Supplementary Information

For

PES and Transport Properties of He…HBr Complex from Kinetic Theory and Molecular Dynamics Simulations

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Table S1. Results of the optimization of HBr structure with different basis sets.

Basis-set	r(A)	μ(Debye)		Q (a.u.)	B (cm^{-1})
			Br	H	
***aug*-cc-pvDz**	1.4266	0.9981	-0.060163	0.060163	8.326655
***aug*-cc-pvTz**	1.4133	0.9503	-0.028062	0.028062	8.481527
***aug*-cc-pvQz**	1.4108	0.9451	-0.111888	0.111888	8.511774
***aug*-cc-pv5z**	1.4093	0.9431	-0.131755	0.131755	8.528347
experimental	1.4144	0.827			8.46488

[a] E: the energy; r: bond length; μ: dipole moment; Q: atomic charge; B: rotational constant.

Table S2. Calculated potential value (U) and distance (R) at minimum points (potential well) of the He-HBr complex at $\theta = 0°$ using CCSD(T) method and different basis sets.

Basic set[a]	E (cm^{-1})	R(A°)
***aug*-cc-pvDz**	-20.07	3.6
***aug*-cc-pvTz**	-28.48	3.5
***aug*-cc-pvQz**	-32.41	3.5
***aug*-cc-pv5z**	-34.10	3.4
***aug*-cc-pvDz-BF**	-35.41	3.4
***aug*-cc-pvTz-BF**	-35.57	3.4
***aug*-cc-pvQz-BF**	-35.67	3.4
***aug*-cc-pv5z-BF**	-35.74	3.4

[a] BF is the mid-bond basis functions of 3s, 3p, 2d, 1f, and 1g with exponents of 0.9, 0.3, and 0.1 for s and p, 0.6 and 0.2 for d, and 0.3 for f and g.

Table S3. Different contributions to the interaction second virial coefficient (B_{12}) of He…HBr complex at different temperatures. B(0) is the classical, and B(1) values are quantum corrections.

***T*(K)**	$B^{(0)}_{calss}$	$B^{(1)}_{r}$	$B^{(1)}_{a\mu}$	$B^{(1)}_{al}$	$B^{(1)}_{q,tot}$	B_{12}
50	-22.3153	0.9532	0.1350	1.0571	2.1453	-20.1700
60	-9.6081	0.6594	0.0834	0.6612	1.4039	-8.2042
70	-1.1966	0.4877	0.0565	0.4521	0.9963	-0.2003
80	4.7349	0.3771	0.0407	0.3286	0.7464	5.4813
90	9.1103	0.3008	0.0308	0.2496	0.5811	9.6914
100	12.4483	0.2455	0.0240	0.1960	0.4656	12.9139
110	15.0621	0.2041	0.0193	0.1580	0.3814	15.4434
120	17.1514	0.1721	0.0158	0.1301	0.3180	17.4694
130	18.8497	0.1468	0.0132	0.1090	0.2690	19.1187
140	20.2493	0.1265	0.0112	0.0926	0.2304	20.4797
150	21.4160	0.1100	0.0096	0.0797	0.1993	21.6154
160	22.3981	0.0964	0.0084	0.0693	0.1740	22.5721
170	23.2315	0.0850	0.0073	0.0608	0.1531	23.3846
180	23.9436	0.0754	0.0065	0.0538	0.1356	24.0793
190	24.5558	0.0672	0.0058	0.0479	0.1209	24.6767
200	25.0848	0.0602	0.0052	0.0430	0.1084	25.1931
300	27.7925	0.0244	0.0022	0.0183	0.0449	27.8374
400	28.5038	0.0124	0.0012	0.0101	0.0237	28.5275
500	28.5644	0.0072	0.0008	0.0064	0.0143	28.5788
600	28.3674	0.0046	0.0005	0.0044	0.0095	28.3769
700	28.0604	0.0031	0.0004	0.0032	0.0067	28.0670
800	27.7072	0.0022	0.0003	0.0025	0.0049	27.7121
900	27.3382	0.0016	0.0002	0.0019	0.0037	27.3419
1000	26.9683	0.0012	0.0002	0.0016	0.0029	26.9713
1200	26.2528	0.0007	0.0001	0.0011	0.0019	26.2548
1400	25.5856	0.0005	0.0001	0.0008	0.0014	25.5870
1600	24.9700	0.0003	0.0001	0.0006	0.0010	24.9710
1800	24.4029	0.0002	0.0001	0.0005	0.0008	24.4037
2000	23.8795	0.0002	0.0000	0.0004	0.0006	23.8801

Table S4. Calculated cross-sections, viscosity η_{12}, and the pair diffusion coefficients D_{12} as a function of temperature for He…HBr complex calculated using a5zBF basis set. All cross sections are in Å^2.

