	7.58390904	0.87299076	--
0.308	24.40221071	15.97570769	7.54268741	0.87662677	--
0.309	24.27252243	15.86604132	7.51927097	0.87993489	--
0.310	24.15710786	15.75427204	7.51229985	0.88319642	--
0.311	24.05513823	15.64257601	7.51857000	0.88662406	--
0.312	23.96459569	15.53327376	7.53361646	0.89035188	--
0.313	23.88361675	15.42932552	7.55259660	0.89439696	--

0.314	23.81116305	15.33415689	7.57113588	0.89866076	--
0.315	23.74749688	15.25144100	7.58599687	0.90295313	--
0.316	23.69432278	15.18473257	7.59557582	0.90700747	--
0.317	23.65390277	15.13650684	7.59991815	0.91054656	--
0.318	23.62826189	15.10764179	7.60041601	0.91331129	--
0.319	23.61797503	15.09686659	7.59908755	0.91512436	--
0.320	23.62118495	15.10041024	7.59792146	0.91591455	--
0.321	23.63325682	15.11245022	7.59804985	0.91575039	--
0.322	23.64707569	15.12587008	7.59928819	0.91483551	--
0.323	23.65386046	15.13331227	7.59991428	0.91348706	--
0.324	23.64500773	15.12835475	7.59689165	0.91257629	--
0.325	23.61261514	15.10655433	7.58643364	0.91243942	--
0.326	23.55185942	15.06620314	7.56491187	0.91358924	--
0.327	23.46115577	15.00838983	7.52952193	0.91614910	--
0.328	23.34271604	14.93644627	7.47923519	0.92001341	--
0.329	23.20220117	14.85525043	7.41500190	0.92499815	--
0.330	23.04764030	14.76990286	7.33996852	0.93086935	--
0.331	22.88801345	14.68473871	7.25899839	0.93739764	--
0.332	22.73185132	14.60264616	7.17802003	0.94429248	--
0.333	22.58597907	14.52466010	7.10309830	0.95128200	--
0.334	22.45513666	14.45036057	7.03965979	0.95810896	--
0.335	22.34179947	14.37851025	6.99160826	0.96459567	--
0.336	22.24662686	14.30783048	6.96100418	0.97063438	--
0.337	22.16930829	14.23790583	6.94795957	0.97623053	--
0.338	22.10918186	14.16967547	6.95079061	0.98147595	--

0.339	22.06558967	14.10524363	6.96657763	0.98653173	--
0.340	22.03816406	14.04775014	6.99161299	0.99159661	--
0.341	22.02628079	14.00015998	7.02211523	0.99685696	--
0.342	22.02877690	13.96467200	7.05456498	1.00246227	--
0.343	22.04321488	13.94178882	7.08594056	1.00848532	--
0.344	22.06566681	13.92983963	7.11398417	1.01491932	--
0.345	22.09068691	13.92525163	7.13691702	1.02166547	--
0.346	22.11185346	13.92303028	7.15347684	1.02855701	--
0.347	22.12252856	13.91775842	7.16264840	1.03538848	--
0.348	22.11690533	13.90458595	7.16371153	1.04192618	--
0.349	22.09090991	13.88017631	7.15613991	1.04796231	--
0.350	22.04293625	13.84330751	7.13973588	1.05331336	--
0.351	21.97380586	13.79465584	7.11475433	1.05787063	--
0.352	21.88650600	13.73656503	7.08188529	1.06158804	--
0.353	21.78558145	13.67223813	7.04243729	1.06449586	--
0.354	21.67600101	13.60474375	6.99820370	1.06669748	--
0.355	21.56241074	13.53644635	6.95128959	1.06836472	--
0.356	21.44862770	13.46862377	6.90396053	1.06976674	--
0.357	21.33907115	13.40135414	6.85939886	1.07205863	--
0.358	21.23477751	13.33409335	6.81955554	1.07486886	--
0.359	21.13533040	13.26608931	6.78489681	1.07806783	--
0.360	21.04150499	13.19715824	6.75612468	1.08191596	--
0.361	20.95456924	13.12796794	6.73355841	1.08669888	--
0.362	20.87643150	13.06024337	6.71724524	1.09255902	--
0.363	20.80921978	12.99638250	6.70693716	1.09948010	--

0.364	20.75494130	12.93907302	6.70214718	1.10727367	--
0.365	20.71475396	12.89049938	6.70218176	1.11560934	--
0.366	20.68851853	12.85185676	6.70614644	1.12404790	--
0.367	20.67460252	12.82299099	6.71307192	1.13207902	--
0.368	20.67009932	12.80254118	6.72188790	1.13922404	--
0.369	20.67099720	12.78799054	6.73149838	1.14507944	--
0.370	20.67430466	12.77752356	6.74097097	1.14939752	--
0.371	20.67604369	12.76803232	6.74949060	1.15211934	--
0.372	20.67245958	12.75601572	6.75663408	1.15341285	--
0.373	20.66189674	12.73958497	6.76228319	1.15362951	--
0.374	20.64407949	12.71774101	6.76666407	1.15326833	--
0.375	20.61934372	12.68987883	6.77013887	1.15291205	--
0.376	20.58773947	12.65519266	6.77303072	1.15309788	--
0.377	20.54846951	12.61250561	6.77527992	1.15426999	--
0.378	20.49969143	12.56034855	6.77627867	1.15666682	--
0.379	20.43859367	12.49720148	6.77470953	1.16031694	--
0.380	20.36197594	12.42206418	6.76858084	1.16501319	--
0.381	20.26741082	12.33522845	6.75555969	1.17036807	--
0.382	20.15408599	12.23873108	6.73329563	1.17588024	--
0.383	20.02398436	12.13675354	6.70008729	1.18104731	--
0.384	19.88199566	12.03532439	6.65523310	1.18542632	--
0.385	19.73599369	11.94162151	6.59967883	1.18875967	--
0.386	19.59569734	11.86291787	6.53593664	1.19097402	--
0.387	19.47146625	11.80530324	6.46811611	1.19222346	--
0.389	19.30487853	11.76460676	6.34118228	1.19328488	--

