

Support Information

Phosphorane Lifetime and Stereo-Electronic Effects Along the Alkaline Hydrolysis of Phosphate Esters

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1) B3LYP/6-31+G(d,p)/EFP optimized structures for all stationary points located along the alkaline hydrolysis of Monoethyl phosphate dianion (MEP) and Diethyl Phosphate monoanion (DEP). Cartesian coordinates are given in Å.

MEP (Reactant)

15	-0.396023544	0.067647991	0.010425218
8	-2.056400329	-1.189975613	-4.628676940
1	-1.867811554	-0.315159912	-4.261410403
8	-0.389989735	-0.072844209	1.695778618
6	0.890488750	-0.380365065	2.281539778
1	1.675470305	0.138379415	1.722879145
1	1.079649333	-1.460133366	2.193309027
6	0.903089929	0.055650762	3.734867329
1	1.889155453	-0.106984062	4.175664094
1	0.175336616	-0.505570783	4.324314363
1	0.682084154	1.121555372	3.800631428
8	0.633337986	1.164774028	-0.310849065
8	-0.016317421	-1.338984128	-0.481844273
8	-1.838500173	0.490384790	-0.309650623
8	-0.715221463	3.332095793	-1.455523218
1	-1.601870960	3.587906445	-1.257301037
1	-0.572360282	2.499728882	-1.034056181
8	-3.219018142	1.994054551	1.461978723
1	-2.645685328	1.648575462	0.796537413
1	-3.741637450	1.271620080	1.771552539
8	-4.498619740	-2.069584805	-3.644419459
1	-3.727644739	-1.748387136	-4.084087584
1	-4.913816853	-1.322364731	-3.244229538
8	-3.578911881	-1.616869972	-0.011890344
1	-3.480160318	-2.322544096	-0.630881955
1	-2.957708256	-0.950518652	-0.258792002
8	0.318686494	-0.897353963	-5.990174191
1	-0.467418874	-1.268616565	-5.622640674

1	0.522758544	-0.131854534	-5.477101411
8	-3.399365368	1.338982341	-2.385159083
1	-2.666934518	0.984432888	-1.906914178
1	-4.148360196	0.807455708	-2.167524897
8	-2.434147581	-0.675120413	3.537939847
1	-2.192156044	0.069517274	4.065038761
1	-1.830912369	-0.701497604	2.812481387
8	-0.840852539	-2.772248219	-2.719496799
1	-1.180114102	-2.284526122	-3.452918371
1	-0.553081748	-2.138455416	-2.082022793
8	-1.684663424	1.352042112	5.001202689
1	-0.810712794	1.241852149	5.340240920
1	-1.658682432	2.095868107	4.420749133
8	3.876950298	-1.866756517	4.310389384
1	4.297410169	-1.564179132	3.521378055
1	2.965991685	-1.996058815	4.099881011
8	3.357548836	2.218080301	5.438737275
1	2.704903867	2.681096639	5.939285844
1	3.429835702	1.356841948	5.818107228
8	3.012135340	2.457101737	2.805407912
1	3.121895902	2.285289391	3.726988940
1	3.389375829	1.723974393	2.345960022
8	-1.499190364	-2.844198130	1.286413833
1	-0.900390414	-2.295201113	0.805873149
1	-2.366218500	-2.510074207	1.120576956
8	3.258015457	2.653800223	-3.687122932
1	2.908967698	3.290519158	-4.290142927
1	2.974179183	2.912598729	-2.824951977
8	1.578361978	-3.578175151	-0.095762732
1	0.973156839	-4.175111712	0.314446893
1	1.121115999	-2.759479465	-0.203196169
8	0.596633284	3.019863297	1.834208606
1	1.423962066	2.839326243	2.251116165
1	0.518733344	2.415887691	1.113082043
8	-0.488013792	3.208389809	-4.066846509
1	-1.350021853	3.022484517	-4.403387412
1	-0.569508539	3.264327334	-3.128172949
8	1.128850208	1.340594851	-4.889580519
1	0.484566848	1.920274705	-4.515750782
1	1.890899916	1.388012556	-4.334683900
8	2.134489645	3.188930262	-1.289740815
1	1.318841744	3.660404943	-1.347261081
1	1.928537266	2.330201905	-0.956502641
8	1.427689417	3.095421829	7.324567271
1	1.906803305	3.100720955	8.137770969
1	1.093623095	2.219831977	7.212226014
8	4.277671046	1.071286323	0.874696919
1	3.830282452	0.688025569	0.137246518
1	4.525309073	1.945038615	0.617576725
8	5.065865915	-1.194125220	2.105844296
1	5.008729930	-0.299444831	1.810613985
1	4.793869026	-1.736313261	1.382706498
8	-1.636528495	3.197162377	3.193538593
1	-2.264911317	2.863773995	2.573163167
1	-0.804734297	3.225779074	2.748366770