T (K)	$\mathfrak{S}^1_D$	$\mathfrak{S}^2_\eta$	$\mathfrak{S}_T$	$\mathfrak{S}_{DPR}$	$\mathfrak{S}_{prod}$	$\mathfrak{S}_{ROT}$	D_{12}(cm^2.s^{-1})	η_{12}(μPa.s)
50	4.9606	0.1623	173.2302	2882.9723	0.0406	12.0523	0.0255	3.5867
100	3.9970	0.1329	12.2429	472.8817	0.0328	9.3653	0.0896	6.1981
110	3.9062	0.1301	9.6967	366.8832	0.0317	9.0434	0.1058	6.6382
120	3.8286	0.1278	8.1371	290.9519	0.0308	8.7617	0.1230	7.0609
130	3.7611	0.1257	7.1309	235.1049	0.0300	8.5128	0.1411	7.4686
140	3.7014	0.1239	6.4509	193.0954	0.0292	8.2908	0.1603	7.8632
150	3.6480	0.1223	5.9719	160.8755	0.0285	8.0915	0.1804	8.2463
160	3.5998	0.1208	5.6215	135.7419	0.0279	7.9112	0.2014	8.6191
170	3.5559	0.1195	5.3565	115.8418	0.0273	7.7471	0.2232	8.9827
180	3.5155	0.1183	5.1498	99.8758	0.0268	7.5970	0.2460	9.3380
190	3.4783	0.1172	4.9842	86.9140	0.0263	7.4590	0.2697	9.6858
200	3.4437	0.1161	4.8484	76.2787	0.0259	7.3316	0.2942	10.0266
210	3.4114	0.1152	4.7346	67.4682	0.0255	7.2135	0.3195	10.3610
220	3.3811	0.1143	4.6375	60.1054	0.0251	7.1036	0.3456	10.6896
230	3.3526	0.1134	4.5533	53.9032	0.0247	7.0010	0.3726	11.0128
240	3.3256	0.1126	4.4793	48.6403	0.0244	6.9048	0.4004	11.3309
250	3.3001	0.1118	4.4135	44.1443	0.0240	6.8146	0.4290	11.6442
260	3.2759	0.1111	4.3543	40.2795	0.0237	6.7295	0.4583	11.9531
270	3.2529	0.1104	4.3006	36.9382	0.0234	6.6492	0.4885	12.2578
280	3.2308	0.1097	4.2516	34.0339	0.0232	6.5733	0.5194	12.5586
290	3.2098	0.1091	4.2064	31.4967	0.0229	6.5012	0.5510	12.8557
300	3.1896	0.1085	4.1646	29.2701	0.0227	6.4328	0.5834	13.1493
325	3.1426	0.1070	4.0722	24.7756	0.0221	6.2755	0.6677	13.8690
350	3.0997	0.1057	3.9930	21.4175	0.0216	6.1351	0.7565	14.5704
375	3.0604	0.1045	3.9238	18.8541	0.0211	6.0085	0.8498	15.2552
400	3.0240	0.1034	3.8626	16.8603	0.0207	5.8936	0.9475	15.9254
425	2.9902	0.1024	3.8076	15.2836	0.0203	5.7886	1.0494	16.5821
450	2.9586	0.1014	3.7579	14.0183	0.0199	5.6920	1.1556	17.2266
475	2.9289	0.1005	3.7126	12.9892	0.0196	5.6028	1.2659	17.8599
500	2.9010	0.0996	3.6709	12.1422	0.0193	5.5200	1.3803	18.4829
525	2.8746	0.0988	3.6324	11.4373	0.0190	5.4427	1.4987	19.0962
550	2.8495	0.0980	3.5967	10.8448	0.0188	5.3704	1.6212	19.7007
575	2.8258	0.0973	3.5634	10.3423	0.0185	5.3026	1.7475	20.2968
600	2.8031	0.0966	3.5323	9.9123	0.0183	5.2387	1.8778	20.8850
625	2.7815	0.0959	3.5031	9.5415	0.0181	5.1783	2.0119	21.4659
650	2.7608	0.0953	3.4756	9.2194	0.0178	5.1212	2.1498	22.0399
675	2.7410	0.0946	3.4496	8.9377	0.0177	5.0670	2.2914	22.6072
700	2.7219	0.0940	3.4250	8.6897	0.0175	5.0154	2.4368	23.1683
725	2.7037	0.0935	3.4016	8.4702	0.0173	4.9663	2.5859	23.7236
750	2.6860	0.0929	3.3794	8.2746	0.0171	4.9194	2.7386	24.2732
775	2.6691	0.0924	3.3581	8.0996	0.0170	4.8745	2.8950	24.8175
800	2.6527	0.0919	3.3378	7.9420	0.0168	4.8315	3.0549	25.3568
825	2.6369	0.0913	3.3184	7.7996	0.0166	4.7901	3.2185	25.8914
850	2.6215	0.0909	3.2997	7.6703	0.0165	4.7504	3.3855	26.4216
875	2.6067	0.0904	3.2816	7.5524	0.0164	4.7121	3.5561	26.9477
900	2.5923	0.0899	3.2642	7.4444	0.0162	4.6751	3.7302	27.4701
925	2.5783	0.0895	3.2473	7.3451	0.0161	4.6393	3.9078	27.9892
950	2.5647	0.0890	3.2309	7.2535	0.0160	4.6046	4.0889	28.5053
975	2.5515	0.0886	3.2149	7.1687	0.0158	4.5709	4.2734	29.0188
1000	2.5386	0.0882	3.1993	7.0900	0.0157	4.5380	4.4614	29.5302

Table S5. Calculated cross-sections, viscosity η_{12}, and the pair diffusion coefficients D_{12} as a function of temperature for He…HBr complex calculated using aQz basis set. All cross sections are in $Å^2$.

T (K)	$\mathfrak{S}^1_D$	$\mathfrak{S}^2_\eta$	$\mathfrak{S}_T$	$\mathfrak{S}_{DPR}$	$\mathfrak{S}_{prod}$	$\mathfrak{S}_{ROT}$	$D_{12}(cm^2.s^{-1})$	$\eta_{12}(\mu Pa.s)$
50	4.8275	0.1588	8.1413	10.4709	0.0374	10.8571	0.0262	3.6664
75	4.2718	0.1414	6.4511	9.3719	0.0335	9.5726	0.0545	5.0417
100	3.9793	0.1325	5.6318	8.8474	0.0307	8.7038	0.0900	6.2157
125	3.7891	0.1267	5.1467	8.5372	0.0286	8.0898	0.1321	7.2659
150	3.6503	0.1225	4.8226	8.3237	0.0270	7.6298	0.1802	8.2316
175	3.5416	0.1192	4.5883	8.1604	0.0258	7.2691	0.2341	9.1354
200	3.4524	0.1166	4.4093	8.0263	0.0247	6.9762	0.2934	9.9912
225	3.3769	0.1143	4.2668	7.9109	0.0239	6.7321	0.3579	10.8085
250	3.3115	0.1123	4.1499	7.8084	0.0231	6.5243	0.4275	11.5938
275	3.2537	0.1106	4.0516	7.7157	0.0224	6.3444	0.5020	12.3520
300	3.2020	0.1090	3.9673	7.6306	0.0218	6.1864	0.5812	13.0869
325	3.1552	0.1076	3.8940	7.5516	0.0213	6.0462	0.6651	13.8014
350	3.1124	0.1063	3.8293	7.4778	0.0209	5.9204	0.7535	14.4978
375	3.0731	0.1051	3.7716	7.4086	0.0204	5.8066	0.8463	15.1780
400	3.0366	0.1039	3.7196	7.3432	0.0200	5.7028	0.9435	15.8436
425	3.0026	0.1029	3.6725	7.2813	0.0197	5.6077	1.0451	16.4959
450	2.9707	0.1019	3.6295	7.2226	0.0193	5.5199	1.1508	17.1361
475	2.9407	0.1010	3.5900	7.1667	0.0190	5.4385	1.2608	17.7652
500	2.9124	0.1002	3.5535	7.1134	0.0187	5.3627	1.3748	18.3839
525	2.8856	0.0993	3.5198	7.0625	0.0184	5.2919	1.4930	18.9930
550	2.8600	0.0986	3.4884	7.0138	0.0182	5.2254	1.6152	19.5933
575	2.8357	0.0978	3.4592	6.9671	0.0179	5.1628	1.7414	20.1853
600	2.8124	0.0971	3.4320	6.9223	0.0177	5.1037	1.8716	20.7696
625	2.7900	0.0964	3.4066	6.8793	0.0175	5.0478	2.0057	21.3467
650	2.7685	0.0958	3.3829	6.8379	0.0172	4.9948	2.1438	21.9170
675	2.7478	0.0952	3.3608	6.7982	0.0170	4.9444	2.2857	22.4810
700	2.7278	0.0946	3.3403	6.7600	0.0168	4.8964	2.4316	23.0391
725	2.7085	0.0940	3.3211	6.7232	0.0167	4.8507	2.5813	23.5917
750	2.6897	0.0934	3.3033	6.6878	0.0165	4.8070	2.7349	24.1392
775	2.6716	0.0929	3.2869	6.6537	0.0163	4.7653	2.8923	24.6820
800	2.6539	0.0923	3.2717	6.6208	0.0162	4.7253	3.0536	25.2205
825	2.6367	0.0918	3.2577	6.5892	0.0160	4.6869	3.2187	25.7550
850	2.6199	0.0913	3.2448	6.5588	0.0159	4.6501	3.3877	26.2858
875	2.6035	0.0908	3.2330	6.5295	0.0158	4.6148	3.5605	26.8135
900	2.5875	0.0904	3.2222	6.5012	0.0157	4.5807	3.7371	27.3384
925	2.5718	0.0899	3.2124	6.4741	0.0156	4.5479	3.9177	27.8609
950	2.5565	0.0894	3.2034	6.4480	0.0155	4.5161	4.1020	28.3814
975	2.5414	0.0890	3.1952	6.4229	0.0154	4.4854	4.2903	28.9005
1000	2.5266	0.0885	3.1877	6.3987	0.0153	4.4557	4.4824	29.4185