0.390	19.27146163	11.77882225	6.29276159	1.19404701	--
0.391	19.27028598	11.80881125	6.26001941	1.19558014	--
0.392	19.29554834	11.84629768	6.24509003	1.19823030	--
0.393	19.33936478	11.88227061	6.24802333	1.20308306	--
0.394	19.39145179	11.90848647	6.26682999	1.21009689	--
0.395	19.44104609	11.91880607	6.29790911	1.21825573	--
0.396	19.47978210	11.90988275	6.33657485	1.22723121	--
0.397	19.50221126	11.88153652	6.37784397	1.23674013	--
0.398	19.50596316	11.83624616	6.41713785	1.24651042	--
0.399	19.49134781	11.77835217	6.45071155	1.25625209	--
0.400	19.46067877	11.71294893	6.47601116	1.26573295	--
0.401	19.41723196	11.64488572	6.49160709	1.27480283	--
0.402	19.36419804	11.57787576	6.49702892	1.28340442	--
0.403	19.30412586	11.51422454	6.49246689	1.29158720	--
0.404	19.23846621	11.45482761	6.47838647	1.29943941	--
0.405	19.16770744	11.39955901	6.45531117	1.30705261	--
0.406	19.09187712	11.34783358	6.42379072	1.31449110	--
0.407	19.01118936	11.29926450	6.38442958	1.32175360	--
0.408	18.92656409	11.25397333	6.33810882	1.32875905	--
0.409	18.84000295	11.21274098	6.28620121	1.33535608	--
0.410	18.75458774	11.17679793	6.23074541	1.34135671	--
0.411	18.67410327	11.14739758	6.17447531	1.34655629	--
0.412	18.60243109	11.12536216	6.12062396	1.35077781	--
0.413	18.54282486	11.11062424	6.07261810	1.35391273	--
0.414	18.49713798	11.10190674	6.03358373	1.35596313	--



0.415	18.46559991	11.09690781	6.00592628	1.35705471	--
0.416	18.44664932	11.09253846	5.99092846	1.35743463	--
0.417	18.43732904	11.08551122	5.98855228	1.35747602	--
0.418	18.43377387	11.07290057	5.99741839	1.35762510	--
0.419	18.43268495	11.05263216	6.01585403	1.35833761	--
0.420	18.43100599	11.02382046	6.04128768	1.36002153	--
0.421	18.42517074	10.98687457	6.06946865	1.36295775	--
0.422	18.41325297	10.94318544	6.09697905	1.36725048	--
0.423	18.39424568	10.89477766	6.12089825	1.37278906	--
0.424	18.36792701	10.84384320	6.13913788	1.37924583	--
0.425	18.33437396	10.79223161	6.15041710	1.38612479	--
0.426	18.29374158	10.74121152	6.15421508	1.39282700	--
0.427	18.24613065	10.69141961	6.15058893	1.39875298	--
0.428	18.19166163	10.64298799	6.14001854	1.40340482	--
0.429	18.13061841	10.59576787	6.12324145	1.40647164	--
0.430	18.06389397	10.54972994	6.10123560	1.40789239	--
0.431	17.99314120	10.50511907	6.07521949	1.40785240	--
0.432	17.92098384	10.46261992	6.04672467	1.40675539	--
0.433	17.85139990	10.42318110	6.01752720	1.40585146	--
0.434	17.78751525	10.38783750	5.98966607	1.40519070	--
0.435	17.73264817	10.35726616	5.96520644	1.40534833	--
0.436	17.68906674	10.33153263	5.94592690	1.40674914	--
0.437	17.65717853	10.30990549	5.93300096	1.40936173	--
0.438	17.63541435	10.29083765	5.92676306	1.41283563	--
0.439	17.62047815	10.27228296	5.92647343	1.41666925	--

0.440	17.60787301	10.25199168	5.93040061	1.42035715	--
0.441	17.59285503	10.22814114	5.93603860	1.42349468	--
0.442	17.57130820	10.19962028	5.94055695	1.42591637	--
0.443	17.54074387	10.16646556	5.94130143	1.42775795	--
0.444	17.50072737	10.12971681	5.93633764	1.42948127	--
0.445	17.45303033	10.09131191	5.92480608	1.43177802	--
0.446	17.40116938	10.05355721	5.90709859	1.43546090	--
0.447	17.34960300	10.01866922	5.88471412	1.44126469	--
0.448	17.30273257	9.98820482	5.85997581	1.44970253	--
0.449	17.26392852	9.96275991	5.83552993	1.46089497	--
0.450	17.23495772	9.94205639	5.81376199	1.47449617	--
0.451	17.21562919	9.92496206	5.79640673	1.48971053	--
0.452	17.20328995	9.90919335	5.78428189	1.50535093	--
0.453	17.19447836	9.89284845	5.77721744	1.52002893	--
0.454	17.18527282	9.87430922	5.77429085	1.53236476	--
0.455	17.17226438	9.85264232	5.77415829	1.54122611	--
0.456	17.15322431	9.82771295	5.77542968	1.54590570	--
0.457	17.12755961	9.80013735	5.77702803	1.54626632	--
0.458	17.09611317	9.77095137	5.77831672	1.54274496	--
0.459	17.06074287	9.74122311	5.77912236	1.53629917	--
0.460	17.02354092	9.71163148	5.77953316	1.52825139	--
0.461	16.98623168	9.68235538	5.77965019	1.52004788	--
0.462	16.94957575	9.65303112	5.77924048	1.51305304	--
0.463	16.91317340	9.62288575	5.77761939	1.50833593	--
0.464	16.87571198	9.59114803	5.77362553	1.50653025	--

