

Supporting information for

Activation of a bromoalkyl ATRP initiator by a variety of inorganic salts: experiments and computations.

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Table S1. Monitoring of the MMA polymerization initiated by EBrPA in the presence of various activators. S2

Figure S1. Monitoring of the initiator and monomer disappearance in the bulk MMA polymerization (70°C, MMA:initiator:Lil = 100:1:1). (a) Polymerization initiated by CPI in the presence Lil, monitored by ¹H NMR. (b) Polymerization initiated by EBrPA in the presence of Lil, monitored by HPLC. S3

Figure S2. NMR spectra recorded during the reaction between EBrPA and Lil in an acetone-*d*₃/toluene 30:70 mixture: (a) EBrPA before addition of Lil; (b) with Lil (1 equiv) after heating at 70°C for 10 min; (c) same as (b), after 20 min. S3

Figure S3. Gibbs energy changes for the process described in Scheme 2, equation 4. S4

Table S2. Summary of the calculated energies for all systems. S5

Table S3. Cartesian coordinates (Å) and views of all optimized geometries. S7

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Figure S4. Correlation between the Br spin density and ΔG_3 for the salt·Br[•] adducts. (a) Li salts. (b) Na salts. (c) K salts. S23

Evaluation of the activation free energy for the MMA propagation at 90°C. S24

Table S5. Eyring analysis of the MMA propagation rate constants. S25

Table S1. Monitoring of the MMA polymerization initiated by EBrPA in the presence of various activators.^a

Additive	Time/h	Conv/%	$10^{-3} M_n(\text{th})$	$M_{n,\text{GPC}}$ (Kg/mol)	$\bar{D}$
KBr	10.5	7.3	1.7	65.7	2.23
	17.5	8.1	1.9	146.8	2.16
	21.5	10.2	2.3	437.8	1.92
	36.0	23.4	4.9	980.6	1.82
Na ₂ CO ₃	4.0	6.8	1.6	355.4	2.79
	5.0	8.3	1.9	401.2	2.39
	18.0	54.5	11.2	663.8	1.65
Cs ₂ SO ₄	10.5	3.7	1.0	97.6	2.78
	12.0	12.6	3.4	127.6	3.90
	13.5	16.8	3.6	505.1	2.11
	17.5	46.9	9.6	912.7	1.72

^aConditions: [MMA]₀/[EBrPA]₀/[Additive]₀ = 200:1:2, T = 90°C.

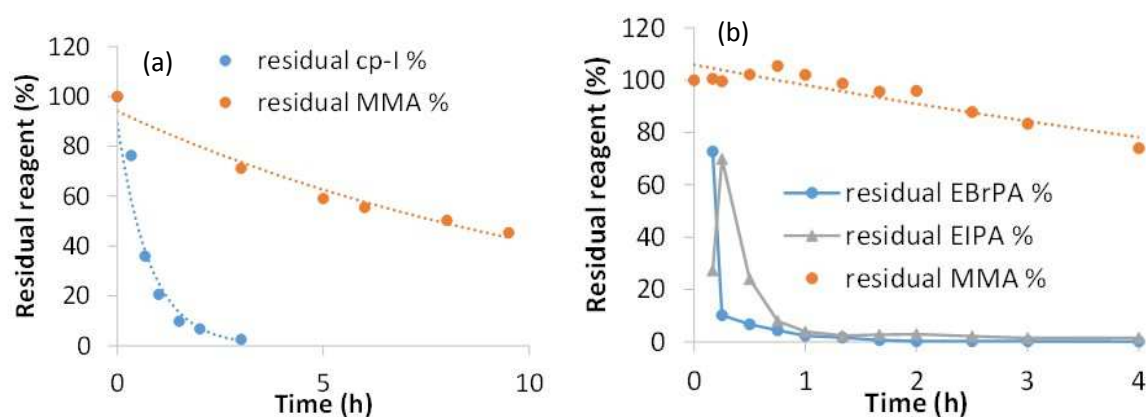


Figure S1. Monitoring of the initiator and monomer disappearance in the bulk MMA polymerization (70°C, MMA:initiator:Lil = 100:1:1). (a) Polymerization initiated by CPI in the presence Lil, monitored by ^1H NMR. (b) Polymerization initiated by EBrPA in the presence of Lil, monitored by HPLC.

In the experiment shown in Figure S1b, the solution was initially stirred at room temperature and then warmed to 70°C after the first sample withdrawal at $t = 15$ min, when ca. 27% of EBrPA had already been converted to EIPA.

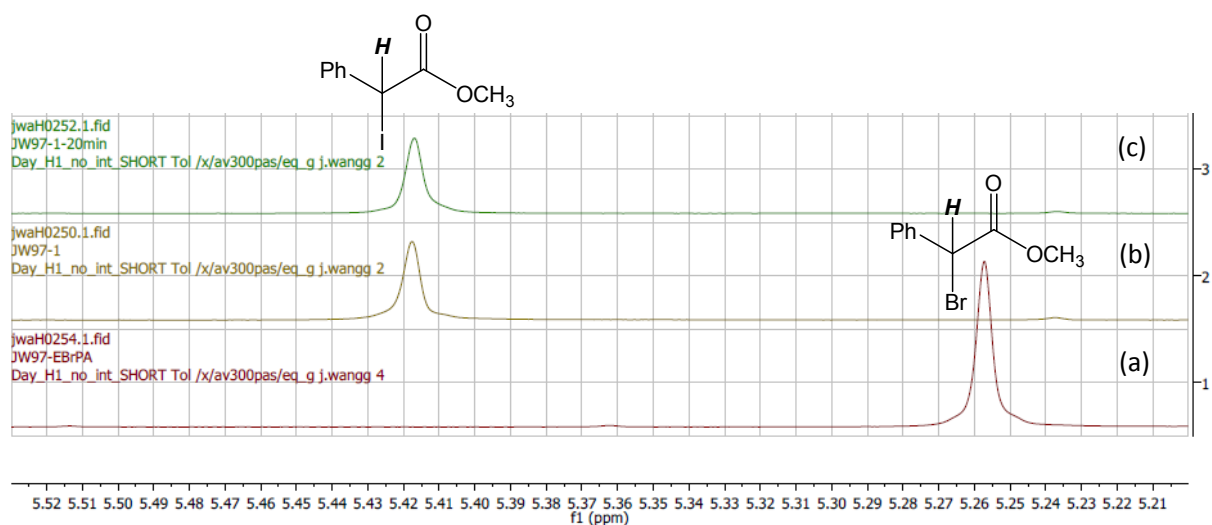


Figure S2. NMR spectra recorded during the reaction between EBrPA and Lil in an acetone- d_3 /toluene 30:70 mixture: (a) EBrPA before addition of Lil; (b) with Lil (1 equiv) after heating at 70°C for 10 min; (c) same as (b), after 20 min.

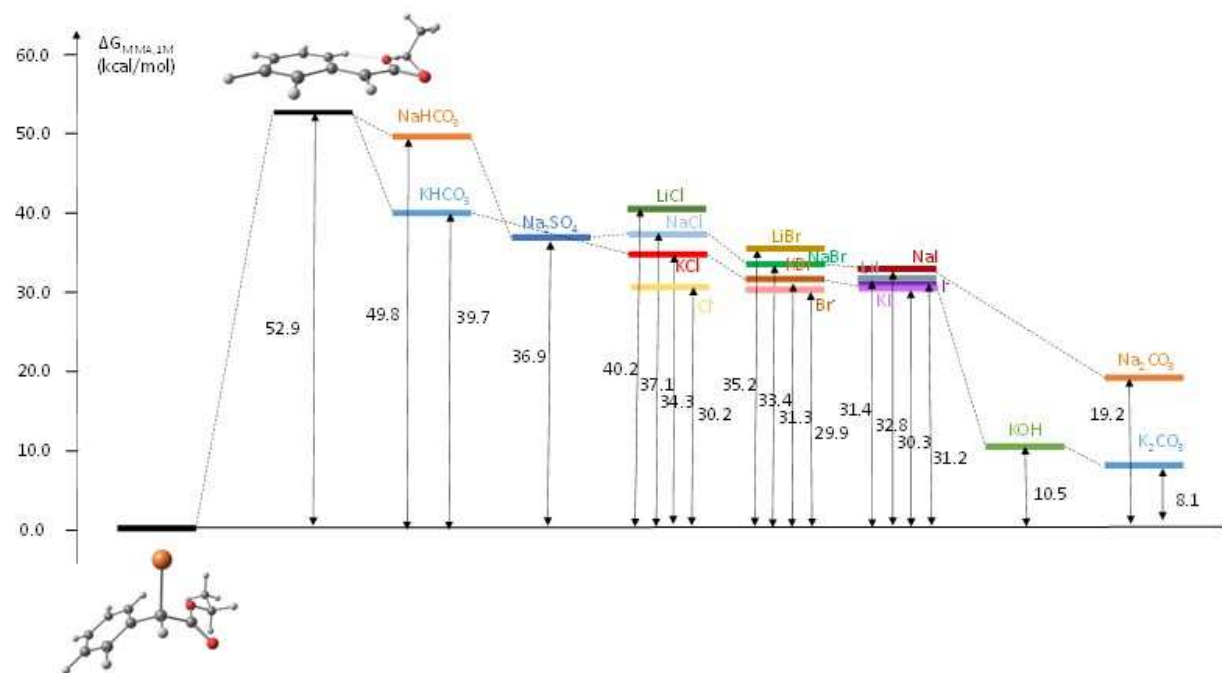


Figure S3. Gibbs energy changes for the process described in Scheme 3, equation 4.

Table S2. Summary of the calculated energies for all systems.

Name	E _{gas} (hartrees)	Thermal (G) correction	E _{solv} (hartrees)	Solv. corr. (kcal/mol)	G _{solv,1M} (hartrees)
1. Reference systems					
PhCH ⁺ COOEt	-538.1384125	0.149067	-538.1454247	-4.40	-537.993250
Br ⁺	-13.13404912	-0.01683	-13.13807409	-2.53	-13.151797
EBrPA	-551.3510607	0.148042	-551.380438	-18.43	-551.229288
EIPA	-549.567547	0.146859	-549.5768351	-5.83	-549.426869
H-MMA ⁺	-346.3861394	0.097631	-346.3809811	3.24	-346.280243
H-MMA-Br	-359.6099685	0.101494	-359.6392533	-18.38	-359.534652
H-MMA-I	-357.8242967	0.100351	-357.8569459	-20.49	-357.753487
H-MMA-MMA ⁺	-692.2314007	0.216028	-692.2239242	4.69	-692.004789
H-MMA-MMA-Br	-705.4423711	0.219840	-705.4682453	-16.24	-705.245298
H-MMA-MMA-I	-703.6562151	0.218858	-703.6863225	-18.89	-703.464357
2. Salts					
Cl ⁻	-460.2487316	-0.015023	-460.3449153	-60.36	-460.356831
LiCl	-467.7929762	-0.019296	-467.8242700	-19.64	-467.840459
NaCl	-622.557275	-0.021603	-622.5873225	-18.85	-622.605818
KCl	-1060.166793	-0.022822	-1060.198603	-19.96	-1060.218318
Br ⁻	-13.26245058	-0.016176	-13.33873317	-47.87	-13.351802
LiBr	-20.77618594	-0.020793	-20.80505342	-18.11	-20.822739
LiBr ₃	-47.13681996	-0.031349	-47.16363675	-16.83	-47.191878
LiBrI ₂	-43.59127951	-0.033437	-43.61513494	-14.97	-43.645464
NaBr	-175.5451109	-0.023039	-175.5723521	-17.09	-175.592284
KBr	-613.157425	-0.024252	-613.1860089	-17.94	-613.207153
I ⁻	-11.488464	-0.016848	-11.56723011	-49.43	-11.580971
LiI	-18.98966267	-0.021765	-19.01836298	-18.01	-19.037020
LiI ₃	-41.80721503	-0.034438	-41.82843039	-13.31	-41.859761
NaI	-173.7614627	-0.023941	-173.7908679	-18.45	-173.811701
KI	-611.3740226	-0.025142	-611.404260	-18.97	-611.426294
Na ₂ CO ₃	-588.5000156	-0.013231	-588.5359972	-22.58	-588.546121
K ₂ CO ₃	-1463.695730	-0.016548	-1463.737926	-26.48	-1463.751366
NaHCO ₃	-426.7602256	0.000188	-426.7774071	-10.78	-426.774112
KHCO ₃	-864.3653831	-0.001528	-864.385185	-12.43	-864.383605
KOH	-675.7152181	-0.007675	-675.7410632	-16.22	-675.745631
Na ₂ SO ₄	-1023.751948	-0.015891	-1023.787019	-22.01	-1023.799802
3. Salt·Br⁺					
Cl ⁻ ·Br ⁺	-473.4479046	-0.024951	-473.5229149	-47.07	-473.544758
NaCl·Br ⁺	-480.966443	-0.026798	-480.9887129	-13.97	-481.012403
NaCl·Br ⁺	-635.732673	-0.02929	-635.7565323	-14.97	-635.782715
KCl·Br ⁺	-1073.345946	-0.030645	-1073.372113	-16.42	-1073.399651
Br ⁻ ·Br ⁺	-26.44847112	-0.025623	-26.51764683	-43.41	-26.540162
LiBr·Br ⁺	-33.95565137	-0.028247	-33.97758208	-13.76	-34.002722
NaBr·Br ⁺	-188.7240667	-0.030705	-188.7475188	-14.72	-188.775116
KBr·Br ⁺	-626.3385996	-0.032122	-626.3643196	-16.14	-626.393334
I ⁻ ·Br ⁺	-24.67556806	-0.027105	-24.74209099	-41.74	-24.766088
LiI·Br ⁺	-32.17732757	-0.029260	-32.19685583	-12.25	-32.223008