Table S6. D_{12} values calculated from classical kinetic theory using the Mason-Monchick approximation.

T(K)	D_{12}(cm^2.s^{-1})	T(K)	D_{12}(cm^2.s^{-1})	T(K)	D_{12}(cm^2.s^{-1})	T(K)	D_{12}(cm^2.s^{-1})
50	0.0234	290	0.5351	530	1.4797	770	2.7615
55	0.0281	295	0.5509	535	1.5032	775	2.7913
60	0.0332	300	0.5668	540	1.5268	780	2.8213
65	0.0386	305	0.5829	545	1.5506	785	2.8514
70	0.0443	310	0.5992	550	1.5745	790	2.8816
75	0.0503	315	0.6156	555	1.5986	795	2.9120
80	0.0566	320	0.6322	560	1.6228	800	2.9424
85	0.0632	325	0.6490	565	1.6472	805	2.9730
90	0.0701	330	0.6660	570	1.6717	810	3.0037
95	0.0773	335	0.6832	575	1.6963	815	3.0345
100	0.0847	340	0.7005	580	1.7211	820	3.0654
105	0.0924	345	0.7180	585	1.7460	825	3.0965
110	0.1004	350	0.7357	590	1.7711	830	3.1277
115	0.1086	355	0.7535	595	1.7963	835	3.1590
120	0.1171	360	0.7716	600	1.8216	840	3.1904
125	0.1258	365	0.7897	605	1.8471	845	3.2219
130	0.1348	370	0.8081	610	1.8727	850	3.2535
135	0.1440	375	0.8266	615	1.8984	855	3.2853
140	0.1535	380	0.8453	620	1.9243	860	3.3171
145	0.1631	385	0.8642	625	1.9503	865	3.3491
150	0.1730	390	0.8832	630	1.9765	870	3.3812
155	0.1832	395	0.9024	635	2.0027	875	3.4134
160	0.1935	400	0.9217	640	2.0292	880	3.4457
165	0.2041	405	0.9412	645	2.0557	885	3.4781
170	0.2149	410	0.9609	650	2.0824	890	3.5107
175	0.2259	415	0.9807	655	2.1092	895	3.5433
180	0.2371	420	1.0007	660	2.1362	900	3.5761
185	0.2486	425	1.0208	665	2.1632	905	3.6090
190	0.2602	430	1.0412	670	2.1905	910	3.6420
195	0.2721	435	1.0616	675	2.2178	915	3.6751
200	0.2841	440	1.0823	680	2.2453	920	3.7083
205	0.2964	445	1.1030	685	2.2729	925	3.7416
210	0.3089	450	1.1240	690	2.3006	930	3.7751
215	0.3216	455	1.1451	695	2.3285	935	3.8086
220	0.3345	460	1.1663	700	2.3565	940	3.8423
225	0.3475	465	1.1877	705	2.3846	945	3.8760
230	0.3608	470	1.2093	710	2.4128	950	3.9099
235	0.3743	475	1.2310	715	2.4412	955	3.9439
240	0.3880	480	1.2529	720	2.4697	960	3.9780
245	0.4018	485	1.2749	725	2.4983	965	4.0122
250	0.4159	490	1.2970	730	2.5270	970	4.0465
255	0.4301	495	1.3193	735	2.5559	975	4.0809
260	0.4446	500	1.3418	740	2.5849	980	4.1154
265	0.4592	505	1.3644	745	2.6140	985	4.1501
270	0.4740	510	1.3872	750	2.6433	990	4.1848
275	0.4890	515	1.4101	755	2.6726	995	4.2196
280	0.5042	520	1.4332	760	2.7021	1000	4.2546
285	0.5196	525	1.4564	765	2.7317		

Table S7. η_{12} values calculated from classical kinetic theory using the Mason-Monchick approximation.