0.465	16.83530162	9.55734471	5.76573415	1.50775700	--
0.466	16.79023461	9.52160476	5.75246204	1.51167183	--
0.467	16.73947253	9.48472974	5.73268234	1.51756543	--
0.468	16.68313549	9.44810818	5.70604893	1.52451205	--
0.469	16.62264397	9.41345743	5.67320219	1.53156609	--
0.470	16.56056735	9.38250629	5.63579730	1.53790057	--
0.471	16.50009353	9.35652333	5.59633067	1.54292580	--
0.472	16.44451986	9.33610603	5.55777794	1.54635629	--
0.473	16.39659347	9.32100992	5.52313876	1.54817950	--
0.474	16.35810206	9.31025992	5.49496026	1.54861338	--
0.475	16.32963480	9.30234838	5.47499782	1.54800684	--
0.476	16.31115904	9.29555790	5.46404460	1.54726294	--
0.477	16.30184671	9.28832100	5.46186463	1.54736986	--
0.478	16.29839167	9.27949096	5.46742690	1.54720932	--
0.479	16.29875755	9.26846746	5.47914871	1.54693312	--
0.480	16.30127840	9.25515455	5.49516323	1.54683789	--
0.481	16.30464664	9.23986886	5.51360361	1.54715944	--
0.482	16.30770588	9.22304674	5.53274568	1.54801849	--
0.483	16.30926800	9.20498757	5.55107352	1.54943121	--
0.484	16.30830941	9.18571990	5.56753530	1.55138572	--
0.485	16.30418203	9.16486402	5.58184318	1.55389347	--
0.486	16.29483111	9.14163414	5.59266408	1.55701554	--
0.487	16.27791241	9.11505617	5.59855530	1.56082648	--
0.488	16.25134197	9.08414042	5.59836757	1.56538728	--
0.489	16.21360043	9.04813190	5.59132440	1.57071830	--

0.490	16.16417034	9.00682402	5.57715978	1.57678238	--
0.491	16.10366648	8.96067022	5.55611684	1.58350386	--
0.492	16.03411336	8.91091085	5.52910464	1.59076019	--
0.493	15.95873626	8.85949502	5.49754941	1.59840053	--
0.494	15.88158981	8.80891273	5.46318754	1.60624966	--
0.495	15.80714438	8.76194038	5.42790242	1.61411334	--
0.496	15.73956953	8.72121894	5.39346149	1.62174833	--
0.497	15.68218294	8.68891662	5.36131930	1.62884634	--
0.498	15.63701796	8.66635666	5.33256350	1.63502873	--
0.499	15.60457005	8.65376364	5.30793490	1.63982627	--
0.500	15.58386103	8.65015544	5.28791283	1.64276573	--
0.501	15.57265861	8.65339594	5.27285949	1.64339163	--
0.502	15.56806347	8.66053542	5.26313411	1.64139771	--
0.503	15.56691749	8.66815352	5.25907019	1.63671470	--
0.504	15.56640029	8.67290200	5.26093247	1.62960692	--
0.505	15.56432594	8.67198165	5.26874331	1.62066563	--
0.506	15.55938101	8.66353178	5.28209831	1.61084255	--
0.507	15.55103411	8.64685598	5.30000664	1.60129365	--
0.508	15.53930580	8.62236890	5.32084868	1.59324458	--
0.509	15.52447771	8.59144789	5.34244482	1.58777951	--
0.510	15.50670880	8.55594571	5.36234258	1.58565684	--
0.511	15.48581794	8.51786943	5.37810222	1.58712744	--
0.512	15.46119369	8.47890385	5.38772647	1.59189006	--
0.513	15.43192242	8.44023830	5.38996399	1.59909010	--
0.514	15.39691432	8.40241211	5.38445159	1.60745739	--

0.515	15.35540187	8.36553477	5.37178418	1.61551562	--
0.516	15.30704575	8.32944969	5.35321717	1.62182310	--
0.517	15.25225353	8.29404491	5.33040291	1.62524475	--
0.518	15.19212298	8.25945344	5.30496066	1.62512568	--
0.519	15.12836062	8.22618547	5.27814582	1.62139888	0.00000986
0.520	15.06300143	8.19503503	5.25062122	1.61459065	0.00008451
0.521	14.99792320	8.16682509	5.22249901	1.60569072	0.00018090
0.522	14.93477550	8.14220884	5.19350521	1.59596982	0.00030260
0.523	14.87575887	8.12136884	5.16328191	1.58778172	0.00047493
0.524	14.82092927	8.10385043	5.13186723	1.58152739	0.00077151
0.525	14.77038188	8.08868221	5.09987001	1.57771914	0.00113899
0.526	14.72445857	8.07444098	5.06871167	1.57676950	0.00150910
0.527	14.68384024	8.05968782	5.04048812	1.57874628	0.00183859
0.528	14.64950199	8.04321510	5.01762866	1.58341618	0.00211551
0.529	14.62266661	8.02435311	5.00245955	1.59033085	0.00235653
0.530	14.60459464	8.00310474	4.99663825	1.59895524	0.00269973
0.531	14.59599182	7.97995842	5.00071589	1.60877588	0.00332789
0.532	14.59634101	7.95579338	5.01384074	1.61930656	0.00418512
0.533	14.60379564	7.93144209	5.03381811	1.63010428	0.00523144
0.534	14.61523813	7.90765750	5.05734815	1.64067868	0.00638623
0.535	14.62589537	7.88413928	5.08059380	1.65046922	0.00757221
0.536	14.63070998	7.86032055	5.09976170	1.65882640	0.00873799
0.537	14.62512979	7.83543508	5.11178037	1.66505276	0.00986183
0.538	14.60588538	7.80877608	5.11473977	1.66849190	0.01094277
0.539	14.57175132	7.78008079	5.10814747	1.66866261	0.01198748