8	2.937056349	-0.155093629	-1.042556752
1	3.111259644	-0.115822924	-1.969373604
1	2.014007863	0.008682472	-0.932841962
8	1.336877460	-4.376212014	-2.721886650
1	1.556282719	-4.180742017	-1.824929981
1	0.566430588	-3.871765781	-2.928826422
8	-2.263162211	-2.670538116	5.310395477
1	-2.420398236	-1.995335374	4.669882757
1	-1.713171360	-3.315530637	4.895217004
8	0.327236690	0.847816308	6.751279251
1	0.753617858	0.008907205	6.678415882
1	-0.461270664	0.708860046	7.251104985
8	-3.243653025	-3.489603400	-1.776934842
1	-3.797144168	-3.192852517	-2.481537511
1	-2.353985218	-3.426306361	-2.085744059
8	-0.652030298	-3.993967702	3.474861426
1	-0.602800383	-4.882107432	3.159167445
1	-0.957264018	-3.466411939	2.754170267
8	3.969424082	-2.341270667	-0.049250640
1	3.522237292	-1.573619270	-0.368019777
1	3.315353328	-3.014406389	0.050540153
8	-4.640110499	-0.258826188	2.079307249
1	-4.465322010	-0.864243464	1.376600084
1	-4.062636232	-0.492284404	2.788461102
8	1.168887742	-1.642813728	6.892914907
1	1.235342424	-2.203907786	6.136848979
1	0.347479546	-1.846760320	7.310734028
8	-4.984209291	3.665622243	0.404180571
1	-4.289473166	3.226490836	0.868275151
1	-4.626966905	3.935866029	-0.426617015
8	3.551403611	-0.246181405	6.421321350
1	2.809308127	-0.663255950	6.829024145
1	3.832482249	-0.815263436	5.722737859
8	-3.445472615	3.863665822	-1.850708480
1	-3.492488104	4.362721018	-2.650465887
1	-3.523051330	2.954773163	-2.093142248
8	1.524883839	-3.108549193	4.716590657
1	2.105466370	-3.845776091	4.818074056
1	0.774484656	-3.418453777	4.235198231
8	1.555999670	4.467589644	-5.125611127
1	1.544610730	5.389200107	-4.922183249
1	0.754210462	4.104592581	-4.784662962
8	3.793500095	-0.043173185	-3.508493810
1	3.426293667	-0.499480482	-4.248643487
1	3.891473790	0.859167774	-3.767454045
8	4.044763973	3.790987701	0.574912996
1	3.595620442	3.713482813	1.401436762
1	3.380798934	3.788468170	-0.095924192
8	-2.870631587	2.435533535	-4.742847944
1	-2.892262792	1.884619062	-5.508944406
1	-3.141764009	1.899034830	-4.015156523
8	2.896486965	-1.532283350	-5.452873283
1	3.052092180	-2.416184076	-5.160666203
1	1.991101812	-1.489002932	-5.716089893
8	5.512311703	3.717966990	4.708820245