NaI·Br [•]	-186.9466224	-0.031638	-186.9669421	-12.75	-186.995473
KI·Br [•]	-624.5611566	-0.033048	-624.5840772	-14.38	-624.614018
Na ₂ CO ₃ ·Br [•]	-601.7122263	-0.023115	-601.7315728	-12.14	-601.751580
K ₂ CO ₃ ·Br [•]	-1476.931979	-0.025882	-1476.951697	-12.37	-1476.974472
NaHCO ₃ ·Br [•]	-439.9191538	-0.009659	-439.9241907	-3.16	-439.930742
KHCO ₃ ·Br [•]	-877.5299424	-0.009518	-877.5499828	-12.58	-877.556393
KOH·Br [•]	-688.9283498	-0.019293	-688.9487699	-12.81	-688.964955
Na ₂ SO ₄ ·Br [•]	-1036.942203	-0.021937	-1036.958212	-10.05	-1036.977041

4. Salt·EBrPA

EBrPA-Cl ⁻	-1011.635822	0.144644	-1011.711218	-47.31	-1011.563466
EBrPA-LiCl	-1019.195627	0.146297	-1019.222913	-17.12	-1019.073509
EBrPA-NaCl	-1173.950832	0.143348	-1173.979261	-17.84	-1173.832805
EBrPA-KCl	-1611.557731	0.142419	-1611.587662	-18.78	-1611.442135
EBrPA-Br ⁻	-564.6360917	0.143311	-564.704510	-42.93	-564.558091
EBrPA-LiBr	-572.1789014	0.144534	-572.2043364	-15.96	-572.056695
EBrPA-NaBr	-726.937809	0.141550	-726.9644937	-16.74	-726.819836
EBrPA-KBr	-1164.546517	0.14015	-1164.574628	-17.64	-1164.431371
EBrPA-I ⁻	-562.8592113	0.141825	-562.9333442	-46.52	-562.788412
EBrPA-LiI	-570.392609	0.143643	-570.4191421	-16.65	-570.272392
EBrPA-NaI	-725.1539249	0.139935	-725.1813286	-17.20	-725.038286
EBrPA-KI	-1162.762887	0.13936	-1162.793175	-19.01	-1162.650707
EBrPA-Na ₂ CO ₃	-1139.903045	0.157703	-1139.93778	-21.80	-1139.780077
EBrPA-K ₂ CO ₃	-2015.104207	0.15479	-2015.142552	-24.06	-2014.987762
EBrPA-NaHCO ₃	-978.1493437	0.168087	-978.1671334	-11.16	-977.9990464
EBrPA-KHCO ₃	-1415.755732	0.167045	-1415.776571	-13.08	-1415.609526
EBrPA-KOH	-1227.091614	0.151318	-1227.125454	-21.23	-1226.974136
EBrPA-Na ₂ SO ₄	-1575.155580	0.157595	-1575.188896	-20.91	-1575.031301

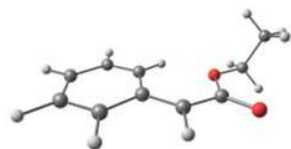
5. Salt·EPA[•]

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EPA [•] -NaCl	-1160.738811	0.143456	-1160.763944	-15.77	-1160.617381
EPA [•] -KCl	-1598.342600	0.142278	-1598.369791	-17.06	-1598.224405
EPA [•] -Br ⁻	-551.4100693	0.141834	-551.483060	-45.80	-551.338118
EPA [•] -LiBr	-33.95565137	-0.028247	-33.97758208	-13.76	-34.002722
EPA [•] -NaBr	-713.7267292	0.141899	-713.7495868	-14.34	-713.604580
EPA [•] -KBr	-1151.332461	0.140581	-1151.357427	-15.67	-1151.213738
EPA [•] -I ⁻	-549.6349965	0.141345	-549.7116907	-48.13	-549.567238
EPA [•] -LiI	-32.17732757	-0.029260	-32.19685583	-12.25	-32.223008
EPA [•] -NaI	-711.9429644	0.141313	-711.9664799	-14.76	-711.822059
EPA [•] -KI	-1149.54908	0.139723	-1149.576494	-17.20	-1149.433663
EPA [•] -Na ₂ CO ₃	-1126.691212	0.157574	-1126.724495	-20.88	-1126.563813
EPA [•] -K ₂ CO ₃	-2001.8902	0.15285	-2001.92626	-22.63	-2001.770302
EPA [•] -NaHCO ₃	-964.9392418	0.166938	-964.9556889	-10.32	-964.785643
EPA [•] -KHCO ₃	-1402.539908	0.16617	-1402.560026	-12.62	-1402.390748
EPA [•] -KOH	-1213.89621	0.154437	-1213.918196	-13.80	-1213.760651
EPA [•] -Na ₂ SO ₄	-1561.935405	0.155894	-1561.970643	-22.11	-1561.811642

Table S3. Cartesian coordinates (Å) and views of all optimized geometries.

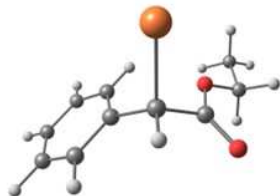
1. Reference systems

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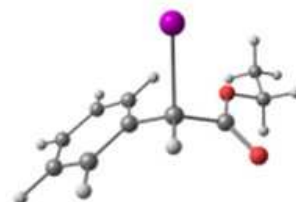
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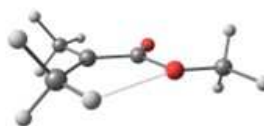
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EIPA



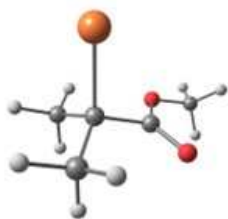
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6	-2.430960000	3.199472000	-1.197907000
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53	-0.860305000	-1.847006000	-0.348373000

H-MMA⁺



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6	-0.288578000	-0.349176000	-0.001525000
8	-0.625731000	-1.528701000	-0.001118000
8	-1.199185000	0.667532000	0.000309000
6	-2.568000000	0.245752000	0.001378000
1	-2.792182000	-0.352466000	-0.886896000
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H-MMA-Br



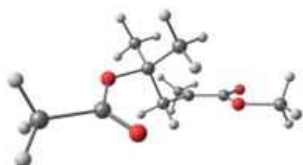
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H-MMA-I



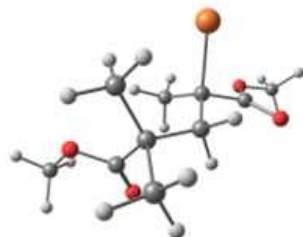
6	0.265899000	0.984008000	0.203809000
6	-0.034835000	2.198468000	-0.667054000
1	-0.973359000	2.666189000	-0.362668000
1	0.777185000	2.925283000	-0.541444000
1	-0.083116000	1.930635000	-1.722308000
6	0.349014000	1.328228000	1.690074000
1	-0.569254000	1.819685000	2.019476000
1	0.524976000	0.444886000	2.303051000
1	1.184805000	2.024221000	1.839521000
6	1.508202000	0.252778000	-0.309258000
8	2.009759000	0.448222000	-1.395049000
8	1.993710000	-0.616212000	0.596034000
6	3.134799000	-1.377860000	0.162429000
1	2.881654000	-1.971681000	-0.719901000
1	3.967854000	-0.714889000	-0.085139000
1	3.391175000	-2.024721000	1.000951000
53	-1.405059000	-0.491876000	-0.072064000

H-MMA-MMA*



6	1.402505000	0.908181000	-0.572310000
6	1.874814000	2.291559000	-0.878810000
1	1.841465000	2.469971000	-1.964988000
1	1.226140000	3.049132000	-0.425439000
1	2.902914000	2.438479000	-0.544604000
6	-0.041589000	0.543821000	-0.733288000
1	-0.507559000	1.232530000	-1.448457000
1	-0.134799000	-0.471069000	-1.122522000
6	2.411715000	-0.082466000	-0.217723000
8	3.601992000	0.159962000	-0.050872000
8	1.897429000	-1.337670000	-0.089055000
6	2.847101000	-2.350129000	0.264505000
1	3.627480000	-2.433877000	-0.497577000
1	3.323229000	-2.119280000	1.222111000
1	2.277686000	-3.277354000	0.333016000
6	-0.897589000	0.621483000	0.569784000
6	-0.857452000	2.017334000	1.191397000
1	0.149128000	2.242252000	1.553007000
1	-1.150315000	2.778008000	0.461844000
1	-1.549551000	2.068813000	2.036383000
6	-0.524600000	-0.442123000	1.604353000
1	0.481644000	-0.248447000	1.984240000
1	-1.227015000	-0.395389000	2.442304000
1	-0.543249000	-1.439127000	1.168620000
8	-2.311465000	0.483241000	0.192033000
6	-2.793576000	-0.647304000	-0.368986000
8	-2.140949000	-1.631765000	-0.645067000
6	-4.281361000	-0.508469000	-0.605871000
1	-4.481411000	0.367311000	-1.229791000
1	-4.795560000	-0.353743000	0.347395000
1	-4.656091000	-1.409678000	-1.090161000

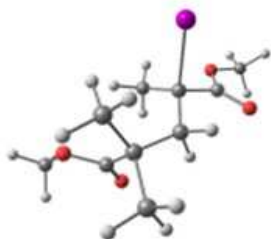
H-MMA-MMA-Br



6	0.745694000	-0.159471000	-0.041499000
6	-0.256012000	-0.043217000	1.119861000
1	-0.326980000	-1.052535000	1.539201000
1	0.192997000	0.577347000	1.897803000
6	0.195682000	-0.764938000	-1.329050000
1	-0.626178000	-0.162673000	-1.720535000
1	0.972820000	-0.836295000	-2.088329000
1	-0.186014000	-1.767485000	-1.109640000
6	1.993803000	-0.898893000	0.474365000
8	2.257519000	-1.048443000	1.647057000
8	2.754873000	-1.365914000	-0.530045000
6	3.971464000	-2.017475000	-0.122161000
1	4.608173000	-1.320725000	0.429339000
1	3.750772000	-2.876628000	0.516425000
1	4.456617000	-2.335101000	-1.044644000
6	-1.707789000	0.435938000	0.864264000
6	-1.813879000	1.816830000	0.199713000
1	-1.240650000	2.546731000	0.777557000
1	-1.425521000	1.821620000	-0.819308000
1	-2.857255000	2.139270000	0.162140000
6	-2.404683000	0.494217000	2.250687000
1	-2.350282000	-0.472919000	2.757651000
1	-1.920275000	1.249006000	2.877999000
1	-3.458614000	0.769494000	2.140894000
6	-2.460759000	-0.658394000	0.096314000
8	-2.360943000	-1.846280000	0.332227000

8	-3.291031000	-0.167839000	-0.846721000
6	-4.062634000	-1.154047000	-1.555938000
1	-3.403227000	-1.844344000	-2.088806000
1	-4.682575000	-1.727952000	-0.862454000
1	-4.682041000	-0.594855000	-2.256948000
35	1.516845000	1.686073000	-0.504795000