0.540	14.52394357	7.74983590	5.09289948	1.66539229	0.01299847
0.541	14.46613520	7.71937878	5.07099088	1.65894300	0.01405177
0.542	14.40379593	7.69071309	5.04508479	1.65005973	0.01520361
0.543	14.34316826	7.66617875	5.01793728	1.63994581	0.01639575
0.544	14.29023666	7.64787018	4.99198860	1.63010955	0.01756823
0.545	14.24967092	7.63713032	4.96899915	1.62216266	0.01867404
0.546	14.22388506	7.63406067	4.94987334	1.61754339	0.01968164
0.547	14.21272281	7.63741620	4.93472459	1.61724085	0.02057658
0.548	14.21347152	7.64468466	4.92299163	1.62161207	0.02136284
0.549	14.22157087	7.65259352	4.91376160	1.63026331	0.02206126
0.550	14.23147404	7.65767920	4.90599505	1.64212254	0.02270354
0.551	14.23775834	7.65704505	4.89872766	1.65559839	0.02332431
0.552	14.23643255	7.64887748	4.89159322	1.66885552	0.02395328
0.553	14.22587827	7.63278870	4.88507950	1.68016144	0.02460984
0.554	14.20431815	7.60986273	4.87769892	1.68813971	0.02530072
0.555	14.17349030	7.58230525	4.86963809	1.69201363	0.02615061
0.556	14.13636212	7.55289844	4.86116072	1.69166992	0.02719419
0.557	14.09641340	7.52438727	4.85268663	1.68760783	0.02824542
0.558	14.05720539	7.49886345	4.84475013	1.68075521	0.02930892
0.559	14.02149363	7.47736658	4.83791574	1.67222903	0.03041651
0.560	13.99069580	7.45973812	4.83267870	1.66307556	0.03160233
0.561	13.96479256	7.44479807	4.82937624	1.65408344	0.03290284
0.562	13.94247242	7.43067467	4.82811137	1.64567823	0.03435327
0.563	13.92157224	7.41537331	4.82861503	1.63794033	0.03597918
0.564	13.89960566	7.39722979	4.83020812	1.63072533	0.03778662

0.565	13.87444439	7.37531974	4.83188944	1.62384998	0.03975974
0.566	13.84476448	7.34969141	4.83239027	1.61724737	0.04186230
0.567	13.81045474	7.32130986	4.83049156	1.61110631	0.04404465
0.568	13.77261346	7.29182867	4.82523052	1.60588145	0.04625260
0.569	13.73339518	7.26323212	4.81617411	1.60221438	0.04843797
0.570	13.69556914	7.23744146	4.80354853	1.60074964	0.05056737
0.571	13.66198696	7.21594465	4.78827606	1.60193242	0.05262779
0.572	13.63515689	7.19955884	4.77182310	1.60597386	0.05462720
0.573	13.61894743	7.18833957	4.75590466	1.61448477	0.05705130
0.574	13.61127919	7.18163918	4.74211727	1.62458797	0.05975273
0.575	13.60983383	7.17830288	4.73163394	1.63423969	0.06244614
0.576	13.61209884	7.17687829	4.72492403	1.64196169	0.06508986
0.577	13.61521513	7.17585924	4.72167580	1.64671238	0.06769337
0.578	13.61633387	7.17390520	4.72090825	1.64797102	0.07025765
0.579	13.61303731	7.16992742	4.72119978	1.64586266	0.07275428
0.580	13.60379643	7.16319073	4.72106249	1.64114106	0.07512363
0.581	13.58815938	7.15325517	4.71929564	1.63506760	0.07729002
0.582	13.56669501	7.13996640	4.71519336	1.62913446	0.07918470
0.583	13.54077520	7.12338409	4.70869100	1.62475184	0.08076818
0.584	13.51218177	7.10377947	4.70023217	1.62297466	0.08204712
0.585	13.48261288	7.08155892	4.69056233	1.62428976	0.08307805
0.586	13.45337674	7.05733964	4.68041708	1.62855071	0.08396202
0.587	13.42504918	7.03184822	4.67024407	1.63503103	0.08482885
0.588	13.39754786	7.00595123	4.66004940	1.64264286	0.08581480
0.589	13.37020948	6.98050178	4.64938514	1.65020019	0.08704121