1	5.372880202	3.785254439	3.777740382
1	4.817279242	3.177418990	5.048844056
8	3.902627489	-4.448675667	4.940025825
1	4.158570698	-3.552439985	4.791253748
1	4.294124972	-4.960640521	4.250460626
8	-1.345525483	3.718938581	7.608871187
1	-1.696902829	4.084399985	6.812723979
1	-0.406996812	3.704607383	7.509689513
8	-1.429538896	-1.691497707	7.652008347
1	-1.825471929	-2.043310493	6.870763665
1	-1.839225606	-0.856225509	7.811242792
8	3.505351081	-3.811908877	-4.218951115
1	4.125382583	-3.440009878	-3.612213507
1	2.755962580	-4.079341127	-3.711235327
8	-0.580667882	-5.174234355	0.586663316
1	-0.792399536	-5.561104134	-0.247830503
1	-1.152620057	-4.431130564	0.694115258
8	-5.397987311	-0.171662902	-1.508608477
1	-4.957209140	-0.800376754	-0.959689584
1	-5.926286367	0.363359578	-0.938056544
8	-6.419999854	1.327897206	0.488434367
1	-5.998410185	0.914741821	1.224941823
1	-6.057632829	2.196799384	0.420776421
8	-2.233521651	1.116128165	7.602422440
1	-2.054644304	1.994031129	7.899352962
1	-2.428807363	1.175932241	6.680920722
8	5.139106574	-2.338425208	-2.584877436
1	4.899539822	-2.416942497	-1.675305415
1	4.884037256	-1.471937082	-2.858768700
8	-0.473476802	0.547185595	-8.138718448
1	0.062030684	1.321859249	-8.075544749
1	-0.104765454	-0.086682739	-7.544461491
8	-2.326942100	4.696246176	5.258285156
1	-3.258274990	4.828595303	5.180946864
1	-2.048141521	4.261745858	4.468121777
8	1.402066950	2.483903821	-7.303792282
1	1.422593751	3.383155677	-7.017779687
1	1.432326770	1.950905571	-6.525412129
8	-2.802547817	0.614269013	-6.653717331
1	-2.687998595	-0.154631062	-6.118414047
1	-2.069386605	0.643151591	-7.247450342

MEP (Transition State)

15	-0.574519628	-0.168959764	-0.548343850
8	-0.628969407	-0.235083034	-2.607998508
1	-0.335871407	0.665194360	-2.791792108
8	-0.534857531	-0.164570813	1.362105845
6	0.721985731	-0.464237276	1.927306198
1	1.523154665	0.049536802	1.374250269
1	0.950333552	-1.545142167	1.852333863
6	0.799414703	-0.045322852	3.396423409
1	1.809931205	-0.189787260	3.792941612

1	0.115692657	-0.625761624	4.021803449
1	0.559505486	1.013971129	3.494817443
8	0.498095070	0.961652044	-0.655530051
8	-0.211565454	-1.678123527	-0.590101802
8	-2.059544056	0.297356207	-0.527155663
8	-0.698731882	3.270309616	-1.544339152
1	-1.521300942	3.592279232	-1.211782145
1	-0.549989746	2.432715087	-1.135450860
8	-3.149815412	1.813350384	1.391665468
1	-2.571062655	1.412189539	0.763180244
1	-3.700730317	1.125934571	1.730532288
8	-3.105579234	-0.865533566	-3.638613718
1	-2.241447031	-0.674834831	-3.310302918
1	-3.685593622	-0.220537603	-3.266535807
8	-3.855731315	-1.678033856	-0.126880003
1	-3.759662987	-2.328429053	-0.804106271
1	-3.194606964	-1.022994315	-0.284094016
8	0.592883498	-0.744999881	-5.007913720
1	0.217468148	-0.830342516	-4.146137413
1	0.836504423	0.161243163	-5.109160175
8	-3.659595138	1.608035613	-2.230382848
1	-2.926977185	1.215476465	-1.783117039
1	-4.439301593	1.221502503	-1.864967394
8	-2.429801760	-0.664324950	3.365265656
1	-2.177164916	0.075914997	3.893562826
1	-1.846230306	-0.680078491	2.623595487
8	-0.603464478	-3.120612358	-2.840180882
1	-0.672120119	-2.647069349	-3.653766695
1	-0.429533667	-2.481242174	-2.167996164
8	-1.661447629	1.340465533	4.867605658
1	-0.782567316	1.198461993	5.181106606
1	-1.625092422	2.082048283	4.284843462
8	3.825344951	-1.915921062	4.248602479
1	4.260440314	-1.597783243	3.473774235
1	2.912186561	-2.008247092	4.028384147
8	3.302786285	2.184678039	5.300499476
1	2.660001403	2.657222353	5.804888136
1	3.368413578	1.324151024	5.682683683
8	2.949023660	2.388649440	2.657777040
1	3.021981320	2.240883552	3.587142886
1	3.367449345	1.656921124	2.233074706
8	-1.693064599	-2.929724737	1.244329584
1	-1.115359808	-2.326450435	0.804789206
1	-2.573327220	-2.632791624	1.077455684
8	3.185950509	2.898395192	-3.760516435
1	2.958073581	3.730379548	-4.143599442
1	2.889564890	2.921928254	-2.864703835
8	1.593245591	-3.635204891	-0.032764435
1	1.029753051	-4.223780660	0.443610601
1	1.096054226	-2.847517078	-0.185168864
8	0.522744131	2.745768649	1.577426635
1	1.363079850	2.609264581	1.984956968
1	0.372214524	2.005488788	1.011560026
8	-0.586530031	3.317748976	-4.142621209
1	-1.445832952	3.102158875	-4.468194321