T(K)	η_{12}(μPa.s)	T(K)	η_{12}(μPa.s)	T(K)	η_{12}(μPa.s)	T(K)	η_{12}(μPa.s)
50	3.2813	290	12.7244	530	19.1748	770	24.7964
55	3.5855	295	12.8731	535	19.2985	775	24.9075
60	3.8806	300	13.0209	540	19.4218	780	25.0184
65	4.1665	305	13.1678	545	19.5448	785	25.1292
70	4.4436	310	13.3139	550	19.6675	790	25.2397
75	4.7124	315	13.4593	555	19.7899	795	25.3500
80	4.9735	320	13.6039	560	19.9120	800	25.4600
85	5.2273	325	13.7477	565	20.0338	805	25.5699
90	5.4743	330	13.8908	570	20.1553	810	25.6796
95	5.7151	335	14.0332	575	20.2764	815	25.7890
100	5.9500	340	14.1750	580	20.3973	820	25.8983
105	6.1795	345	14.3160	585	20.5179	825	26.0073
110	6.4040	350	14.4564	590	20.6382	830	26.1161
115	6.6238	355	14.5962	595	20.7582	835	26.2248
120	6.8392	360	14.7353	600	20.8779	840	26.3332
125	7.0505	365	14.8739	605	20.9974	845	26.4414
130	7.2579	370	15.0118	610	21.1166	850	26.5494
135	7.4618	375	15.1492	615	21.2354	855	26.6573
140	7.6623	380	15.2860	620	21.3541	860	26.7649
145	7.8597	385	15.4222	625	21.4724	865	26.8723
150	8.0541	390	15.5579	630	21.5905	870	26.9795
155	8.2456	395	15.6931	635	21.7083	875	27.0865
160	8.4345	400	15.8277	640	21.8259	880	27.1934
165	8.6209	405	15.9619	645	21.9432	885	27.3000
170	8.8048	410	16.0955	650	22.0602	890	27.4064
175	8.9866	415	16.2287	655	22.1770	895	27.5127
180	9.1661	420	16.3613	660	22.2935	900	27.6187
185	9.3436	425	16.4935	665	22.4098	905	27.7246
190	9.5192	430	16.6253	670	22.5258	910	27.8303
195	9.6929	435	16.7566	675	22.6416	915	27.9357
200	9.8648	440	16.8874	680	22.7571	920	28.0410
205	10.0350	445	17.0178	685	22.8724	925	28.1461
210	10.2036	450	17.1478	690	22.9874	930	28.2510
215	10.3707	455	17.2774	695	23.1022	935	28.3557
220	10.5362	460	17.4065	700	23.2168	940	28.4603
225	10.7003	465	17.5353	705	23.3311	945	28.5646
230	10.8630	470	17.6636	710	23.4452	950	28.6688
235	11.0244	475	17.7916	715	23.5590	955	28.7728
240	11.1845	480	17.9192	720	23.6726	960	28.8766
245	11.3434	485	18.0463	725	23.7860	965	28.9802
250	11.5011	490	18.1732	730	23.8992	970	29.0836
255	11.6577	495	18.2996	735	24.0121	975	29.1868
260	11.8131	500	18.4257	740	24.1248	980	29.2899
265	11.9675	505	18.5514	745	24.2373	985	29.3928
270	12.1208	510	18.6768	750	24.3496	990	29.4955
275	12.2731	515	18.8018	755	24.4616	995	29.5980
280	12.4245	520	18.9264	760	24.5734	1000	29.7004
285	12.5749	525	19.0508	765	24.6850		

Table S8. Comparison of the ab-initio PES computed at CCSDT/a5zBF level of theory with with LJ(12,6) and Vashishta force fields.

θ	AAD%		SD%	
	Vashishta	LJ (12-6)	Vashishta	LJ (12-6)
0	2.1783	29.415	14.759	54.236
40	0.8299	26.178	9.1099	51.165
90	0.59071	52.938	7.6858	72.758
130	1.1951	57.749	10.932	75.992
180	4.3629	23.005	20.888	47.963

Table S9. Comparison of the viscosity coefficients obtained from MM, CC, LJ (12,6) and Vashishta methods for He-HBr complex at some temperatures.

T	***CC-a5zBF***	***CC-aQz***	***MM***	***LJ***	***Vashishta***
100	6.1967	6.2157	5.9500	-	-
200	10.0265	9.9912	9.8648	9.9431	10.0076
300	13.1493	13.0869	13.0209	13.1180	13.1443
400	15.9254	15.8436	15.8277	16.0250	15.9302
500	18.4829	18.3839	18.4257	18.4050	18.2441
600	20.8850	20.7696	20.8779	21.1620	21.0049
700	23.1683	23.0391	23.2168	22.9890	23.1662
800	25.3568	25.2205	25.4600	25.0240	25.4214
900	27.4701	27.3384	27.6187	27.3150	27.3765
1000	29.5302	29.4185	29.7004	29.7740	29.6524

Table S10. Comparison of the diffusion coefficients obtained from MM, CC, LJ(12,6) and Vashishta methods for He-HBr complex at some temperatures.

T	***CC-a5zBF***	***CC-aQz***	***MM***	***LJ***	***Vashishta***
100	0.089514	0.090001	0.084738	0.120740	0.115394
200	0.294131	0.293410	0.284146	0.307230	0.265632
300	0.583432	0.581188	0.566783	0.675410	0.675552
400	0.947456	0.943539	0.921698	1.112300	0.782145
500	1.380273	1.374846	1.341810	1.356100	1.370313
600	1.877764	1.871579	1.821597	2.375600	2.054817
700	2.436812	2.431562	2.356450	2.953400	2.287700
800	3.054944	3.053579	2.942427	4.011100	3.278650
900	3.730226	3.737142	3.576119	6.000900	3.663817
1000	4.461364	4.482411	4.254566	6.617900	5.676470

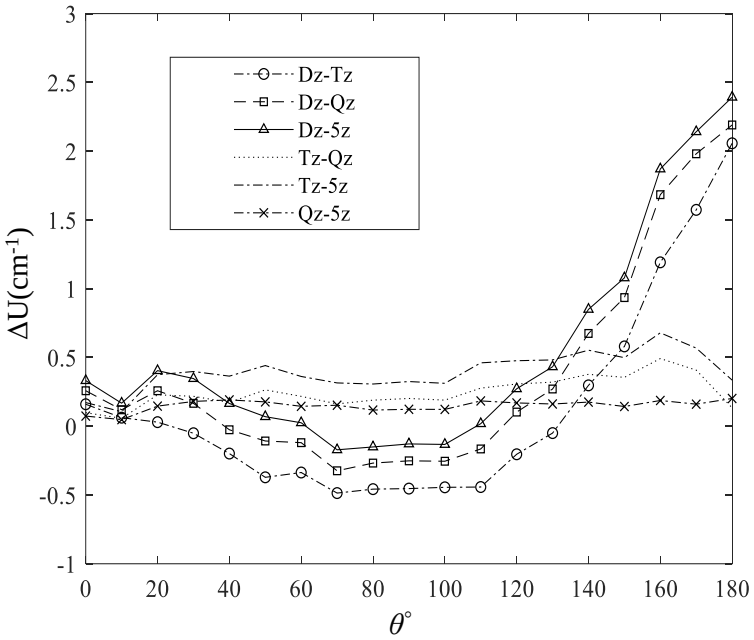

Fig. S1. The difference between the potential well-depth of the He…HBr PES calculated using aXzBF (X = D, T, Q, and 5) basis sets and RCCSD(T) methods. Note that, Qz-5z represents the difference between the well-depth of the potentials calculated at aQzBF and a5zBF.