0.590	13.34213723	6.95629166	4.63748321	1.65669894	0.08859479
0.591	13.31257241	6.93386177	4.62359750	1.66154904	0.09051377
0.592	13.28117530	6.91342820	4.60726238	1.66467340	0.09278497
0.593	13.24820705	6.89479275	4.58857418	1.66649267	0.09534892
0.594	13.21519890	6.87737249	4.56828757	1.66775935	0.09880943
0.595	13.18326523	6.86034544	4.54776783	1.66934983	0.10285792
0.596	13.15348241	6.84283588	4.52873626	1.67200380	0.10698297
0.597	13.12708464	6.82416571	4.51290499	1.67611395	0.11099041
0.598	13.10496624	6.80411516	4.50161554	1.68162588	0.11470743
0.599	13.08756709	6.78305915	4.49553026	1.68805472	0.11802305
0.600	13.07488006	6.76202217	4.49449211	1.69457357	0.12089228
0.601	13.06652183	6.74255358	4.49753499	1.70021209	0.12332165
0.602	13.06185030	6.72642448	4.50310457	1.70407677	0.12534838
0.603	13.06010127	6.71529249	4.50936965	1.70552858	0.12702262
0.604	13.06037189	6.71026160	4.51455078	1.70429335	0.12839160
0.605	13.06168704	6.71157729	4.51725897	1.70049462	0.12949928
0.606	13.06289571	6.71846452	4.51661775	1.69459544	0.13038123
0.607	13.06263178	6.72913782	4.51232119	1.68728526	0.13107066
0.608	13.05930403	6.74103947	4.50453437	1.67932519	0.13160549
0.609	13.05126896	6.75129418	4.49371800	1.67143439	0.13203531
0.610	13.03700909	6.75718896	4.48042542	1.66418680	0.13242693
0.611	13.01543961	6.75665984	4.46515844	1.65797340	0.13286607
0.612	12.98621528	6.74864858	4.44831131	1.65301426	0.13345183
0.613	12.94998681	6.73329331	4.43020817	1.64939144	0.13429144
0.614	12.90834219	6.71180327	4.41115730	1.64708050	0.13548140



0.615	12.86378549	6.68621309	4.39162002	1.64601244	0.13710044
0.616	12.81927004	6.65891847	4.37223281	1.64606909	0.13918923
0.617	12.77778729	6.63219531	4.35387235	1.64709224	0.14174612
0.618	12.74187569	6.60778287	4.33753586	1.64887482	0.14478121
0.619	12.71385642	6.58665864	4.32422897	1.65114260	0.14890730
0.620	12.69361278	6.56904978	4.31476830	1.65357673	0.15328353
0.621	12.67996599	6.55386947	4.30958060	1.65584745	0.15772138
0.622	12.67119641	6.53990496	4.30862545	1.65764944	0.16206012
0.623	12.66527838	6.52581516	4.31158496	1.65876429	0.16615237
0.624	12.66163069	6.51051108	4.31920483	1.65908797	0.16986469
0.625	12.65641578	6.49342828	4.32791471	1.65903244	0.17308329
0.626	12.64984692	6.47464795	4.33602614	1.66050414	0.17572312
0.627	12.63865351	6.45487617	4.34236714	1.66075067	0.17773219
0.628	12.62358662	6.43524166	4.34613555	1.66020745	0.17910002
0.629	12.60588431	6.41702234	4.34696925	1.65916218	0.17986094
0.630	12.58697896	6.40135831	4.34491753	1.65777609	0.18009594
0.631	12.56818703	6.38900786	4.34039957	1.65606282	0.17992859
0.632	12.55045381	6.38017538	4.33410301	1.65391945	0.17951261
0.633	12.53426106	6.37449780	4.32682923	1.65122006	0.17901410
0.634	12.51957991	6.37110267	4.31934171	1.64787951	0.17859417
0.635	12.50600661	6.36880559	4.31226286	1.64391609	0.17838857
0.636	12.49287082	6.36632238	4.30594874	1.63948542	0.17849549
0.637	12.47949391	6.36250573	4.30050708	1.63489706	0.17896331
0.638	12.46528394	6.35655329	4.29575636	1.63054303	0.17979051
0.639	12.44986843	6.34810460	4.29131308	1.62684469	0.18092754

0.640	12.43313085	6.33727860	4.28665489	1.62417702	0.18228896
0.641	12.41523248	6.32461838	4.28126021	1.62279220	0.18376658
0.642	12.39652563	6.31091732	4.27469278	1.62280200	0.18524937
0.643	12.37748319	6.29704928	4.26670291	1.62415742	0.18664108
0.644	12.35863010	6.28377185	4.25730523	1.62668233	0.18787573
0.645	12.34041773	6.27153114	4.24676172	1.63015295	0.18892461
0.646	12.32321363	6.26037748	4.23558700	1.63430332	0.18985864
0.647	12.30859084	6.24997452	4.22441281	1.63891405	0.19217507
0.648	12.29464898	6.23963367	4.21394760	1.64380153	0.19413583
0.649	12.28104641	6.22850535	4.20478155	1.64882477	0.19579738
0.650	12.26744835	6.21579156	4.19734261	1.65384426	0.19733183
0.651	12.25349491	6.20093230	4.19180383	1.65869204	0.19893208
0.652	12.23889006	6.18380066	4.18806618	1.66313985	0.20075504
0.653	12.22349094	6.16476170	4.18580508	1.66691240	0.20289253
0.654	12.20732298	6.14463949	4.18452448	1.66968721	0.20536479
0.655	12.19068610	6.12463148	4.18366071	1.67116951	0.20813364
0.656	12.17398360	6.10601412	4.18264129	1.67114171	0.21111611
0.657	12.15771045	6.08995671	4.18099181	1.66951874	0.21419677
0.658	12.14223404	6.07723553	4.17832960	1.66640115	0.21724718
0.659	12.12776113	6.06812605	4.17442188	1.66207345	0.22014421
0.660	12.11414820	6.06228638	4.16912903	1.65696664	0.22279175
0.661	12.10098650	6.05885365	4.16242709	1.65160975	0.22513590
0.662	12.08766015	6.05661182	4.15438133	1.64653677	0.22717529
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0.664	12.05774635	6.05033489	4.13492100	1.63895538	0.23056179