H-MMA-MMA-I



6	-0.481159000	0.457122000	-0.004120000
6	0.532905000	0.331442000	1.147674000
1	0.741104000	1.363756000	1.451242000
1	0.036822000	-0.136139000	2.000165000
6	0.109124000	0.833521000	-1.360415000
1	0.831248000	0.087212000	-1.695525000
1	-0.668553000	0.935167000	-2.115495000
1	0.629651000	1.792167000	-1.256015000
6	-1.593028000	1.417509000	0.444472000
8	-1.810804000	1.711719000	1.599720000
8	-2.289931000	1.908832000	-0.596333000
6	-3.391645000	2.764006000	-0.242835000
1	-4.122757000	2.210820000	0.352924000
1	-3.041050000	3.623234000	0.334368000
1	-3.828803000	3.084220000	-1.188181000
53	-1.649037000	-1.467145000	-0.270470000
6	1.912578000	-0.343968000	0.928065000
6	1.846821000	-1.793768000	0.426192000
1	1.216667000	-2.388084000	1.093218000
1	1.435900000	-1.871609000	-0.581028000
1	2.847695000	-2.232443000	0.409832000
6	2.633399000	-0.325245000	2.303056000
1	2.707069000	0.693400000	2.692809000
1	2.080260000	-0.939092000	3.020719000
1	3.644432000	-0.735748000	2.213732000
6	2.763315000	0.561192000	0.026699000
8	2.839396000	1.767151000	0.154184000
8	3.456577000	-0.120384000	-0.908294000
6	4.300565000	0.683823000	-1.751868000
1	3.702841000	1.413173000	-2.305111000
1	5.041940000	1.220410000	-1.154281000
1	4.785348000	-0.014105000	-2.434231000

2. Salts

LiCl



3	0.000000000	0.000000000	-1.747950000
17	0.000000000	0.000000000	0.308462000

NaCl



11	0.000000000	0.000000000	-1.444280000
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17	0.000000000	0.000000000	0.934534000
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KCl



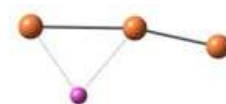
19	0.000000000	0.000000000	1.294104000
17	0.000000000	0.000000000	-1.446351000

LiBr



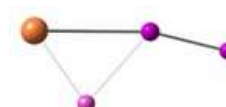
3	0.000000000	0.000000000	-2.055833000
35	0.000000000	0.000000000	0.176214000

LiBr₃



3	-0.229720000	-2.172368000	0.000000000
35	0.000000000	0.302389000	0.000000000
35	2.078724000	-1.794054000	0.000000000
35	-2.059033000	1.677868000	0.000000000

LiBrI₂



3	2.673711000	-0.071652000	0.000000000
53	0.000000000	0.338341000	0.000000000
35	2.506807000	2.252680000	0.000000000
53	-1.806781000	-1.821904000	0.000000000

NaBr



11	0.000000000	0.000000000	-1.940070000
35	0.000000000	0.000000000	0.609736000

KBr



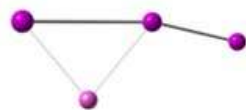
19	0.000000000	0.000000000	-1.901137000
35	0.000000000	0.000000000	1.032046000

LiI



3	0.000000000	0.000000000	-2.302131000
53	0.000000000	0.000000000	0.130309000

LiI₃



3	-0.005427000	-2.361298000	0.000000000
53	0.000000000	0.317174000	0.000000000
53	-2.503988000	-1.848146000	0.000000000
53	2.504295000	1.664630000	0.000000000

NaI



11	0.000000000	0.000000000	-2.270801000
53	0.000000000	0.000000000	0.471298000

KI



19	0.000000000	0.000000000	-2.314721000
53	0.000000000	0.000000000	0.829806000

Na₂CO₃



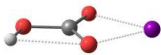
6	0.000019000	0.563900000	0.000142000
8	-1.129685000	1.164272000	-0.000423000
8	1.129825000	1.163917000	0.000371000
8	-0.000045000	-0.797635000	0.000436000
11	2.142408000	-0.710336000	-0.000331000
11	-2.142488000	-0.710375000	-0.000026000

K₂CO₃



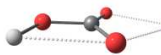
6	-0.000017000	0.806697000	0.000564000
8	-1.127679000	1.417867000	-0.000061000
8	1.127651000	1.417826000	-0.000249000
8	-0.000006000	-0.546181000	0.000005000
19	-2.484142000	-0.609386000	-0.000071000
19	2.484162000	-0.609365000	0.000021000

NaHCO₃



6	-0.559106000	0.041724000	-0.000039000
8	0.050772000	1.144266000	-0.000089000
8	-1.922431000	0.097515000	0.000095000
8	-0.021823000	-1.113486000	-0.000099000
11	1.883292000	-0.040956000	0.000078000
1	-2.213725000	-0.826198000	0.000121000

KHCO₃



6	-0.996273000	0.041576000	-0.000331000
8	-0.408900000	1.152119000	-0.000650000
8	-2.371733000	0.084679000	0.000781000
8	-0.463912000	-1.111922000	-0.000729000
1	-2.642815000	-0.844646000	0.000965000

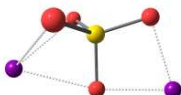
19	1.819832000	-0.021254000	0.000305000
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KOH



19	0.000080000	0.749991000	0.000000000
8	0.000080000	-1.476495000	0.000000000
1	-0.002156000	-2.437877000	0.000000000

Na₂SO₄



16	-0.045809000	0.436067000	0.000105000
8	-0.872675000	0.709213000	1.229585000
8	-0.872400000	0.709164000	-1.229742000
8	1.303107000	1.117430000	-0.000064000
8	0.231805000	-1.113370000	-0.000123000
11	2.381808000	-0.781367000	0.000098000
11	-2.162331000	-0.887412000	0.000000000

3. salt·Br⁺ adducts

Cl⁻·Br⁺



35	0.000000000	0.000000000	0.942248000
17	0.000000000	0.000000000	-1.939923000

LiCl·Br⁺



35	0.000000000	1.007306000	0.000000000
17	-0.280704000	-1.932314000	0.000000000
3	1.590658000	-0.802121000	0.000000000

NaCl·Br⁺



35	0.000000000	1.148810000	0.000000000
17	-0.975282000	-1.624496000	0.000000000
11	1.507254000	-1.144719000	0.000000000

KCl·Br⁺



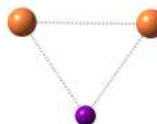
35	0.000000000	1.148810000	0.000000000
17	-0.975282000	-1.624496000	0.000000000
19	1.507254000	-1.144719000	0.000000000

Br·Br[•]

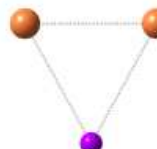
35	0.000000000	0.000000000	1.520459000
35	0.000000000	0.000000000	-1.520459000

LiBr·Br[•]

35	0.000000000	-1.546569000	0.000000000
35	-0.149328000	1.539412000	0.000000000
3	1.742154000	0.083496000	0.000000000

NaBr·Br[•]

35	0.000000000	-1.570925000	0.000000000
35	-0.598702000	1.452388000	0.000000000
11	1.904961000	0.377164000	0.000000000

KBr·Br[•]

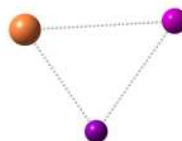
35	0.000000000	-1.635165000	0.000000000
35	-1.093516000	1.216576000	0.000000000
19	2.014372000	0.771084000	0.000000000

I·Br[•]

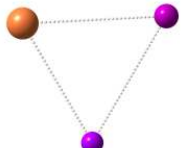
53	0.000000000	0.000000000	1.277893000
35	0.000000000	0.000000000	-1.935096000

LiI·Br[•]

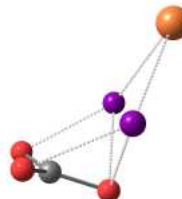
53	0.000000000	1.323159000	0.000000000
35	-0.152632000	-1.952978000	0.000000000
3	1.780711000	-0.591058000	0.000000000

NaI·Br[•]

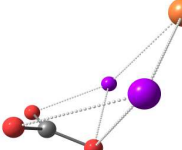
53	0.000000000	-1.382990000	0.000000000
35	0.603878000	1.826390000	0.000000000
11	-1.921429000	0.852256000	0.000000000

KI·Br[•]

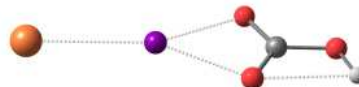
53	0.000000000	-1.478423000	0.000000000
35	1.090986000	1.567836000	0.000000000
19	-2.009711000	1.235901000	0.000000000

Na₂CO₃·Br[•]

35	-1.860702000	-0.000481000	-0.131459000
8	2.253586000	1.112868000	-0.645409000
6	2.074334000	0.001167000	-0.053607000
8	1.587582000	-0.004571000	1.132834000
8	2.257709000	-1.108263000	-0.650330000
11	0.175801000	1.803548000	0.283427000
11	0.177613000	-1.802680000	0.282568000

K₂CO₃·Br[•]

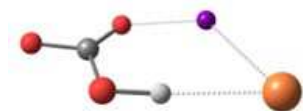
35	2.077760000	0.000759000	-0.181568000
8	-2.491793000	1.099389000	-0.697679000
6	-2.253486000	-0.000442000	-0.098810000
8	-1.709703000	0.000849000	1.056527000
8	-2.490231000	-1.102331000	-0.695126000
19	-0.147979000	-2.187628000	0.253567000
19	-0.150276000	2.187251000	0.253694000

NaHCO₃·Br[•] (more stable)

8	-2.188756000	-1.079143000	0.000429000
6	-2.819638000	0.019286000	-0.000076000

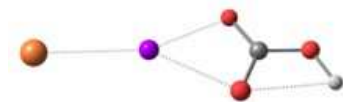
8	-4.158319000	0.034890000	-0.000944000
1	-4.461979000	-0.886742000	-0.001096000
8	-2.211517000	1.124525000	0.000235000
35	2.619898000	-0.014846000	-0.000259000
11	-0.167989000	0.058952000	0.001170000

NaHCO₃·Br[•] (less stable)



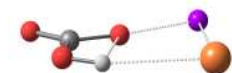
8	-1.703398000	0.958797000	0.001104000
6	-2.060569000	-0.241239000	0.000220000
8	-1.300452000	-1.293675000	0.000468000
1	-0.314888000	-1.050382000	0.001560000
8	-3.335299000	-0.424994000	-0.001107000
35	1.719540000	-0.351102000	-0.000090000
11	0.291599000	1.896850000	-0.000313000

KHCO₃·Br[•] (less stable)



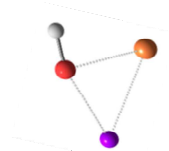
8	-2.188756000	-1.079143000	0.000429000
6	-2.819638000	0.019286000	-0.000076000
8	-4.158319000	0.034890000	-0.000944000
1	-4.461979000	-0.886742000	-0.001096000
8	-2.211517000	1.124525000	0.000235000
35	2.879032586	-0.015572354	-0.000246383
19	-0.019951537	0.061166491	0.001239562

KHCO₃·Br[•] (more stable)



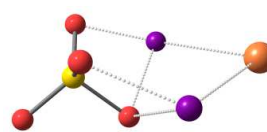
8	-0.972200000	0.527419000	0.001288000
6	-2.102819000	-0.115972000	0.000051000
8	-2.070710000	-1.453227000	-0.000543000
1	-1.136809000	-1.731199000	0.000037000
8	-3.157149000	0.513148000	-0.000220000
35	1.329840000	-0.995582000	0.000010000
19	0.884726000	2.135458000	-0.000257000

KOH·Br[•]



35	0.000000000	1.204195000	0.000000000
19	-0.754345000	-1.794919000	0.000000000
8	1.509069000	-0.961374000	0.000000000
1	2.259995000	-0.352362000	0.000000000

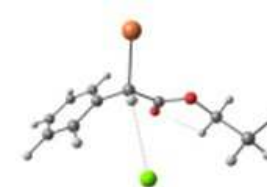
Na₂SO₄·Br[•]



16	1.821017000	0.000037000	-0.079473000
8	3.043806000	-0.001393000	0.788769000
8	1.638320000	1.248461000	-0.875529000
8	1.637165000	-1.247081000	-0.877357000
8	0.705058000	-0.000259000	1.041231000
11	-0.284124000	-1.982371000	0.038631000
11	-0.284150000	1.982778000	0.038733000
35	-2.259430000	-0.000083000	-0.005610000