1	-0.630257885	3.258673736	-3.201623630
8	1.216051703	1.790465198	-5.226118469
1	0.540341057	2.296440122	-4.803882807
1	2.027413814	2.009352113	-4.796399377
8	2.089686338	3.042928808	-1.337390095
1	1.277038422	3.522766298	-1.352810975
1	1.884584618	2.171564727	-1.038163799
8	1.403140355	3.078557279	7.217216972
1	1.892426655	3.072599749	8.024336467
1	1.081184774	2.200662947	7.088668934
8	4.339920695	1.047409237	0.812135001
1	3.861373845	0.663195313	0.095022021
1	4.562451008	1.926345111	0.549779436
8	5.082029142	-1.213941317	2.087400265
1	5.046250511	-0.312958517	1.808422958
1	4.782632013	-1.735315575	1.359795499
8	-1.601395668	3.151340913	3.026136657
1	-2.244663758	2.769211001	2.450757348
1	-0.777608202	3.127424266	2.566048992
8	2.944183140	-0.135815717	-1.080076961
1	3.179563877	-0.055684590	-1.990600638
1	2.014531977	0.018018253	-1.025650134
8	1.698126928	-4.576035606	-2.567100670
1	1.825720590	-4.331788645	-1.664359437
1	0.895352680	-4.166743494	-2.848013339
8	-2.338419492	-2.605610889	5.198234850
1	-2.447226932	-1.944345619	4.533578820
1	-1.797967437	-3.281895993	4.822165056
8	0.330513473	0.826377122	6.612062143
1	0.746507757	-0.018676279	6.551136297
1	-0.466802277	0.701593236	7.101546596
8	-3.338849513	-3.190287760	-2.287058212
1	-3.456277885	-2.480122155	-2.897593914
1	-2.428847385	-3.437155306	-2.329848351
8	-0.744623147	-4.002712903	3.423981249
1	-0.677649110	-4.886375038	3.099121027
1	-1.088333864	-3.479350990	2.717699644
8	3.930819769	-2.313793546	-0.047673013
1	3.474529375	-1.554190643	-0.372759095
1	3.281585060	-2.987420479	0.077224947
8	-4.736391038	-0.353916790	2.131615453
1	-4.644679517	-0.960972137	1.414711515
1	-4.059662734	-0.565599484	2.754598353
8	1.120882077	-1.675598743	6.823818604
1	1.186278623	-2.240570155	6.070553014
1	0.281266668	-1.847062187	7.219450637
8	-4.815591902	3.715618116	0.704993235
1	-4.113642328	3.140646076	0.964901683
1	-4.560676076	4.099884170	-0.118557599
8	3.498013671	-0.266372124	6.332992939
1	2.753106770	-0.674566596	6.744538119
1	3.776848746	-0.845117862	5.641485291
8	-3.418020390	4.129181549	-1.671789454
1	-3.441662566	4.669685779	-2.445206986
1	-3.578822344	3.243263631	-1.954933634