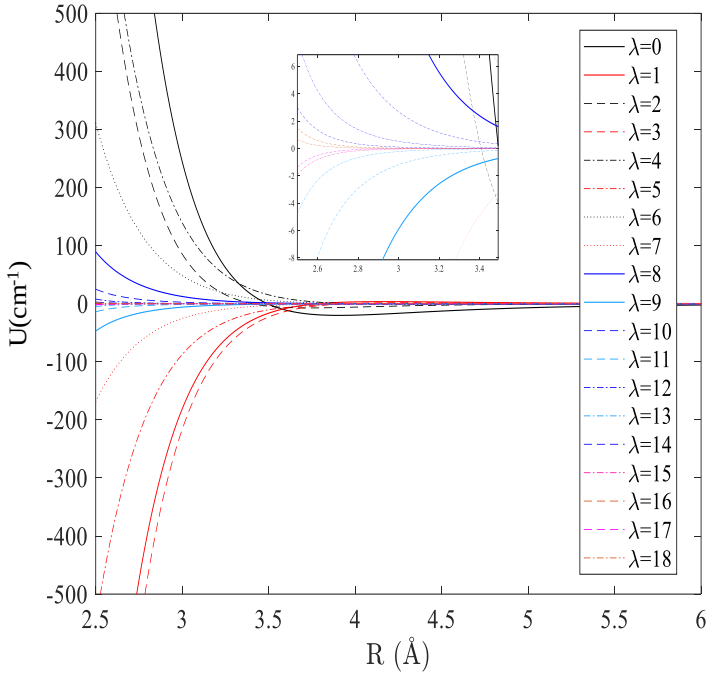

Fig. S2. Fitted expansion coefficients of the PES V_λ (R) for λ = 0-18.

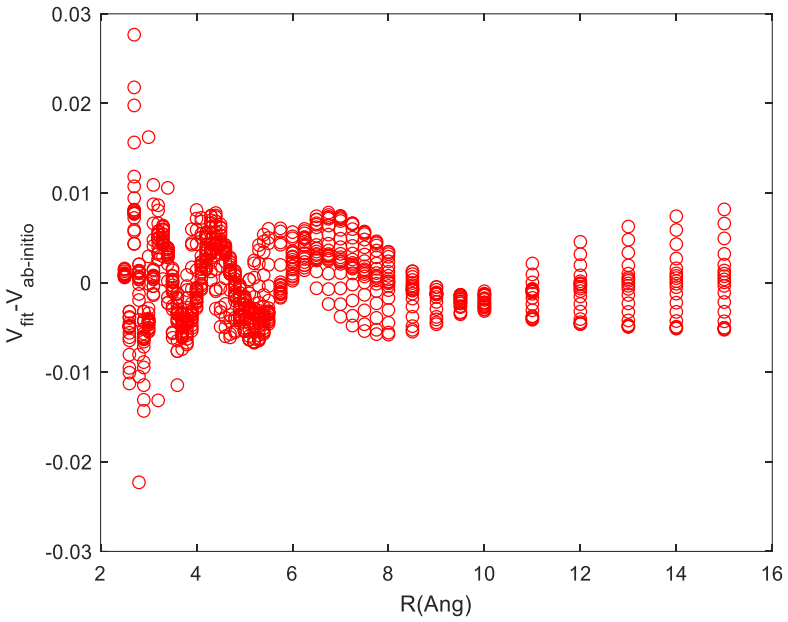

Fig. S3. Deviation of the ab-initio potentials and fitted values for He…HBr PES.

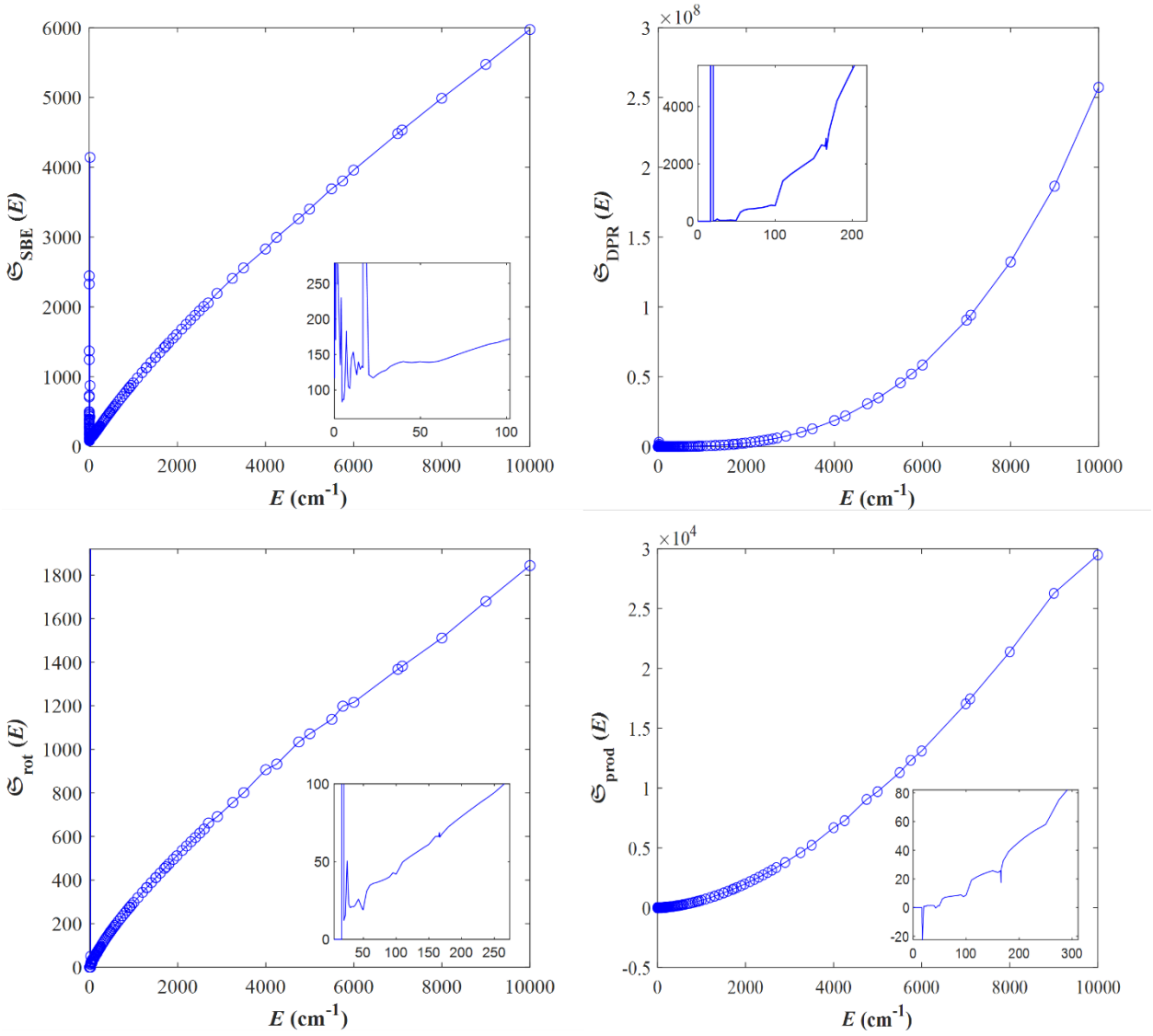

Fig. S4. Different SBE cross sections as function of energy.