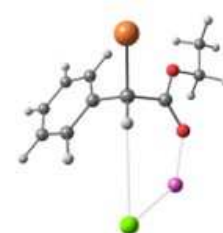
4. EBrPA-salt adducts

EBrPA·Cl[•]



6	3.531439000	0.120062000	-1.225334000
6	2.260343000	-0.388022000	-0.969516000
6	1.425287000	0.231967000	-0.029862000
6	1.866900000	1.384204000	0.634028000
6	3.142112000	1.891399000	0.371409000
6	3.978674000	1.260785000	-0.550319000
1	4.173698000	-0.371002000	-1.952462000
1	1.907312000	-1.273468000	-1.487626000
1	1.178377000	1.897547000	1.302040000
1	3.476194000	2.788200000	0.887003000
1	4.971852000	1.657152000	-0.749745000
6	0.044136000	-0.269526000	0.263128000
1	-0.417369000	0.244019000	1.109728000
6	-0.924600000	-0.167440000	-0.911311000
8	-0.599740000	0.082305000	-2.053614000
8	-2.181020000	-0.360145000	-0.490133000
6	-3.251959000	0.112243000	-1.331972000
1	-2.835884000	0.775132000	-2.094847000
1	-3.696021000	-0.755773000	-1.836950000
6	-4.238334000	0.835344000	-0.429991000
1	-3.707541000	1.628180000	0.108843000
1	-5.052752000	1.261761000	-1.028411000
1	-4.669217000	0.146170000	0.303648000
35	0.098964000	-2.253715000	0.825175000
17	-1.385312000	2.531691000	1.293298000

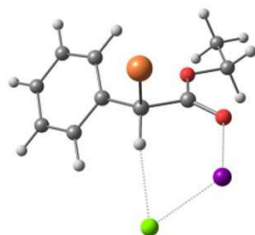
EBrPA·LiCl



6	0.825172000	-3.255347000	-0.479908000
6	0.139909000	-2.100208000	-0.113191000
6	0.836158000	-0.891817000	0.039781000

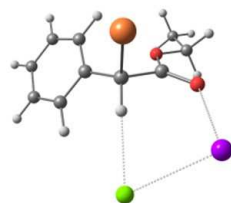
6	2.219550000	-0.846910000	-0.181562000
6	2.898037000	-2.009522000	-0.553923000
6	2.205754000	-3.211901000	-0.701702000
1	0.284899000	-4.191115000	-0.589411000
1	-0.929073000	-2.129386000	0.071038000
1	2.751086000	0.095581000	-0.080282000
1	3.969631000	-1.970704000	-0.724593000
1	2.737750000	-4.115001000	-0.986685000
6	0.124803000	0.388627000	0.407511000
1	0.842183000	1.204766000	0.511303000
6	-0.862564000	0.776188000	-0.679487000
8	-0.579441000	1.606882000	-1.548817000
8	-1.999454000	0.116900000	-0.673328000
6	-2.942339000	0.380418000	-1.756107000
1	-3.201227000	1.442635000	-1.729947000
1	-2.437808000	0.173086000	-2.704389000
6	-4.138942000	-0.517400000	-1.522297000
1	-4.603965000	-0.300233000	-0.557218000
1	-4.879370000	-0.353097000	-2.310701000
1	-3.843365000	-1.569903000	-1.538381000
35	-0.793111000	0.293406000	2.191731000
3	0.999064000	2.582150000	-1.721261000
17	2.756992000	2.802039000	-0.581475000

EBrPA·NaCl



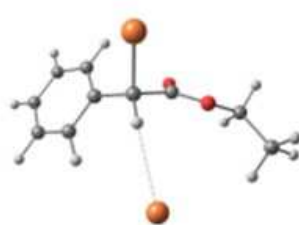
6	-3.540075000	-1.003798000	0.312916000
6	-2.322456000	-0.366686000	0.531599000
6	-1.157626000	-0.848184000	-0.084162000
6	-1.224385000	-1.980846000	-0.908365000
6	-2.449436000	-2.613178000	-1.128491000
6	-3.606531000	-2.126605000	-0.519875000
1	-4.439316000	-0.628982000	0.793058000
1	-2.266020000	0.501327000	1.179540000
1	-0.315568000	-2.355819000	-1.372992000
1	-2.495140000	-3.487605000	-1.770606000
1	-4.558862000	-2.621769000	-0.686940000
6	0.182034000	-0.211541000	0.088654000
1	0.949469000	-0.786180000	-0.445960000
6	0.368354000	1.247355000	-0.299338000
8	1.477201000	1.737684000	-0.500518000
8	-0.756442000	1.933476000	-0.413923000
6	-0.644773000	3.333149000	-0.799672000
1	-0.036936000	3.848158000	-0.049508000
1	-0.117551000	3.383832000	-1.756745000
6	-2.055443000	3.878893000	-0.883098000
1	-2.559064000	3.803403000	0.084501000
1	-2.026018000	4.932078000	-1.177827000
1	-2.640342000	3.326299000	-1.623126000
35	0.847497000	-0.295192000	2.019681000
11	3.323495000	0.410983000	-0.568460000
17	2.777675000	-1.724968000	-1.656157000

EBrPA·KCl



6	-3.737154000	-0.948542000	0.366338000
6	-2.514593000	-0.312847000	0.559234000
6	-1.357711000	-0.812707000	-0.057685000
6	-1.436515000	-1.962120000	-0.858209000
6	-2.667415000	-2.591919000	-1.052583000
6	-3.816364000	-2.088156000	-0.442490000
1	-4.630119000	-0.559529000	0.847129000
1	-2.447833000	0.569034000	1.187293000
1	-0.532371000	-2.347898000	-1.324104000
1	-2.723693000	-3.478708000	-1.676861000
1	-4.772632000	-2.582259000	-0.590032000
6	-0.014001000	-0.181355000	0.090481000
1	0.741968000	-0.765032000	-0.454051000
6	0.182966000	1.276298000	-0.300498000
8	1.291279000	1.764364000	-0.480896000
8	-0.948461000	1.956568000	-0.448723000
6	-0.829111000	3.346380000	-0.854834000
1	-0.233863000	3.876245000	-0.104358000
1	-0.285513000	3.383427000	-1.803703000
6	-2.237554000	3.893109000	-0.971937000
1	-2.758104000	3.832817000	-0.012168000
1	-2.202916000	4.941558000	-1.282996000
1	-2.810340000	3.328580000	-1.712517000
35	0.668142000	-0.280996000	2.027800000
19	3.554046000	0.243186000	-0.325255000
17	2.327397000	-1.909423000	-1.723338000

EBrPA·Br⁻



6	3.687851000	0.703407000	-1.271871000
6	2.608857000	-0.116227000	-0.952355000
6	1.583731000	0.357509000	-0.121040000
6	1.642184000	1.667387000	0.371662000
6	2.724963000	2.487303000	0.044811000
6	3.750677000	2.008096000	-0.770348000
1	4.479867000	0.327481000	-1.914763000
1	2.550451000	-1.127620000	-1.338828000
1	0.812254000	2.048616000	0.960808000
1	2.757382000	3.505053000	0.424228000
1	4.593619000	2.647677000	-1.021683000
6	0.396832000	-0.482359000	0.231571000
1	-0.263608000	0.008731000	0.946653000
6	-0.444279000	-0.933824000	-0.960008000
8	-0.071956000	-0.934255000	-2.115126000
8	-1.661295000	-1.295354000	-0.542882000
6	-2.695004000	-1.423719000	-1.539694000
1	-2.476080000	-0.737817000	-2.362580000
1	-2.676878000	-2.447912000	-1.934837000
6	-4.002800000	-1.079779000	-0.850190000
1	-3.926736000	-0.072338000	-0.429194000

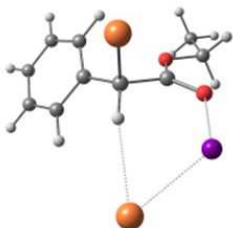
1	-4.829685000	-1.120965000	-1.568654000
1	-4.210076000	-1.783265000	-0.037525000
35	0.986131000	-2.199548000	1.201873000
35	-2.085062000	2.127047000	0.639419000

EBrPA·LiBr



6	-1.535809000	-3.262723000	-0.646685000
6	-1.505602000	-1.938963000	-0.217009000
6	-0.275811000	-1.313530000	0.037449000
6	0.920456000	-2.020857000	-0.144263000
6	0.881528000	-3.346729000	-0.581012000
6	-0.342050000	-3.968740000	-0.831006000
1	-2.489607000	-3.746916000	-0.834568000
1	-2.427676000	-1.388882000	-0.061286000
1	1.871949000	-1.529731000	0.040956000
1	1.811007000	-3.890124000	-0.721006000
1	-0.369201000	-5.001683000	-1.165699000
6	-0.197298000	0.129673000	0.472354000
1	0.838705000	0.413460000	0.665704000
6	-0.733047000	1.048159000	-0.612169000
8	0.018854000	1.672005000	-1.368655000
8	-2.040685000	1.074797000	-0.732204000
6	-2.610380000	1.869575000	-1.816583000
1	-2.289234000	2.906292000	-1.682058000
1	-2.198677000	1.501281000	-2.760787000
6	-4.113522000	1.708889000	-1.731986000
1	-4.487401000	2.062607000	-0.767655000
1	-4.589055000	2.292676000	-2.525544000
1	-4.398973000	0.660590000	-1.854198000
35	-1.144844000	0.485197000	2.208607000
3	1.875168000	1.695103000	-1.424968000
35	3.611887000	0.807151000	-0.232225000

EBrPA·NaBr



6	3.503477000	1.930555000	0.079448000
6	2.580287000	0.930665000	0.368981000
6	1.238169000	1.082740000	-0.010019000
6	0.830614000	2.252039000	-0.667655000
6	1.761848000	3.249877000	-0.961181000
6	3.096737000	3.090907000	-0.589079000
1	4.540993000	1.809595000	0.376858000
1	2.890702000	0.032015000	0.891060000
1	-0.212867000	2.372106000	-0.948267000
1	1.440004000	4.150886000	-1.474427000
1	3.820413000	3.869619000	-0.812212000
6	0.195957000	0.046491000	0.255007000

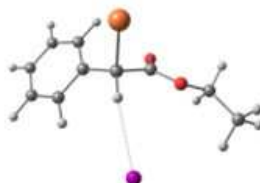
1	-0.787205000	0.396895000	-0.079663000
6	0.381522000	-1.355713000	-0.307950000
8	-0.545811000	-2.157297000	-0.393461000
8	1.612608000	-1.627486000	-0.704123000
6	1.855048000	-2.950642000	-1.264076000
1	1.585072000	-3.695992000	-0.509787000
1	1.194328000	-3.083419000	-2.125571000
6	3.321328000	-3.004944000	-1.640063000
1	3.953541000	-2.856520000	-0.760362000
1	3.553993000	-3.982023000	-2.073697000
1	3.560922000	-2.231775000	-2.374770000
35	-0.109763000	-0.260583000	2.252332000
11	-2.687209000	-1.567573000	0.072825000
35	-3.236091000	0.806535000	-0.929762000

EBrPA·KBr



6	3.797964000	1.582987000	0.291730000
6	2.777191000	0.658970000	0.490850000
6	1.465419000	0.964889000	0.097785000
6	1.186263000	2.210323000	-0.483375000
6	2.215734000	3.131533000	-0.686273000
6	3.519535000	2.820553000	-0.300113000
1	4.811649000	1.342548000	0.598941000
1	2.987862000	-0.300259000	0.951648000
1	0.166200000	2.445230000	-0.778247000
1	1.994011000	4.091973000	-1.141713000
1	4.319191000	3.539719000	-0.453469000
6	0.325297000	0.017887000	0.269629000
1	-0.608277000	0.474861000	-0.082532000
6	0.397839000	-1.368748000	-0.357615000
8	-0.578829000	-2.100963000	-0.449137000
8	1.600171000	-1.690306000	-0.818302000
6	1.727981000	-2.983010000	-1.471383000
1	1.444206000	-3.760720000	-0.755236000
1	1.021590000	-3.018134000	-2.306129000
6	3.168549000	-3.106614000	-1.924188000
1	3.849762000	-3.056922000	-1.070243000
1	3.315504000	-4.065466000	-2.430318000
1	3.424889000	-2.302773000	-2.619323000
35	-0.079209000	-0.332606000	2.252737000
19	-3.087481000	-1.326871000	0.246010000
35	-2.770101000	1.377693000	-1.110176000