0.665	12.04014068	6.04409654	4.12403734	1.63692220	0.23209114
0.666	12.02052510	6.03493607	4.11285601	1.63607864	0.23363760
0.667	11.99909538	6.02277019	4.10177082	1.63624672	0.23526872
0.668	11.97624657	6.00788724	4.09114683	1.63714443	0.23701201
0.669	11.95248820	5.99084109	4.08126674	1.63846536	0.23885043
0.670	11.92827643	5.97228543	4.07226709	1.63993366	0.24072780
0.671	11.90395700	5.95286996	4.06411693	1.64136100	0.24256042
0.672	11.87969589	5.93314570	4.05659762	1.64266924	0.24425949
0.673	11.85558455	5.91357835	4.04936111	1.64390682	0.24574902
0.674	11.83168800	5.89455288	4.04199529	1.64520621	0.24698650
0.675	11.80820426	5.87644167	4.03412261	1.64676824	0.24797169
0.676	11.78548484	5.85963658	4.02545631	1.64878907	0.24875236
0.677	11.76407500	5.84456747	4.01588649	1.65140415	0.24941586
0.678	11.74565303	5.83166360	4.00549971	1.65462933	0.25110662
0.679	11.73073502	5.82126615	3.99454526	1.65832159	0.25389151
0.680	11.71832536	5.81354749	3.98339171	1.66216496	0.25654842
0.681	11.70821493	5.80839157	3.97246515	1.66569296	0.25902348
0.682	11.70099355	5.80539481	3.96218739	1.66942936	0.26136346
0.683	11.69484819	5.80383575	3.95292585	1.67187989	0.26360324
0.684	11.68815402	5.80278172	3.94492803	1.67210262	0.26574496
0.685	11.67970991	5.80121978	3.93838748	1.66974904	0.26775565
0.686	11.66858956	5.79819278	3.93336161	1.66485049	0.26957833
0.687	11.65431564	5.79297730	3.92981832	1.65775170	0.27114795
0.688	11.63692218	5.78513097	3.92764414	1.64909621	0.27241267
0.689	11.61692905	5.77458741	3.92660644	1.63972661	0.27335136

0.690	11.59521222	5.76159521	3.92638936	1.63057092	0.27398190
0.691	11.57279958	5.74664570	3.92658776	1.62251808	0.27436016
0.692	11.55067466	5.73035734	3.92675236	1.61629687	0.27457427
0.693	11.52964145	5.71339294	3.92644279	1.61238800	0.27472762
0.694	11.51018765	5.69632333	3.92529490	1.61097215	0.27492196
0.695	11.49250896	5.67960905	3.92305738	1.61195180	0.27524169
0.696	11.47661577	5.66359014	3.91966643	1.61500577	0.27574163
0.697	11.46251590	5.64846102	3.91535404	1.61968942	0.27644576
0.698	11.45070327	5.63434459	3.91096982	1.62552682	0.27734846
0.699	11.44050129	5.62129670	3.90621561	1.63210027	0.27842943
0.700	11.43140269	5.60932790	3.90093182	1.63907047	0.27966520