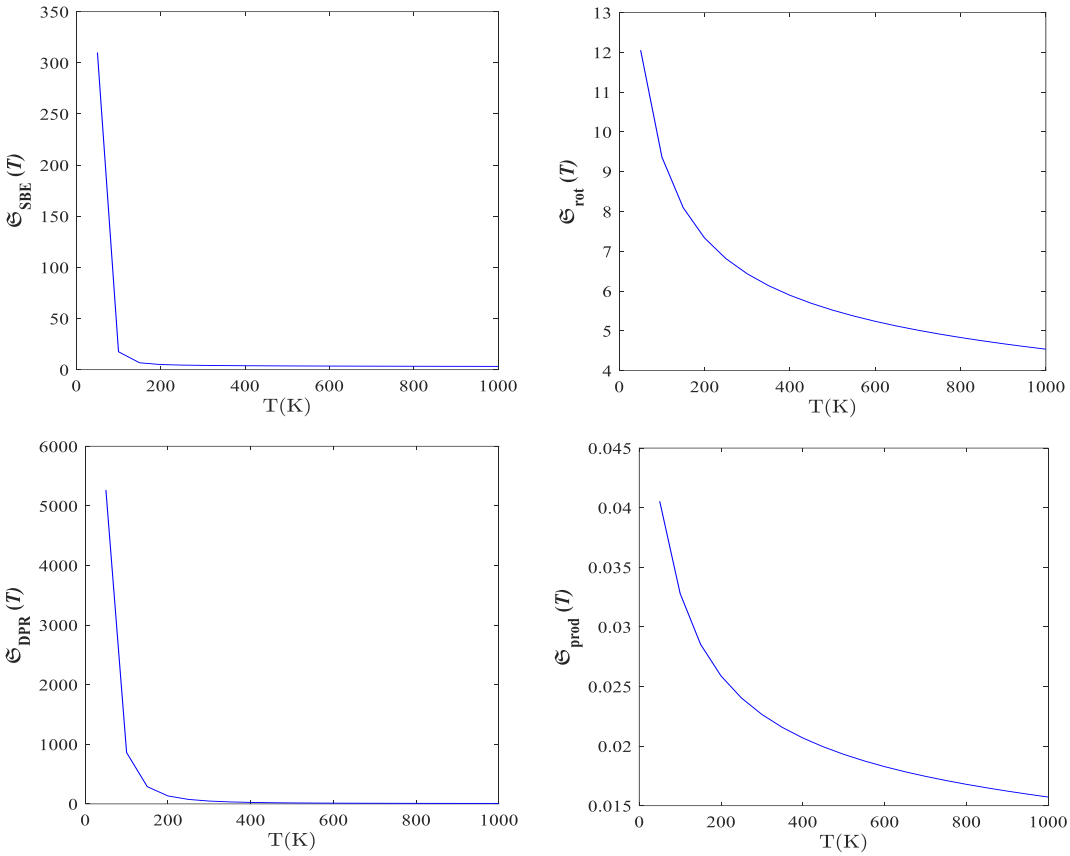

Fig. S5. Different SBE cross sections as function of temperature.

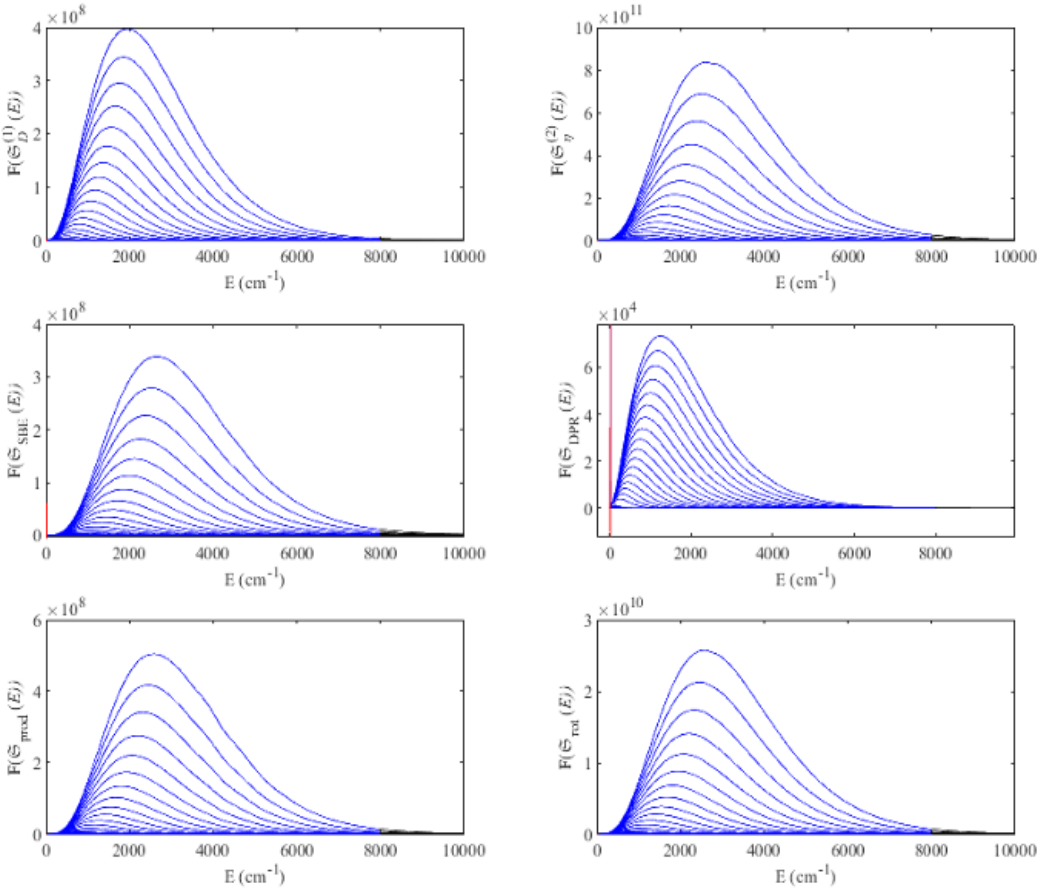

Fig. S6. The integration function of temperature dependent cross sections at different temperatures as function of energy. The height of the peaks increases with increasing temperature from 50 K and the highest peak belongs to the temperature of 1000 K.