EBrPA·I⁻



6	-3.634937000	-1.622073000	-1.301436000
6	-2.848127000	-0.521611000	-0.973195000
6	-1.735575000	-0.675188000	-0.133054000
6	-1.412646000	-1.945286000	0.360696000

6	-2.202948000	-3.047126000	0.026222000
6	-3.316405000	-2.888435000	-0.799078000
1	-4.496444000	-1.494579000	-1.952010000
1	-3.083950000	0.462000000	-1.362758000
1	-0.516897000	-2.069364000	0.962722000
1	-1.938483000	-4.029783000	0.406823000
1	-3.931962000	-3.746845000	-1.057329000
6	-0.858327000	0.477780000	0.235783000
1	-0.064926000	0.193301000	0.926235000
6	-0.229217000	1.218496000	-0.941929000
8	-0.627199000	1.176904000	-2.087646000
8	0.842529000	1.897861000	-0.526355000
6	1.725621000	2.408032000	-1.546043000
1	1.841151000	1.641700000	-2.317965000
1	1.265894000	3.291691000	-2.006624000
6	3.043731000	2.717399000	-0.861962000
1	3.433137000	1.804176000	-0.402695000
1	3.766812000	3.092177000	-1.595189000
1	2.910081000	3.475513000	-0.083585000
35	-1.931012000	1.889799000	1.284019000
53	2.556441000	-1.322510000	0.378447000

EBrPA·LiI

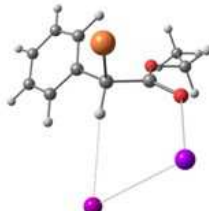
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6	-2.114567000	-1.829359000	-0.349797000
6	-0.843120000	-1.351124000	0.001650000
6	0.274581000	-2.189219000	-0.108743000
6	0.117219000	-3.496980000	-0.572227000
6	-1.147815000	-3.971619000	-0.920622000
1	-3.250285000	-3.505191000	-1.071437000
1	-2.977955000	-1.179987000	-0.246956000
1	1.260501000	-1.815785000	0.154278000
1	0.986578000	-4.141819000	-0.656724000
1	-1.267431000	-4.990514000	-1.277201000
6	-0.640424000	0.068360000	0.473532000
1	0.412890000	0.250395000	0.695327000
6	-1.057730000	1.048185000	-0.609091000
8	-0.234654000	1.539983000	-1.388593000
8	-2.346912000	1.275690000	-0.704433000
6	-2.807953000	2.141939000	-1.786955000
1	-2.299679000	3.105246000	-1.690355000
1	-2.507291000	1.687160000	-2.735393000
6	-4.310560000	2.258507000	-1.643565000
1	-4.574413000	2.692999000	-0.675925000
1	-4.703703000	2.904075000	-2.434375000
1	-4.786910000	1.278052000	-1.727695000
35	-1.588688000	0.462375000	2.198872000
3	1.605834000	1.384914000	-1.470306000
53	3.470041000	0.445194000	-0.117022000

EBrPA·NaI



6	3.995489000	1.718172000	-0.173247000
6	3.039703000	0.796840000	0.242646000
6	1.684450000	1.006471000	-0.053135000
6	1.299160000	2.154374000	-0.758261000
6	2.261537000	3.074625000	-1.177940000
6	3.608333000	2.858372000	-0.886518000
1	5.043152000	1.551505000	0.059186000
1	3.336592000	-0.086794000	0.798273000
1	0.247875000	2.320633000	-0.978685000
1	1.955459000	3.959617000	-1.727366000
1	4.356940000	3.576356000	-1.208715000
6	0.614998000	0.050234000	0.362738000
1	-0.371504000	0.400381000	0.033381000
6	0.714441000	-1.406440000	-0.077692000
8	-0.169108000	-2.229453000	0.143171000
8	1.810845000	-1.685014000	-0.760567000
6	1.942347000	-3.038826000	-1.285271000
1	1.912305000	-3.736345000	-0.442734000
1	1.079445000	-3.241197000	-1.926197000
6	3.254673000	-3.089403000	-2.039846000
1	4.093511000	-2.864248000	-1.375650000
1	3.400391000	-4.090209000	-2.456968000
1	3.257244000	-2.366633000	-2.859895000
35	0.394454000	-0.004202000	2.390247000
11	-2.263962000	-1.657510000	0.794487000
53	-3.110159000	0.557091000	-0.760270000

EBrPA·KI



6	3.976111000	1.859972000	0.248531000
6	3.071810000	0.819277000	0.434172000
6	1.706391000	1.019827000	0.180404000
6	1.257295000	2.276761000	-0.248261000
6	2.169485000	3.316570000	-0.438315000
6	3.526666000	3.110649000	-0.190783000
1	5.031857000	1.700136000	0.447210000
1	3.415985000	-0.151142000	0.776615000
1	0.197650000	2.431445000	-0.436446000
1	1.815288000	4.286040000	-0.775386000
1	4.235407000	3.921268000	-0.334343000
6	0.688289000	-0.058032000	0.351171000
1	-0.313521000	0.315187000	0.104005000
6	0.852915000	-1.371906000	-0.404981000
8	-0.012789000	-2.236854000	-0.422030000
8	1.993948000	-1.463188000	-1.074981000
6	2.187236000	-2.657458000	-1.882979000
1	2.152784000	-3.529275000	-1.221972000
1	1.354042000	-2.733690000	-2.587777000
6	3.524807000	-2.505891000	-2.578068000
1	4.333883000	-2.415839000	-1.848047000

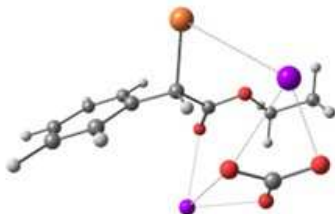
1	3.717004000	-3.382790000	-3.203563000
1	3.530804000	-1.616551000	-3.213721000
35	0.479412000	-0.589102000	2.320768000
19	-2.512245000	-1.946611000	0.559118000
53	-2.870439000	1.009832000	-0.762376000

EBrPA·Na₂CO₃



6	4.173103000	0.750667000	-1.290058000
6	2.839054000	0.392611000	-1.114972000
6	2.305697000	0.269112000	0.176004000
6	3.125147000	0.502220000	1.286209000
6	4.461867000	0.861793000	1.109578000
6	4.987080000	0.986057000	-0.177742000
1	4.579089000	0.846835000	-2.292487000
1	2.205718000	0.202992000	-1.977433000
1	2.714873000	0.401705000	2.287587000
1	5.090791000	1.044575000	1.975660000
1	6.027430000	1.265165000	-0.315765000
6	0.869355000	-0.113062000	0.373899000
1	0.530955000	0.036504000	1.398108000
6	-0.084940000	0.709293000	-0.492734000
8	-0.093674000	1.924260000	-0.326313000
8	-0.788832000	0.047154000	-1.379516000
6	-1.776850000	0.800419000	-2.175941000
1	-2.285273000	1.501850000	-1.512581000
1	-1.212761000	1.340744000	-2.942880000
6	-2.747499000	-0.212706000	-2.742631000
1	-3.321774000	-0.652559000	-1.922840000
1	-3.444687000	0.302341000	-3.411150000
1	-2.228544000	-0.988714000	-3.314609000
35	0.675905000	-2.133466000	0.144898000
6	-3.114283000	0.537945000	0.807768000
8	-3.765340000	-0.493055000	0.406759000
8	-3.449109000	1.740452000	0.519352000
8	-1.983659000	0.341134000	1.522269000
11	-1.605220000	2.518145000	1.322720000
11	-2.203323000	-1.792308000	1.082761000

EBrPA·K₂CO₃



6	-4.291645000	0.328926000	0.976063000
6	-2.996965000	-0.176340000	1.064731000
6	-2.127038000	-0.085041000	-0.031169000
6	-2.575026000	0.519340000	-1.215039000
6	-3.872008000	1.033027000	-1.300395000
6	-4.731935000	0.936795000	-0.205032000
1	-4.959405000	0.252766000	1.829076000
1	-2.649281000	-0.634322000	1.984712000
1	-1.900953000	0.587569000	-2.065578000

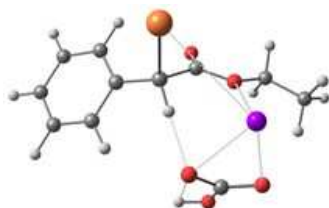
1	-4.209761000	1.498232000	-2.222094000
1	-5.742618000	1.329262000	-0.269996000
6	-0.717116000	-0.581020000	0.029451000
1	-0.139957000	-0.221535000	-0.832532000
6	0.104779000	-0.052189000	1.203312000
8	-0.282241000	0.884195000	1.884537000
8	1.300231000	-0.614412000	1.290443000
6	2.265170000	0.049515000	2.184776000
1	2.272538000	1.109704000	1.918365000
1	1.907068000	-0.092390000	3.208990000
6	3.616484000	-0.581971000	1.926100000
1	3.951624000	-0.295326000	0.924740000
1	4.336290000	-0.191026000	2.652637000
1	3.577625000	-1.671795000	2.036525000
35	-0.650777000	-2.610601000	-0.091698000
6	2.328361000	1.501035000	-0.763047000
8	3.393815000	0.828105000	-1.003934000
8	2.296624000	2.477259000	0.069565000
8	1.181369000	1.136403000	-1.368650000
19	-0.112478000	3.018816000	-0.092030000
19	2.280756000	-1.194867000	-1.810581000

EBrPA·NaHCO₃



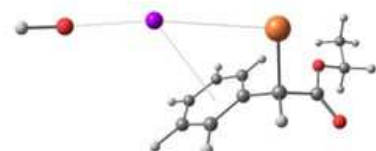
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6	3.035982000	0.615240000	0.730206000
6	2.052873000	-0.270730000	0.262970000
6	2.384302000	-1.613478000	0.027689000
6	3.680503000	-2.069272000	0.266343000
6	4.654064000	-1.184749000	0.733513000
1	5.086455000	0.843603000	1.328905000
1	2.779249000	1.651082000	0.917755000
1	1.618328000	-2.293557000	-0.336012000
1	3.928815000	-3.110970000	0.086713000
1	5.664916000	-1.537132000	0.917533000
6	0.653181000	0.150994000	-0.008609000
1	0.009482000	-0.703783000	-0.241864000
6	-0.033908000	0.999862000	1.052803000
8	0.495131000	1.503577000	2.014154000
8	-1.367880000	1.069693000	0.810882000
6	-2.164474000	1.721753000	1.846885000
1	-1.964169000	1.209429000	2.791866000
1	-1.820555000	2.755738000	1.942333000
6	-3.620448000	1.615667000	1.440483000
1	-3.901416000	0.570743000	1.277829000
1	-4.250225000	2.035273000	2.230723000
1	-3.817363000	2.188707000	0.526184000
35	0.543423000	1.249591000	-1.763503000
6	-2.585979000	-2.140279000	-0.122072000
8	-3.580272000	-1.372659000	-0.130758000
8	-2.686845000	-3.266964000	0.642587000
8	-1.492077000	-1.960857000	-0.753916000
1	-1.851416000	-3.739367000	0.515695000
11	-2.341606000	0.065933000	-1.278665000

EBrPA·KHCO₃



6	4.374276000	-0.168341000	0.901050000
6	3.100023000	0.390429000	0.851271000
6	2.084431000	-0.253059000	0.128431000
6	2.358558000	-1.455249000	-0.541797000
6	3.636260000	-2.012143000	-0.484435000
6	4.645031000	-1.368171000	0.234092000
1	5.159358000	0.330027000	1.462004000
1	2.880697000	1.313462000	1.374910000
1	1.558012000	-1.946276000	-1.090166000
1	3.843062000	-2.945037000	-1.000638000
1	5.641590000	-1.798529000	0.276347000
6	0.696303000	0.272917000	0.035496000
1	0.053742000	-0.430744000	-0.500751000
6	0.015523000	0.658675000	1.340341000
8	0.564799000	0.900839000	2.389415000
8	-1.327940000	0.640421000	1.177976000
6	-2.114556000	0.822228000	2.389351000
1	-1.774550000	0.087486000	3.124471000
1	-1.909979000	1.820221000	2.789807000
6	-3.569953000	0.616325000	2.019224000
1	-3.704278000	-0.359017000	1.541670000
1	-4.188847000	0.665910000	2.920344000
1	-3.917262000	1.405172000	1.339967000
35	0.608445000	1.963172000	-1.153092000
6	-2.028861000	-2.212220000	-0.434774000
8	-3.192333000	-1.776506000	-0.285215000
8	-1.647201000	-3.233468000	0.400679000
8	-1.151027000	-1.794094000	-1.261742000
1	-0.743339000	-3.454667000	0.134698000
19	-2.597178000	0.366056000	-1.579624000