### Fortran code of the analytical PES

```

!-----
      module para
      implicit none

      integer,parameter :: NL=3,NAmax=20,Ndim=3

      double precision :: Weit(20,20,3),B(20,3)

      double precision :: Emax,Emin,Rmin(3),Rmax(3)

      integer :: NA(3)

      !----- <init Network beg> -----

      !Weights

      DATA Weit(1,1,1) / 0.198504083299D+01/

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DATA Weit(2,1,1) / -0.210400597083D+01/  
DATA Weit(3,1,1) / 0.108378865973D+00/  
DATA Weit(4,1,1) / -0.116784674135D+01/  
DATA Weit(5,1,1) / -0.186738597314D+01/  
DATA Weit(6,1,1) / 0.127238088895D+01/  
DATA Weit(7,1,1) / 0.383125374157D+01/  
DATA Weit(8,1,1) / 0.354474302513D+00/  
DATA Weit(9,1,1) / 0.539473146258D+00/  
DATA Weit(10,1,1) / -0.302215294661D+00/  
DATA Weit(11,1,1) / 0.219572372888D-01/  
DATA Weit(12,1,1) / 0.820506676505D+00/  
DATA Weit(13,1,1) / -0.226499109109D+01/  
DATA Weit(14,1,1) / -0.219959100762D+01/  
DATA Weit(15,1,1) / 0.211814986083D+01/  
DATA Weit(16,1,1) / -0.934644394238D+00/  
DATA Weit(17,1,1) / -0.731403070152D+01/  
DATA Weit(18,1,1) / 0.110845367294D+01/  
DATA Weit(19,1,1) / 0.418743276523D+01/  
DATA Weit(20,1,1) / -0.138460023730D+01/  
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DATA Weit(7,2,1) / -0.119242459750D+01/  
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DATA Weit(17,16,3) / 0.000000000000D+00/  
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DATA Weit(19,16,3) / 0.000000000000D+00/  
DATA Weit(20,16,3) / 0.000000000000D+00/  
DATA Weit(1,17,3) / 0.109990266728D+00/  
DATA Weit(2,17,3) / 0.000000000000D+00/  
DATA Weit(3,17,3) / 0.000000000000D+00/  
DATA Weit(4,17,3) / 0.000000000000D+00/  
DATA Weit(5,17,3) / 0.000000000000D+00/  
DATA Weit(6,17,3) / 0.000000000000D+00/

DATA Weit(7,17,3) / 0.000000000000D+00/  
DATA Weit(8,17,3) / 0.000000000000D+00/  
DATA Weit(9,17,3) / 0.000000000000D+00/  
DATA Weit(10,17,3) / 0.000000000000D+00/  
DATA Weit(11,17,3) / 0.000000000000D+00/  
DATA Weit(12,17,3) / 0.000000000000D+00/  
DATA Weit(13,17,3) / 0.000000000000D+00/  
DATA Weit(14,17,3) / 0.000000000000D+00/  
DATA Weit(15,17,3) / 0.000000000000D+00/  
DATA Weit(16,17,3) / 0.000000000000D+00/  
DATA Weit(17,17,3) / 0.000000000000D+00/  
DATA Weit(18,17,3) / 0.000000000000D+00/  
DATA Weit(19,17,3) / 0.000000000000D+00/  
DATA Weit(20,17,3) / 0.000000000000D+00/  
DATA Weit(1,18,3) / 0.453818794088D+00/  
DATA Weit(2,18,3) / 0.000000000000D+00/  
DATA Weit(3,18,3) / 0.000000000000D+00/  
DATA Weit(4,18,3) / 0.000000000000D+00/  
DATA Weit(5,18,3) / 0.000000000000D+00/  
DATA Weit(6,18,3) / 0.000000000000D+00/  
DATA Weit(7,18,3) / 0.000000000000D+00/  
DATA Weit(8,18,3) / 0.000000000000D+00/  
DATA Weit(9,18,3) / 0.000000000000D+00/  
DATA Weit(10,18,3) / 0.000000000000D+00/  
DATA Weit(11,18,3) / 0.000000000000D+00/

DATA Weit(12,18,3) / 0.000000000000D+00/  
DATA Weit(13,18,3) / 0.000000000000D+00/  
DATA Weit(14,18,3) / 0.000000000000D+00/  
DATA Weit(15,18,3) / 0.000000000000D+00/  
DATA Weit(16,18,3) / 0.000000000000D+00/  
DATA Weit(17,18,3) / 0.000000000000D+00/  
DATA Weit(18,18,3) / 0.000000000000D+00/  
DATA Weit(19,18,3) / 0.000000000000D+00/  
DATA Weit(20,18,3) / 0.000000000000D+00/  
DATA Weit(1,19,3) / -0.171240668725D+01/  
DATA Weit(2,19,3) / 0.000000000000D+00/  
DATA Weit(3,19,3) / 0.000000000000D+00/  
DATA Weit(4,19,3) / 0.000000000000D+00/  
DATA Weit(5,19,3) / 0.000000000000D+00/  
DATA Weit(6,19,3) / 0.000000000000D+00/  
DATA Weit(7,19,3) / 0.000000000000D+00/  
DATA Weit(8,19,3) / 0.000000000000D+00/  
DATA Weit(9,19,3) / 0.000000000000D+00/  
DATA Weit(10,19,3) / 0.000000000000D+00/  
DATA Weit(11,19,3) / 0.000000000000D+00/  
DATA Weit(12,19,3) / 0.000000000000D+00/  
DATA Weit(13,19,3) / 0.000000000000D+00/  
DATA Weit(14,19,3) / 0.000000000000D+00/  
DATA Weit(15,19,3) / 0.000000000000D+00/  
DATA Weit(16,19,3) / 0.000000000000D+00/

DATA Weit(17,19,3) / 0.000000000000D+00/  
DATA Weit(18,19,3) / 0.000000000000D+00/  
DATA Weit(19,19,3) / 0.000000000000D+00/  
DATA Weit(20,19,3) / 0.000000000000D+00/  
DATA Weit(1,20,3) / 0.695926470002D+01/  
DATA Weit(2,20,3) / 0.000000000000D+00/  
DATA Weit(3,20,3) / 0.000000000000D+00/  
DATA Weit(4,20,3) / 0.000000000000D+00/  
DATA Weit(5,20,3) / 0.000000000000D+00/  
DATA Weit(6,20,3) / 0.000000000000D+00/  
DATA Weit(7,20,3) / 0.000000000000D+00/  
DATA Weit(8,20,3) / 0.000000000000D+00/  
DATA Weit(9,20,3) / 0.000000000000D+00/  
DATA Weit(10,20,3) / 0.000000000000D+00/  
DATA Weit(11,20,3) / 0.000000000000D+00/  
DATA Weit(12,20,3) / 0.000000000000D+00/  
DATA Weit(13,20,3) / 0.000000000000D+00/  
DATA Weit(14,20,3) / 0.000000000000D+00/  
DATA Weit(15,20,3) / 0.000000000000D+00/  
DATA Weit(16,20,3) / 0.000000000000D+00/  
DATA Weit(17,20,3) / 0.000000000000D+00/  
DATA Weit(18,20,3) / 0.000000000000D+00/  
DATA Weit(19,20,3) / 0.000000000000D+00/  
DATA Weit(20,20,3) / 0.000000000000D+00/

!Bias

DATA B(1,1) / -0.678881866854D+00/

DATA B(2,1) / -0.842120035075D+00/

DATA B(3,1) / 0.543005822679D+01/

DATA B(4,1) / -0.252350222139D+01/

DATA B(5,1) / -0.639978624972D+01/

DATA B(6,1) / -0.551214118113D+01/

DATA B(7,1) / -0.435184067451D+01/

DATA B(8,1) / -0.112889847070D+01/

DATA B(9,1) / -0.754329758734D+00/

DATA B(10,1) / 0.156936276533D+00/

DATA B(11,1) / -0.477260470878D+00/

DATA B(12,1) / -0.276532245392D+01/

DATA B(13,1) / 0.149454941373D+00/

DATA B(14,1) / -0.253295086502D+01/

DATA B(15,1) / 0.116846781476D+01/

DATA B(16,1) / -0.284176924338D+01/

DATA B(17,1) / -0.533918719513D+01/

DATA B(18,1) / 0.195764562334D+01/

DATA B(19,1) / 0.252538972436D+01/

DATA B(20,1) / -0.109058126182D+01/

DATA B(1,2) / 0.120256508778D+01/

DATA B(2,2) / 0.683881956269D+01/

DATA B(3,2) / 0.695392650023D+00/

DATA B(4,2) / 0.111142843003D+01/

DATA B(5,2) / -0.133409396350D+01/  
DATA B(6,2) / -0.372647204922D+00/  
DATA B(7,2) / 0.193291431403D+01/  
DATA B(8,2) / -0.332607191548D+01/  
DATA B(9,2) / 0.116422285177D+02/  
DATA B(10,2) / 0.141699863472D+01/  
DATA B(11,2) / -0.205051650087D+00/  
DATA B(12,2) / -0.323588617263D+01/  
DATA B(13,2) / 0.114283201724D+01/  
DATA B(14,2) / -0.267246391695D+00/  
DATA B(15,2) / 0.194498008489D+01/  
DATA B(16,2) / 0.670816353728D+00/  
DATA B(17,2) / -0.591233864571D+00/  
DATA B(18,2) / 0.222427824801D+00/  
DATA B(19,2) / 0.705062683524D+00/  
DATA B(20,2) / 0.258933232336D+00/  
DATA B(1,3) / 0.937432064599D+00/  
DATA B(2,3) / 0.000000000000D+00/  
DATA B(3,3) / 0.000000000000D+00/  
DATA B(4,3) / 0.000000000000D+00/  
DATA B(5,3) / 0.000000000000D+00/  
DATA B(6,3) / 0.000000000000D+00/  
DATA B(7,3) / 0.000000000000D+00/  
DATA B(8,3) / 0.000000000000D+00/  
DATA B(9,3) / 0.000000000000D+00/

DATA B(10,3) / 0.000000000000D+00/  
DATA B(11,3) / 0.000000000000D+00/  
DATA B(12,3) / 0.000000000000D+00/  
DATA B(13,3) / 0.000000000000D+00/  
DATA B(14,3) / 0.000000000000D+00/  
DATA B(15,3) / 0.000000000000D+00/  
DATA B(16,3) / 0.000000000000D+00/  
DATA B(17,3) / 0.000000000000D+00/  
DATA B(18,3) / 0.000000000000D+00/  
DATA B(19,3) / 0.000000000000D+00/  
DATA B(20,3) / 0.000000000000D+00/

!Number of nodes

DATA NA(1) / 20/  
DATA NA(2) / 20/  
DATA NA(3) / 1/

!Normalize parameter

DATA Emin /-0.205636567030D+00/  
DATA Emax /0.407803432970D+00/  
DATA Rmin(1) / 0.289864902665D-01/  
DATA Rmax(1) / 0.191285052986D+01/  
DATA Rmin(2) / 0.724647511360D-01/  
DATA Rmax(2) / 0.145881936068D+01/  
DATA Rmin(3) / 0.126028218550D-02/

DATA Rmax(3) / 0.530452762651D+00/

!----- <init Network end> -----

end module para

!-----

subroutine pes\_oh2\_3bond(r,v,n)

use para

implicit none

integer,intent(in) :: n

double precision,intent(in) :: r(Ndim,n)

double precision,intent(out) :: v(n)

double precision :: r\_tmp(Ndim,n)

integer i

if(Ndim.ne.3) stop 'Ndim.ne.3'

r\_tmp(1,:)=1.0d0/r(1,:)

r\_tmp(2,:)=1.0d0/r(2,:)+1.0d0/r(3,:)

r\_tmp(3,:)=1.0d0/(r(2,:)\*r(3,:))

call pes\_oh2(r\_tmp,v,n)

do i=1,n

    if(r(1,i).lt.0.9d0.or.r(2,i).lt.1.5d0.or.r(3,i).lt.1.5d0) v(i)=1.0d0

enddo

return

end subroutine pes\_oh2\_3bond

!-----