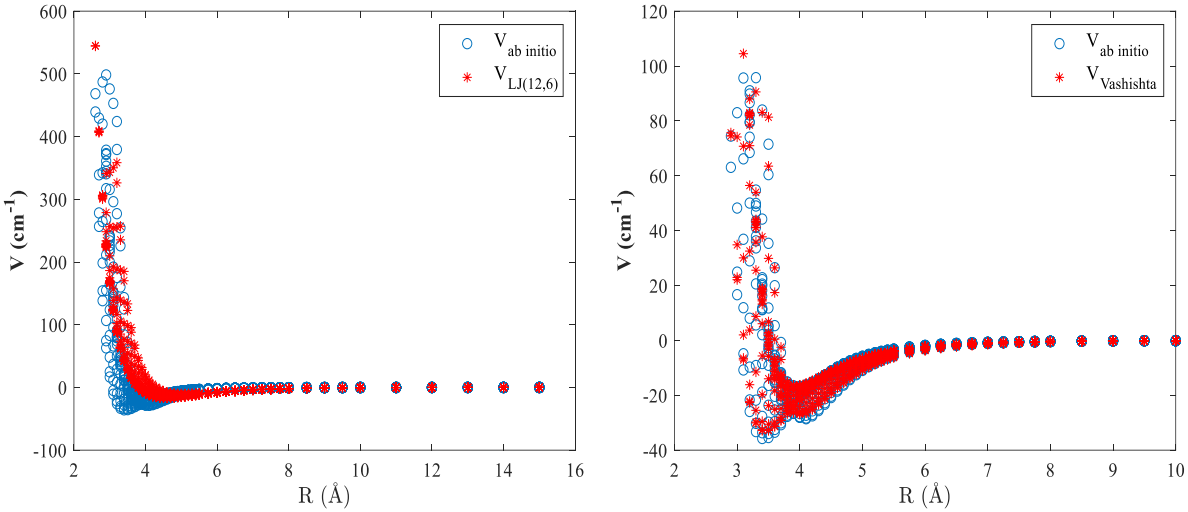

Fig. S7. Comparison of the ab-initio potentials with LJ(12,6) and Vashishta potential models.

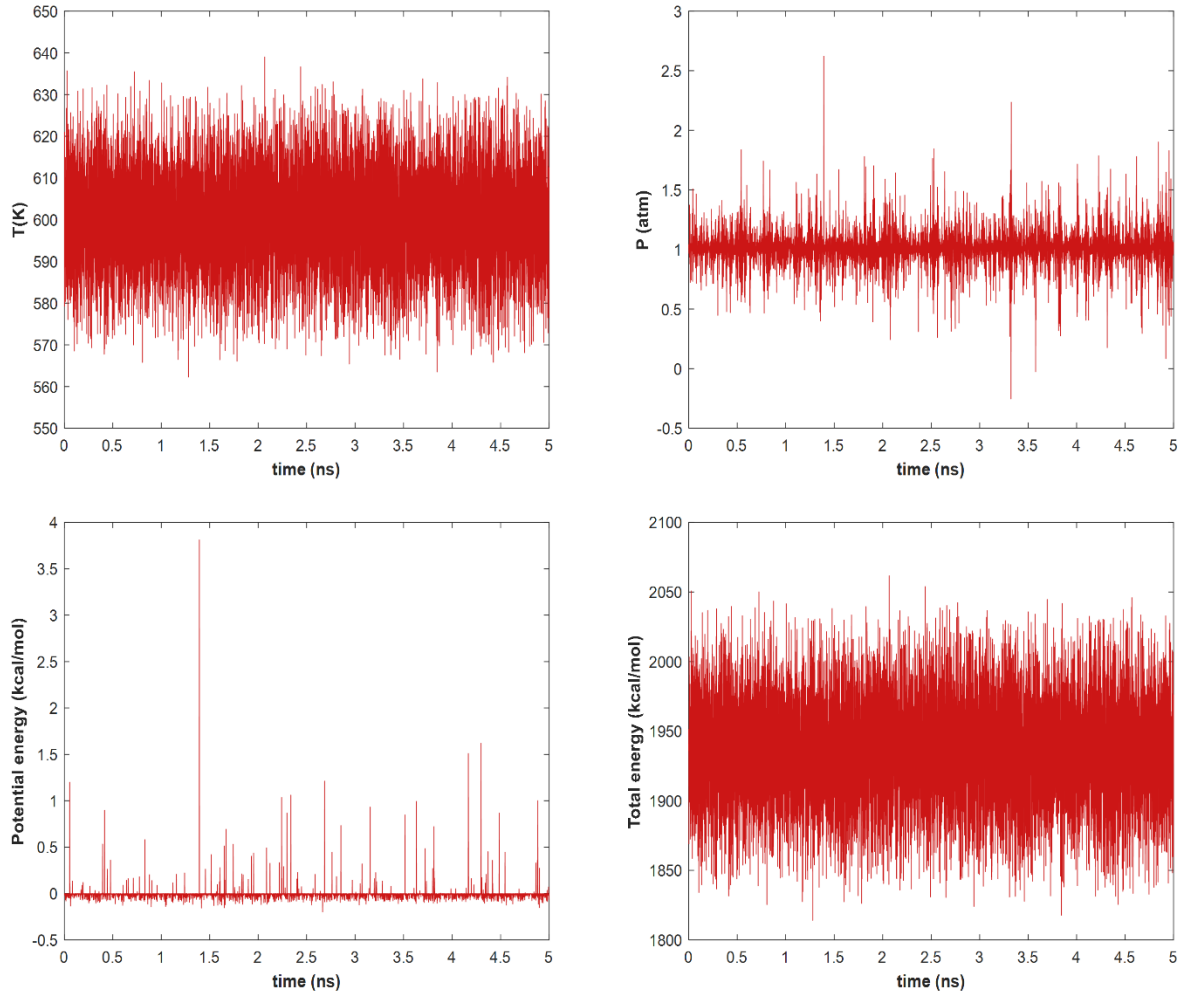

Fig. S8. Calculated thermodynamical parameters (temperature, pressure, potential energy, total energy) as a function of simulation time using LJ(12,6) potential at T = 600 K.