EBrPA·KOH



6	1.149126000	-2.361570000	0.919780000
6	0.150313000	-1.454655000	0.562479000
6	0.184486000	-0.829739000	-0.696860000
6	1.227931000	-1.135836000	-1.585909000
6	2.225927000	-2.043686000	-1.224101000
6	2.190895000	-2.655383000	0.031885000
1	1.119393000	-2.835594000	1.896430000
1	-0.649275000	-1.216506000	1.254177000
1	1.266908000	-0.650877000	-2.557583000
1	3.038351000	-2.255447000	-1.911177000
1	2.976725000	-3.345222000	0.321799000
6	-0.832880000	0.196018000	-1.110003000
1	-0.727910000	0.449171000	-2.162504000
35	-0.477622000	1.976073000	-0.175510000
6	-2.293756000	-0.196119000	-0.907610000
8	-3.022141000	-0.426207000	-1.846721000
8	-2.648951000	-0.288621000	0.379442000
6	-4.023933000	-0.688432000	0.630055000
1	-4.187635000	-1.671385000	0.177357000
1	-4.686626000	0.024602000	0.130536000
6	-4.216192000	-0.701568000	2.132788000

1	-5.243959000	-0.991048000	2.371392000
1	-3.538224000	-1.417446000	2.606647000
1	-4.027587000	0.288850000	2.556082000
19	2.902835000	0.855334000	0.823798000
8	5.118456000	0.581353000	0.569757000
1	6.072327000	0.500601000	0.472693000

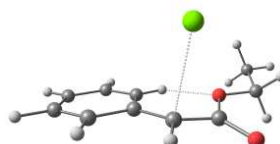
EBrPA·Na₂SO₄



6	-2.695098000	-1.233055000	1.452847000
6	-1.606484000	-0.356495000	1.403293000
6	-1.698719000	0.836712000	0.674131000
6	-2.890652000	1.133600000	-0.001417000
6	-3.967871000	0.247269000	0.026370000
6	-3.876244000	-0.942985000	0.758778000
1	-2.608071000	-2.146369000	2.035593000
1	-0.684848000	-0.643464000	1.892588000
1	-2.970325000	2.052929000	-0.573871000
1	-4.882461000	0.494903000	-0.504403000
1	-4.724832000	-1.620406000	0.810655000
6	-0.555750000	1.834324000	0.647500000
1	-0.879745000	2.774844000	1.094535000
6	0.674715000	1.402992000	1.447972000
8	0.597227000	1.414715000	2.655852000
8	1.761481000	1.041777000	0.757740000
6	2.859624000	0.520324000	1.594045000
1	3.117190000	1.299117000	2.315848000
1	2.468013000	-0.360083000	2.104214000
6	4.008040000	0.163671000	0.674716000
1	4.321736000	1.024949000	0.071746000
1	4.865466000	-0.143044000	1.281700000
1	3.737024000	-0.684786000	0.037801000
35	-0.113050000	2.466103000	-1.242900000
11	1.748177000	0.060458000	-1.601615000
8	-0.007444000	-1.062731000	-0.934388000
16	0.895223000	-2.199567000	-0.326862000
8	0.153628000	-3.486637000	-0.621835000
11	-1.734742000	-2.395731000	-1.060275000
8	2.213290000	-2.087876000	-1.070068000
8	1.058925000	-1.959156000	1.134732000

5. EPA⁺·salt adducts

EPA⁺·Cl⁻



6	-2.388023000	-1.844846000	-0.484395000
6	-1.199363000	-1.214560000	-0.131546000
6	-1.201297000	0.082146000	0.448119000
6	-2.470097000	0.697227000	0.628724000
6	-3.651065000	0.061976000	0.271016000
6	-3.625845000	-1.222544000	-0.287104000
1	-2.348739000	-2.839199000	-0.925696000
1	-0.252009000	-1.707541000	-0.301552000
1	-2.501466000	1.701289000	1.043329000

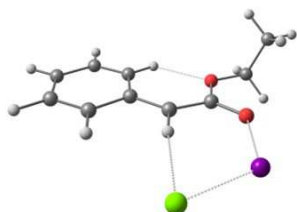
1	-4.601035000	0.571031000	0.421726000
1	-4.549297000	-1.722510000	-0.569056000
6	-0.040662000	0.798543000	0.890855000
1	-0.203929000	1.731276000	1.413490000
6	1.345210000	0.386066000	0.952532000
8	2.201558000	0.926348000	1.643824000
8	1.656803000	-0.706373000	0.173766000
6	3.047612000	-1.015902000	0.102473000
1	3.428085000	-1.281077000	1.097729000
1	3.600133000	-0.128570000	-0.226751000
6	3.198068000	-2.165200000	-0.880880000
1	4.252921000	-2.442243000	-0.990306000
1	2.642786000	-3.044705000	-0.537707000
1	2.807259000	-1.876578000	-1.860928000
17	0.515951000	2.464800000	-1.303751000

EPA[•]LiCl



6	3.324978000	-1.307172000	-0.031219000
6	1.947420000	-1.170116000	-0.107159000
6	1.347042000	0.121079000	-0.047099000
6	2.208603000	1.250773000	0.093204000
6	3.583274000	1.097745000	0.167572000
6	4.150940000	-0.182200000	0.105721000
1	3.767460000	-2.297893000	-0.078454000
1	1.318231000	-2.043071000	-0.211754000
1	1.764134000	2.240881000	0.141703000
1	4.219201000	1.971213000	0.274030000
1	5.228551000	-0.303157000	0.164034000
6	-0.045866000	0.392434000	-0.111933000
1	-0.349338000	1.436301000	-0.045819000
6	-1.170717000	-0.503476000	-0.245238000
8	-2.351061000	-0.088198000	-0.264668000
8	-0.901905000	-1.810189000	-0.352271000
6	-2.024409000	-2.728203000	-0.452346000
1	-1.590655000	-3.620881000	-0.907490000
1	-2.770597000	-2.303393000	-1.127793000
6	-2.611275000	-3.022020000	0.919172000
1	-3.039935000	-2.116013000	1.353317000
1	-3.403584000	-3.772003000	0.829462000
1	-1.842041000	-3.409693000	1.592935000
3	-2.864534000	1.685284000	-0.128090000
17	-1.937885000	3.567993000	0.093621000

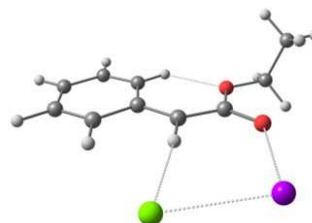
EPA[•]NaCl



6	3.579829000	-1.127243000	-0.037287000
6	2.194824000	-1.140308000	-0.105133000
6	1.460217000	0.079037000	-0.048695000
6	2.193635000	1.297450000	0.080118000
6	3.577723000	1.293027000	0.145980000
6	4.279952000	0.081529000	0.087466000
1	4.126958000	-2.064612000	-0.081639000

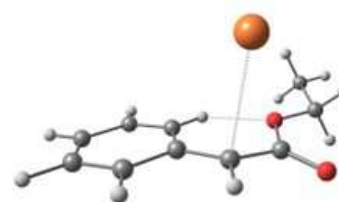
1	1.661531000	-2.076226000	-0.200706000
1	1.640305000	2.232068000	0.126109000
1	4.116444000	2.230708000	0.243443000
1	5.364820000	0.077786000	0.139050000
6	0.046282000	0.203793000	-0.107408000
1	-0.348523000	1.217023000	-0.042997000
6	-0.986576000	-0.798614000	-0.234504000
8	-2.198818000	-0.505352000	-0.255510000
8	-0.579735000	-2.077103000	-0.334365000
6	-1.602458000	-3.099159000	-0.436575000
1	-1.082555000	-3.949448000	-0.883346000
1	-2.383718000	-2.754579000	-1.118730000
6	-2.170939000	-3.444230000	0.931544000
1	-2.688604000	-2.581069000	1.356150000
1	-2.885743000	-4.268561000	0.840919000
1	-1.373390000	-3.750728000	1.614280000
11	-3.029745000	1.558762000	-0.104723000
17	-1.530991000	3.478188000	0.130905000

EPA[•]KCl



6	-3.933770000	0.512378000	-0.046448000
6	-2.580873000	0.810851000	-0.110863000
6	-1.611777000	-0.231535000	-0.054773000
6	-2.076197000	-1.576560000	0.070478000
6	-3.432514000	-1.855816000	0.132713000
6	-4.369446000	-0.815314000	0.074585000
1	-4.662690000	1.316823000	-0.090206000
1	-2.251282000	1.836987000	-0.203611000
1	-1.337960000	-2.374797000	0.116360000
1	-3.766699000	-2.884748000	0.227257000
1	-5.432078000	-1.035312000	0.123760000
6	-0.201580000	-0.065805000	-0.109389000
1	0.381307000	-0.983754000	-0.045087000
6	0.613722000	1.120694000	-0.229452000
8	1.856393000	1.071566000	-0.238109000
8	-0.044546000	2.296100000	-0.337488000
6	0.756335000	3.496299000	-0.432688000
1	0.088395000	4.228817000	-0.891904000
1	1.602068000	3.310891000	-1.100218000
6	1.227210000	3.952675000	0.940632000
1	1.896203000	3.207077000	1.376550000
1	1.768527000	4.900722000	0.855843000
1	0.375007000	4.098482000	1.610536000
19	3.406812000	-1.083354000	-0.070099000
17	1.515785000	-3.180353000	0.149918000

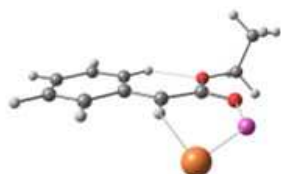
EPA[•]Br⁻



6	-2.721133000	-1.714308000	-0.915212000
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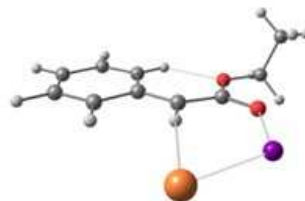
6	-1.484489000	-1.387558000	-0.370221000
6	-1.356388000	-0.329192000	0.568322000
6	-2.543079000	0.377067000	0.905615000
6	-3.772620000	0.045002000	0.354883000
6	-3.877067000	-1.009551000	-0.560869000
1	-2.784930000	-2.528973000	-1.633737000
1	-0.598517000	-1.932529000	-0.664991000
1	-2.469430000	1.208771000	1.600899000
1	-4.657094000	0.613730000	0.633316000
1	-4.838712000	-1.270097000	-0.995854000
6	-0.140696000	0.059740000	1.218088000
1	-0.204271000	0.837764000	1.967642000
6	1.179180000	-0.541319000	1.179135000
8	2.056359000	-0.324025000	2.006213000
8	1.385804000	-1.413307000	0.139272000
6	2.732285000	-1.870922000	-0.006812000
1	3.027705000	-2.454572000	0.874660000
1	3.401879000	-1.005689000	-0.062630000
6	2.783284000	-2.702377000	-1.277602000
1	3.799044000	-3.075654000	-1.450283000
1	2.106074000	-3.560311000	-1.207995000
1	2.481459000	-2.096514000	-2.136754000
35	0.811538000	2.388664000	-0.590289000