```

subroutine pes_oh2(r,v,n)

use para

implicit none

integer,intent(in) :: n

double precision,intent(in) :: r(Ndim,n)

double precision,intent(out) :: v(n)

double precision Rnormalize(Ndim,n)

integer i

v=0.0

do i=1,Ndim

    Rnormalize(i,:)=2.0D0*(r(I,:)-Rmin(I))/(Rmax(I)-Rmin(I))-1.0D0

enddo

CALL Y_A(NAmax,NA,NL,Weit,B,Rnormalize,Ndim,N,V)

v=(v+1.0d0)*0.5d0*(Emax-Emin)+Emin

return

end subroutine pes_oh2

```

!-----

```

SUBROUTINE Y_A(NAmax,NA,NL,W,B,Xin,NROWin,Np,Eout)

IMPLICIT REAL*8(A-H,O-Z)

DIMENSION NA(NL),W(NAmax,NAmax,NL),B(NAmax,NL),Xin(NROWin,Np)

DIMENSION A(NAmax,Np,NL),Y(NAmax,Np,NL),Eout(Np)

ALPHA=1.0D0;BETA=0.0D0

CALL DGEMM('N','N',NA(1),Np,NROWin,ALPHA,W,

$  NAmax,Xin,NROWin,BETA,Y,NAmax)

DO I2=1,Np

```

```

      Y(1:NA(1),I2,1)=Y(1:NA(1),I2,1)+B(1:NA(1),1)
ENDDO

DO I2=1,Np

DO I1=1,NA(1)

      A(I1,I2,1)=DTANH(Y(I1,I2,1))

ENDDO;ENDDO

DO I3=2,NL

      CALL DGEMM('N','N',NA(I3),Np,NA(I3-1),ALPHA,W(1,1,I3),
$      NAmax,A(1,1,I3-1),NAmax,BETA,Y(1,1,I3),NAmax)

DO I2=1,Np

      Y(1:NA(I3),I2,I3)=Y(1:NA(I3),I2,I3)+B(1:NA(I3),I3)

DO I1=1,NA(I3)

      A(I1,I2,I3)=DTANH(Y(I1,I2,I3))

ENDDO

ENDDO

ENDDO

Eout=Y(1,1:Np,NL)

RETURN

END SUBROUTINE Y_A

```