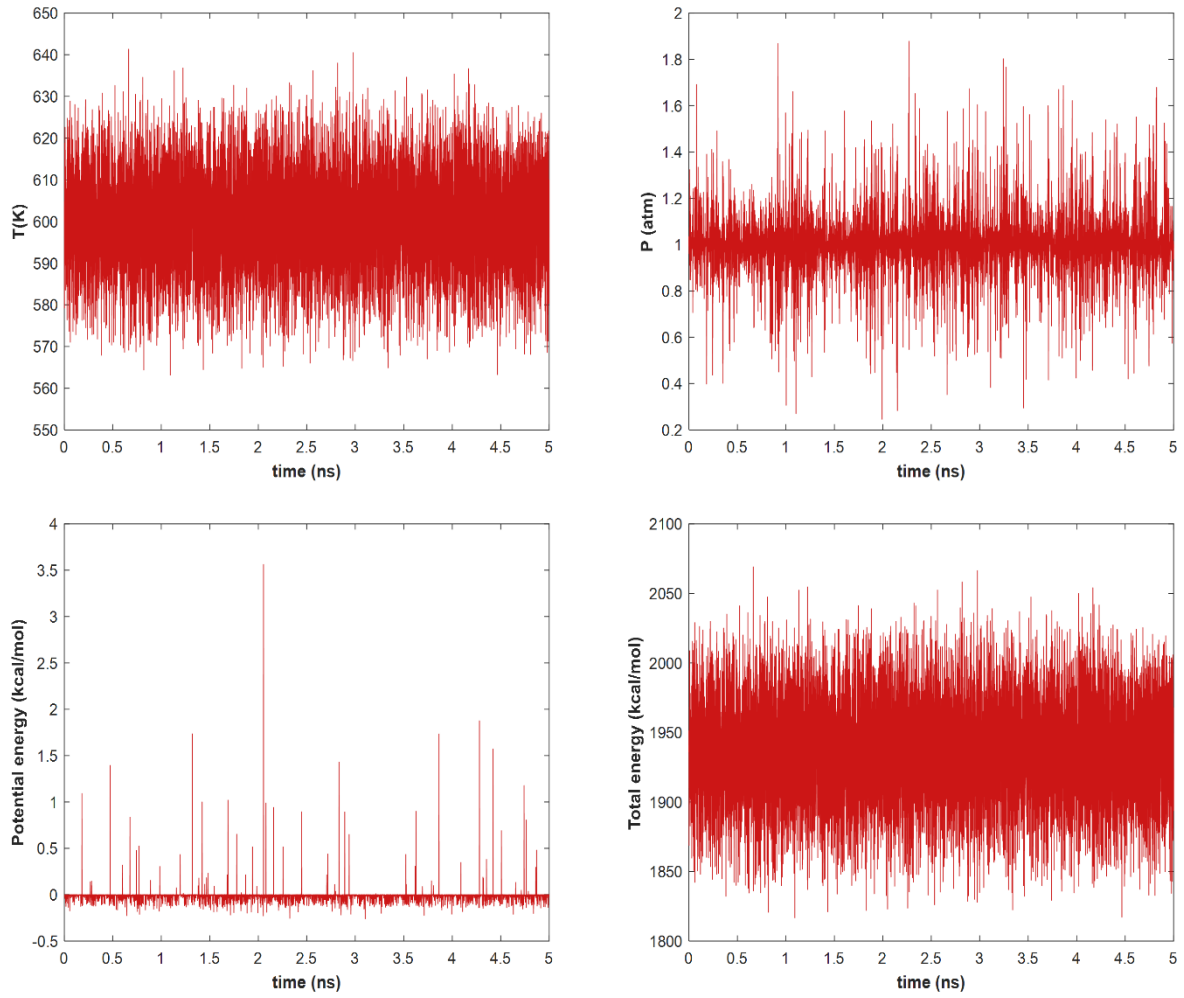

Fig. S9. Calculated thermodynamical parameters (temperature, pressure, potential energy, total energy) as a function of simulation time using Vashishta potential at T = 600 K.

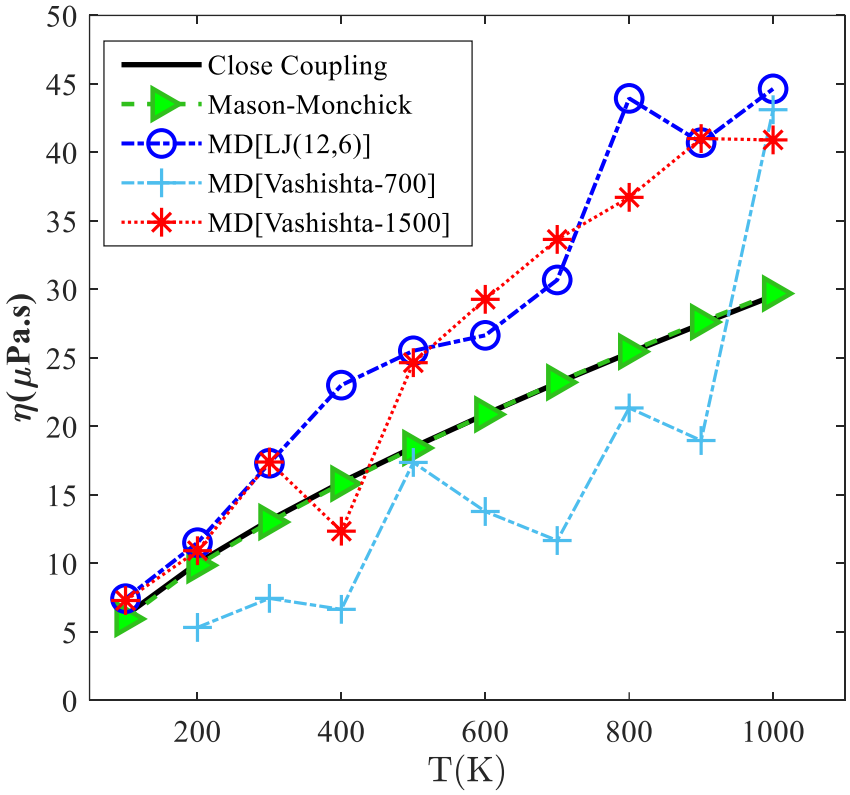

Fig. S10. calculated viscosity coefficient from different methods for He…HBr complex. Vashishta-700 and Vashishta-1500 represents MD simulation with time correlation length (τ) of 700 and 1500 fs.