EPA[•]LiBr



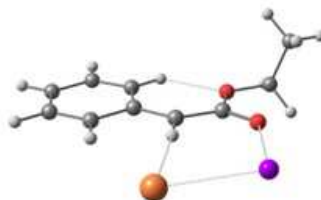
6	-3.891411000	-1.261426000	-0.019223000
6	-2.824835000	-0.379847000	-0.102745000
6	-1.484759000	-0.863281000	-0.054613000
6	-1.288018000	-2.270876000	0.081547000
6	-2.364071000	-3.139057000	0.164004000
6	-3.672974000	-2.640302000	0.114036000
1	-4.906789000	-0.877987000	-0.057343000
1	-3.002460000	0.681633000	-0.204764000
1	-0.271819000	-2.653365000	0.119989000
1	-2.191036000	-4.205795000	0.267293000
1	-4.517244000	-3.320215000	0.178522000
6	-0.312954000	-0.064288000	-0.129634000
1	0.641489000	-0.584925000	-0.077066000
6	-0.158750000	1.365316000	-0.260745000
8	0.967413000	1.910603000	-0.301395000
8	-1.276441000	2.095285000	-0.340811000
6	-1.141202000	3.539796000	-0.434992000
1	-2.090761000	3.862013000	-0.866817000
1	-0.329988000	3.775524000	-1.127658000
6	-0.906859000	4.155259000	0.935526000
1	0.047027000	3.819255000	1.348330000
1	-0.882396000	5.246310000	0.850790000
1	-1.709615000	3.879367000	1.624986000
3	2.612152000	1.088238000	-0.193831000
35	3.489267000	-1.016611000	0.054397000

EPA[•]NaBr



6	-3.699684000	-1.907408000	-0.036933000
6	-2.829972000	-0.829580000	-0.102606000
6	-1.421221000	-1.037348000	-0.050782000
6	-0.946754000	-2.378646000	0.071427000
6	-1.829281000	-3.444716000	0.135745000
6	-3.211028000	-3.216631000	0.081734000
1	-4.771147000	-1.733907000	-0.077696000
1	-3.214317000	0.177070000	-0.192522000
1	0.126069000	-2.548341000	0.112719000
1	-1.447153000	-4.456755000	0.228004000
1	-3.903183000	-4.052024000	0.131989000
6	-0.428861000	-0.022662000	-0.108611000
1	0.604823000	-0.357750000	-0.050020000
6	-0.549203000	1.411948000	-0.232877000
8	0.446349000	2.162967000	-0.258974000
8	-1.795653000	1.906835000	-0.324049000
6	-1.942654000	3.345724000	-0.423684000
1	-2.928826000	3.479591000	-0.873510000
1	-1.180445000	3.736034000	-1.102606000
6	-1.856959000	4.000310000	0.946548000
1	-0.862355000	3.857275000	1.375313000
1	-2.046010000	5.074985000	0.858045000
1	-2.600307000	3.572461000	1.625072000
11	2.588483000	1.582250000	-0.159423000
35	3.338219000	-0.921079000	0.077237000

EPA[•]KBr



6	-3.844468000	-1.882793000	-0.059227000
6	-2.978269000	-0.801196000	-0.111580000
6	-1.569422000	-1.004607000	-0.052641000
6	-1.088518000	-2.344696000	0.062347000
6	-1.968965000	-3.413842000	0.113132000
6	-3.351139000	-3.190995000	0.052585000
1	-4.916533000	-1.713210000	-0.105082000
1	-3.365187000	0.205160000	-0.196256000
1	-0.014134000	-2.508540000	0.107882000
1	-1.583213000	-4.425144000	0.199815000
1	-4.040547000	-4.029432000	0.092344000
6	-0.579315000	0.013561000	-0.096330000
1	0.451857000	-0.326403000	-0.031849000
6	-0.695252000	1.449087000	-0.214738000
8	0.300213000	2.194396000	-0.229329000
8	-1.947265000	1.944686000	-0.314913000
6	-2.087354000	3.380984000	-0.414343000
1	-3.068440000	3.522787000	-0.873515000
1	-1.316236000	3.770727000	-1.084107000
6	-2.012013000	4.036485000	0.956753000
1	-1.021790000	3.887249000	1.393617000
1	-2.195800000	5.112266000	0.868105000
1	-2.762842000	3.610764000	1.628485000

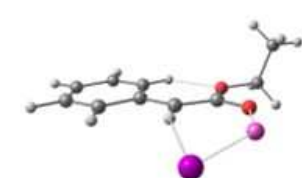
19	2.873596000	1.629027000	-0.125154000
35	2.955979000	-1.389209000	0.094762000

EPA••I⁻



6	3.390392000	0.645409000	-1.078477000
6	2.169409000	0.911083000	-0.469086000
6	1.684434000	0.089429000	0.583218000
6	2.500798000	-1.008299000	0.970036000
6	3.716990000	-1.266632000	0.354334000
6	4.178137000	-0.439459000	-0.677518000
1	3.731829000	1.291257000	-1.884748000
1	1.567898000	1.746891000	-0.798822000
1	2.143640000	-1.665911000	1.757794000
1	4.309645000	-2.121039000	0.673309000
1	5.128826000	-0.641950000	-1.164198000
6	0.461297000	0.296714000	1.299120000
1	0.255621000	-0.361717000	2.133549000
6	-0.494385000	1.386613000	1.226182000
8	-1.308299000	1.643413000	2.105162000
8	-0.415846000	2.144721000	0.086340000
6	-1.446291000	3.125551000	-0.063538000
1	-1.356697000	3.884548000	0.724589000
1	-2.422752000	2.645004000	0.058909000
6	-1.288205000	3.727777000	-1.449434000
1	-2.062283000	4.482460000	-1.628457000
1	-0.308167000	4.204402000	-1.558080000
1	-1.376191000	2.947517000	-2.210678000
53	-1.604786000	-1.726899000	-0.335928000

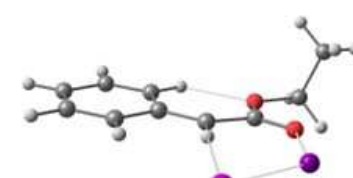
EPA••LiI



6	-4.121519000	-1.850244000	0.004568000
6	-3.232313000	-0.790380000	-0.082276000
6	-1.826649000	-1.025819000	-0.058852000
6	-1.377866000	-2.376274000	0.058057000
6	-2.278900000	-3.424597000	0.143370000
6	-3.656703000	-3.168717000	0.116917000
1	-5.189746000	-1.655512000	-0.014398000
1	-3.599320000	0.223006000	-0.167086000
1	-0.309086000	-2.570082000	0.079403000
1	-1.915287000	-4.443709000	0.231098000
1	-4.363925000	-3.990017000	0.183955000
6	-0.819012000	-0.028679000	-0.138699000
1	0.213462000	-0.369681000	-0.096949000
6	-0.922661000	1.405415000	-0.262233000
8	0.089226000	2.142674000	-0.294786000
8	-2.152080000	1.922881000	-0.346740000
6	-2.281286000	3.368195000	-0.440873000
1	-3.264532000	3.511879000	-0.893255000
1	-1.512709000	3.749686000	-1.116850000
6	-2.192895000	4.011990000	0.933488000
1	-1.201735000	3.858691000	1.366580000

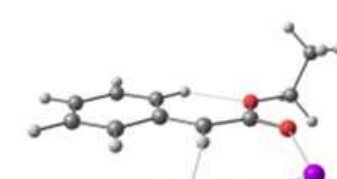
1	-2.370604000	5.088718000	0.848552000
1	-2.943901000	3.589225000	1.606645000
3	1.856579000	1.648730000	-0.194815000
53	3.276402000	-0.399777000	0.038645000

EPA••NaI



6	3.821167000	2.425558000	-0.036401000
6	3.142176000	1.218509000	-0.101782000
6	1.718333000	1.190493000	-0.051756000
6	1.028159000	2.434947000	0.068026000
6	1.721706000	3.632419000	0.131886000
6	3.122252000	3.635992000	0.079836000
1	4.906573000	2.431956000	-0.075887000
1	3.688176000	0.289445000	-0.191178000
1	-0.058050000	2.425444000	0.107550000
1	1.177040000	4.567232000	0.222240000
1	3.666434000	4.574497000	0.129772000
6	0.908464000	0.025487000	-0.110890000
1	-0.166105000	0.184361000	-0.056457000
6	1.261843000	-1.369946000	-0.233053000
8	0.400908000	-2.272072000	-0.264660000
8	2.572164000	-1.655105000	-0.316379000
6	2.952331000	-3.051331000	-0.411809000
1	3.951616000	-3.022957000	-0.851409000
1	2.270479000	-3.560051000	-1.097735000
6	2.959557000	-3.710266000	0.958961000
1	1.950530000	-3.728859000	1.377279000
1	3.320182000	-4.740458000	0.874775000
1	3.617394000	-3.167760000	1.643740000
11	-1.809505000	-2.094069000	-0.185712000
53	-3.170193000	0.369965000	0.053780000

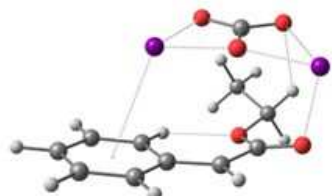
EPA••KI



6	3.696896000	2.695538000	-0.066906000
6	3.127442000	1.432293000	-0.117485000
6	1.712200000	1.278483000	-0.056995000
6	0.913442000	2.457066000	0.056800000
6	1.499490000	3.711846000	0.106008000
6	2.893568000	3.839995000	0.044458000
1	4.777324000	2.798100000	-0.114113000
1	3.753160000	0.554323000	-0.202527000
1	-0.167987000	2.349714000	0.102533000
1	0.873780000	4.595050000	0.192003000
1	3.352509000	4.823668000	0.082913000
6	1.007805000	0.045612000	-0.099087000
1	-0.075226000	0.116301000	-0.037061000
6	1.477656000	-1.316284000	-0.212818000
8	0.698430000	-2.285390000	-0.228817000
8	2.813228000	-1.484604000	-0.305841000

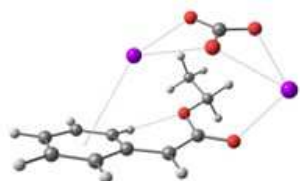
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1	4.298633000	-2.737439000	-0.839374000
1	2.665753000	-3.414304000	-1.067016000
6	3.379584000	-3.487574000	0.983921000
1	2.377734000	-3.583643000	1.408909000
1	3.823426000	-4.485515000	0.906605000
1	3.994414000	-2.886060000	1.659425000
19	-1.922118000	-2.450006000	-0.158746000
53	-3.006425000	0.597920000	0.070302000

EPA⁺·Na₂CO₃



6	-3.022938000	1.291826000	0.647750000
6	-1.850271000	1.082101000	-0.073288000
6	-1.736752000	-0.023252000	-0.969132000
6	-2.873978000	-0.872482000	-1.106835000
6	-4.037531000	-0.651007000	-0.381718000
6	-4.121335000	0.430854000	0.506446000
1	-3.082309000	2.138527000	1.325786000
1	-1.005156000	1.744144000	0.054214000
1	-2.815177000	-1.718723000	-1.785886000
1	-4.884890000	-1.318958000	-0.506057000
1	-5.031716000	0.606676000	1.071343000
6	-0.551955000	-0.380736000	-1.679404000
1	-0.594467000	-1.267418000	-2.303039000
6	0.791552000	0.188248000	-1.613734000
8	1.757817000	-0.392496000	-2.126562000
8	0.880597000	1.346723000	-0.964978000
6	2.201531000	1.893475000	-0.654184000
1	2.883418000	1.065257000	-0.466355000
1	2.527599000	2.469941000	-1.526885000
6	2.035715000	2.732319000	0.596750000
1	1.709524000	2.085617000	1.417133000
1	2.999630000	3.177937000	0.862534000
1	1.313784000	3.541895000	0.441676000
6	1.558887000	-0.748654000	1.412081000
8	0.959196000	-0.010062000	2.276754000
8	2.801129000	-0.639360000	1.124654000
8	0.825950000	-1.659659000	0.738659000
11	2.549598000	-1.931715000	-0.608808000
11	-0.929172000	-0.917576000	1.783256000
0	-2.940467500	0.209673333	-0.229462833

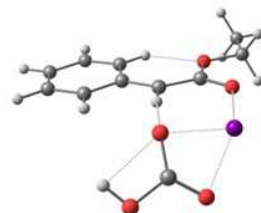
EPA⁺·K₂CO₃



6	-3.814827000	0.884733000	-0.525049000
6	-2.608542000	0.337041000	-0.954856000
6	-2.162334000	-0.933838000	-0.478027000
6	-3.042110000	-1.622191000	0.411048000
6	-4.238703000	-1.061297000	0.836980000

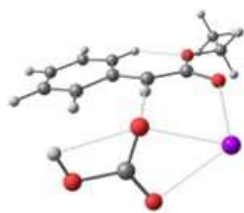
6	-4.635610000	0.205205000	0.384249000
1	-4.124365000	1.851512000	-0.914487000
1	-1.996305000	0.871946000	-1.669468000
1	-2.746951000	-2.602070000	0.777859000
1	-4.872108000	-1.612933000	1.526753000
1	-5.572914000	0.641270000	0.715619000
6	-0.903148000	-1.534612000	-0.794108000
1	-0.768477000	-2.577439000	-0.526564000
6	0.283799000	-0.935394000	-1.322442000
8	1.325725000	-1.567622000	-1.569642000
8	0.226207000	0.418781000	-1.485794000
6	1.421996000	1.078110000	-1.976291000
1	2.275820000	0.789602000	-1.360167000
1	1.597622000	0.748607000	-3.006658000
6	1.182685000	2.572066000	-1.872368000
1	1.125721000	2.856366000	-0.818381000
1	2.025785000	3.108187000	-2.319666000
1	0.268812000	2.866380000	-2.399786000
6	2.209326000	0.795080000	1.300741000
8	1.647200000	1.943475000	1.392841000
8	3.401438000	0.670800000	0.847683000
8	1.539700000	-0.280044000	1.623364000
19	3.134838000	-1.837239000	0.272451000
19	-0.739574000	1.040714000	1.489026000
0	-3.417021000	-0.365057833	-0.054275833

EPA⁺·NaHCO₃



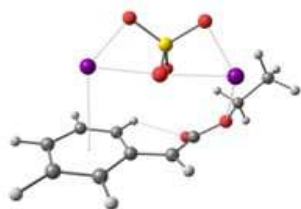
6	3.183979000	-2.406218000	0.214361000
6	2.492313000	-1.208897000	0.104171000
6	1.085686000	-1.208058000	-0.119894000
6	0.426477000	-2.469582000	-0.224823000
6	1.130819000	-3.657173000	-0.111743000
6	2.514896000	-3.633682000	0.108561000
1	4.256581000	-2.390614000	0.385232000
1	3.015880000	-0.266411000	0.187386000
1	-0.646703000	-2.475131000	-0.395760000
1	0.609026000	-4.605967000	-0.193586000
1	3.068088000	-4.563973000	0.197633000
6	0.261713000	-0.057478000	-0.248552000
1	-0.798540000	-0.236244000	-0.423052000
6	0.588914000	1.350231000	-0.179480000
8	-0.275882000	2.238619000	-0.283600000
8	1.883132000	1.664612000	0.006199000
6	2.206047000	3.073499000	0.088316000
1	1.891580000	3.562289000	-0.839436000
1	1.634555000	3.519301000	0.908726000
6	3.702607000	3.173979000	0.310748000
1	4.249754000	2.713954000	-0.517103000
1	3.998405000	4.225193000	0.378977000
1	3.991160000	2.672935000	1.239170000
6	-3.712061000	-0.267169000	0.170909000
8	-3.996738000	0.753409000	0.842745000
8	-4.371346000	-1.421668000	0.498630000
8	-2.869428000	-0.334606000	-0.784889000
1	-4.047373000	-2.082975000	-0.129421000
11	-2.497150000	1.871638000	-0.336990000

EPA⁺·KHCO₃



6	-2.969624000	2.677911000	0.187778000
6	-2.425738000	1.412318000	0.023859000
6	-1.025060000	1.249303000	-0.177195000
6	-0.213047000	2.423242000	-0.191584000
6	-0.771151000	3.679882000	-0.018241000
6	-2.153184000	3.817263000	0.167332000
1	-4.040871000	2.785002000	0.333552000
1	-3.063411000	0.539090000	0.038993000
1	0.861606000	2.312961000	-0.303842000
1	-0.132163000	4.557930000	-0.020620000
1	-2.590567000	4.802560000	0.299899000
6	-0.351609000	0.009555000	-0.358084000
1	0.708283000	0.062412000	-0.599634000
6	-0.828789000	-1.351663000	-0.226068000
8	-0.061593000	-2.325760000	-0.236877000
8	-2.160768000	-1.512490000	-0.074451000
6	-2.632289000	-2.868188000	0.088024000
1	-2.330540000	-3.456635000	-0.784871000
1	-2.149916000	-3.310017000	0.966515000
6	-4.140075000	-2.800283000	0.238090000
1	-4.596923000	-2.347523000	-0.646589000
1	-4.548941000	-3.807777000	0.361774000
1	-4.416181000	-2.205087000	1.113295000
6	3.202052000	0.623839000	0.102031000
8	3.404125000	0.002289000	1.165802000
8	3.400503000	1.995994000	0.142670000
8	2.810929000	0.157587000	-1.015422000
1	3.271384000	2.280263000	-0.773957000
19	2.617567000	-2.210169000	0.060319000

EPA⁺·Na₂SO₄



6	-3.181534000	-0.504697000	-1.314433000
6	-1.942615000	-1.040857000	-0.976878000
6	-1.639062000	-1.348605000	0.380308000
6	-2.645934000	-1.118992000	1.357693000
6	-3.881828000	-0.584968000	1.008601000
6	-4.158723000	-0.266132000	-0.331843000
1	-3.389352000	-0.262210000	-2.352739000
1	-1.176513000	-1.170890000	-1.728884000
1	-2.430915000	-1.346869000	2.398264000
1	-4.636019000	-0.421576000	1.773366000

1	-5.127354000	0.139851000	-0.608982000
6	-0.337240000	-1.735775000	0.802325000
1	-0.126506000	-1.766845000	1.866942000
6	0.775314000	-1.967853000	-0.118269000
8	0.690600000	-2.500545000	-1.205483000
8	1.975540000	-1.536214000	0.401871000
6	3.061208000	-1.531158000	-0.577458000
1	3.358964000	-2.567588000	-0.761024000
1	2.663809000	-1.096081000	-1.496129000
6	4.193685000	-0.689939000	-0.019264000
1	4.510273000	-1.042619000	0.971194000
1	5.061529000	-0.762195000	-0.681766000
1	3.901962000	0.366197000	0.013579000
11	2.007481000	0.539214000	1.708270000
8	0.022593000	1.118735000	0.939788000
16	0.723554000	1.688257000	-0.357721000
8	-0.139619000	2.852102000	-0.788306000
11	-1.917842000	1.880648000	0.164136000
8	2.113883000	2.092547000	0.089038000
8	0.757953000	0.602636000	-1.378338000
0	-2.908282667	-0.810708500	0.020574667

EPA⁺·KOH



6	-3.482266000	1.362313000	-0.233954000
6	-2.100136000	1.281740000	-0.127789000
6	-1.469953000	0.025398000	0.090662000
6	-2.294757000	-1.136711000	0.177112000
6	-3.673305000	-1.038012000	0.063374000
6	-4.276550000	0.211050000	-0.138060000
1	-3.952557000	2.329280000	-0.391877000
1	-1.491958000	2.174442000	-0.196131000
1	-1.787196000	-2.093372000	0.298215000
1	-4.286499000	-1.933007000	0.124636000
1	-5.356829000	0.287959000	-0.225315000
6	-0.071719000	-0.214157000	0.224614000
1	0.197575000	-1.258606000	0.500140000
6	1.051146000	0.651639000	-0.048485000
8	2.207445000	0.213232000	-0.178289000
8	0.784520000	1.976352000	-0.172408000
6	1.902025000	2.848660000	-0.448144000
1	1.446248000	3.745094000	-0.876272000
1	2.548501000	2.380584000	-1.195860000
6	2.678384000	3.170126000	0.821248000
1	3.131327000	2.261140000	1.223325000
1	3.473657000	3.891135000	0.603905000
1	2.016160000	3.601547000	1.577587000
19	2.482597000	-2.520113000	-0.375622000
8	0.434707000	-3.073717000	0.609382000
1	-0.098374000	-3.403257000	1.341529000

Table S4. Interaction Gibbs energies for the formation of salt·EBrPA (ΔG_5) and salt·EPA* (ΔG_6)

Salt/Anion	ΔG_5 (kcal/mol)	ΔG_6 (kcal/mol)
Cl ⁻	+14.2	+4.6
LiCl	-2.4	-15.8
NaCl	+1.4	-11.5
KCl	+3.4	-8.1
Br ⁻	+14.4	+4.4
LiBr	-2.9	-16.7
NaBr	+1.1	-12.0
KBr	+3.2	-8.4
I ⁻	+13.7	+4.4
LiI	-3.8	-17.7
NaI	+1.7	-10.7
KI	+3.1	-8.9
Na ₂ CO ₃	-1.0	-15.3
K ₂ CO ₃	-2.5	-16.1
NaHCO ₃	4.7	-11.5
KHCO ₃	4.1	-8.7
Na ₂ SO ₄	0.6	-11.7
KOH	2.4	-13.7

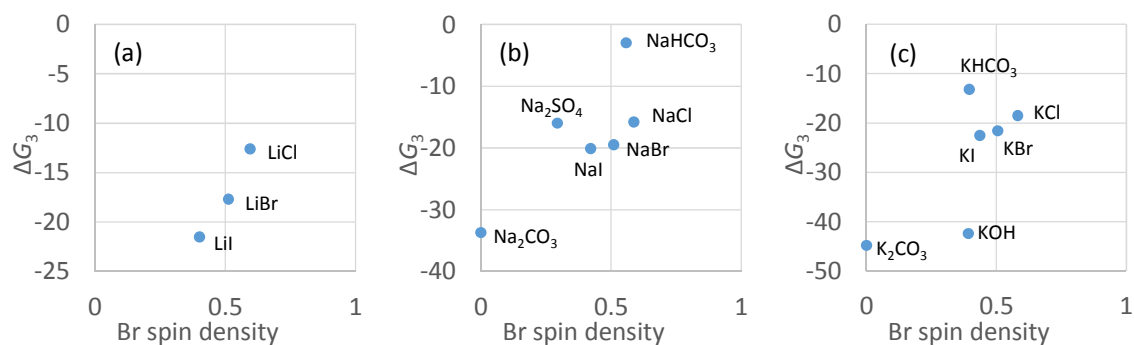


Figure S4. Correlation between the Br spin density and ΔG_3 for the salt·Br[•] adducts. (a) Li salts. (b) Na salts. (c) K salts.

Evaluation of the activation free energy for the MMA propagation at 90°C.

The rate constants at different temperature were extracted from the equation

$$k_p = (10^{6.427} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}) \cdot \exp\left(\frac{-22.36 \text{ kJ} \cdot \text{mol}^{-1}}{RT}\right),$$

which is available in the literature (S. Beuermann, M. Buback, T. P. Davis, R. G. Gilbert, R. A. Hutchinson, O. F. Olaj, G. T. Russell, J. Schweer and A. M. vanHerk, *Macromol. Chem. Phys.* **1997**, *198*, 1545-1560). The data were then used to optimize thermodynamic activation parameters through use of the Eyring equation and the Solver and the Solver Aid macro in Excel, as shown in Table S5.

Table S5. Eyring analysis of the MMA propagation rate constants.

k_p	T	1/T	$\ln(kh/k_B T)$	$\ln(kh/k_B T)_{\text{calc}}$	$(y-y_c)^2$
141.6251	273.15	3.66E-03	-24.4158	-24.4081	5.8E-05
200.5167	283.15	3.53E-03	-24.1040	-24.1016	5.65E-06
277.2415	293.15	3.41E-03	-23.8147	-23.8160	1.7E-06
375.2175	303.15	3.30E-03	-23.5456	-23.5492	1.31E-05
498.0972	313.15	3.19E-03	-23.2948	-23.2995	2.23E-05
649.7266	323.15	3.09E-03	-23.0605	-23.0653	2.28E-05
834.1006	333.15	3.00E-03	-22.8412	-22.8450	1.52E-05
1055.317	343.15	2.91E-03	-22.6355	-22.6377	4.8E-06
1317.534	353.15	2.83E-03	-22.4423	-22.4420	5.85E-08
1624.923	363.15	2.75E-03	-22.2605	-22.2572	1.1E-05
1981.629	373.15	2.68E-03	-22.0892	-22.0822	4.86E-05
$\Delta H^* (\text{cal} \cdot \text{mol}^{-1}) =$			4715.285	9.21283	SUM = 0.000203 0.005
$\Delta S^* (\text{cal} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) =$			-31.2852	0.02893	

From the results ($\Delta H^* = 4.715 \pm 0.009 \text{ kcal} \cdot \text{mol}^{-1}$; $\Delta S^* = -31.29 \pm 0.03 \text{ kcal} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$), the ΔG^* value at 90°C (363.15 K) is calculated as $16.08 \pm 0.01 \text{ kcal} \cdot \text{mol}^{-1}$.