8	1.458647994	-3.138505304	4.645696938
1	2.025102763	-3.890129038	4.716895343
1	0.701599876	-3.414919615	4.154421323
8	1.470995982	5.021243511	-4.525688978
1	1.370560612	5.673828418	-3.851208342
1	0.685233291	4.498395477	-4.516448730
8	4.021557797	0.125029515	-3.456995478
1	3.702391935	-0.387287087	-4.182628516
1	4.028211170	1.024726787	-3.742265535
8	3.972861002	3.774843875	0.492358104
1	3.535621729	3.643012474	1.318385195
1	3.315147217	3.690115667	-0.179290734
8	-3.016039547	2.480294772	-4.711161689
1	-3.049921999	1.778052356	-5.340912451
1	-3.330260121	2.127362596	-3.894104308
8	3.118285053	-1.526476825	-5.262052834
1	3.329356027	-2.396333338	-4.962591409
1	2.177191157	-1.455613839	-5.247940050
8	5.451633532	3.659280298	4.506111224
1	5.295360397	3.710279347	3.576672545
1	4.761841750	3.126504283	4.868347983
8	3.842421487	-4.517827107	4.790307066
1	4.077835200	-3.611048007	4.675370123
1	4.203601531	-4.987129990	4.055336159
8	-1.342233460	3.758077624	7.451540351
1	-1.674605067	4.104494002	6.638888358
1	-0.403100306	3.718738579	7.365751003
8	-1.498060310	-1.641867572	7.537084268
1	-1.892269237	-1.980935280	6.749359148
1	-1.882479189	-0.793378767	7.689292440
8	3.821749853	-3.789351350	-4.043541585
1	4.418627869	-3.378437831	-3.438756361
1	3.106647661	-4.129600729	-3.529987625
8	-0.613942786	-5.223587149	0.648523676
1	-0.712696696	-5.567565086	-0.224863579
1	-1.172964277	-4.465272201	0.706246007
8	-5.628332654	0.195168749	-1.211503836
1	-5.189864611	-0.552575679	-0.838003502
1	-6.066645095	0.635498166	-0.500961323
8	-6.465467351	1.511298011	0.984259326
1	-5.973998088	1.015134199	1.619206481
1	-6.040235801	2.350451124	0.907587071
8	-2.240656868	1.154829457	7.449761217
1	-2.056105480	2.032272955	7.744569878
1	-2.406117504	1.209488164	6.522122463
8	5.339279365	-2.229577333	-2.406808130
1	5.005369970	-2.324644465	-1.529115012
1	5.114300655	-1.357659515	-2.689690352
8	-0.823523016	-0.581802697	-7.311782718
1	-0.347382485	0.152256699	-7.665796070
1	-0.351645694	-0.867297174	-6.545817215
8	-2.280535773	4.691318056	5.061024028
1	-3.211351859	4.819295328	4.971125833
1	-1.992232051	4.241074374	4.283180827
8	0.579488694	1.746372109	-7.794957177

1	0.004150087	2.489174978	-7.885000714
1	0.958159736	1.799567643	-6.932022109
8	-3.114266927	0.205613442	-6.141697795
1	-3.143005057	-0.356402194	-5.383943879
1	-2.364471874	-0.061260201	-6.649107187

MEP (Final Product)

15	-0.733310174	-0.147619279	-1.753851709
8	-1.473732037	-0.356978405	-3.299122658
1	-1.120270094	0.311085389	-3.900761768
8	-0.236413397	-0.470339542	2.011815202
6	0.998888931	-0.665819694	2.579313800
1	1.830511524	-0.218385118	1.984183677
1	1.290361277	-1.748672224	2.643442622
6	1.076779003	-0.089921715	4.005546582
1	2.065981967	-0.165163481	4.460111056
1	0.357293140	-0.605482854	4.648209259
1	0.813285095	0.970176829	3.981589864
8	0.616083730	0.493061165	-2.096209146
8	-0.716200705	-1.585637671	-1.229039615
8	-1.723123780	0.766041095	-0.998923740
8	-0.918258056	3.361662581	-1.453775060
1	-1.679122648	3.856048417	-1.193878595
1	-1.025489852	2.492998218	-1.100501766
8	-2.950561186	1.772986051	1.257991468
1	-2.319537856	1.477397021	0.621347819
1	-3.424870172	1.009005067	1.544770991
8	-4.131770925	-1.054022319	-3.691225336
1	-3.277391782	-0.719149025	-3.470375586
1	-4.751912201	-0.595033309	-3.147504507
8	-3.362157591	-1.521850506	-0.260812177
1	-3.317302345	-2.232977790	-0.879814961
1	-2.606193718	-0.978570057	-0.416515198
8	1.014298103	-0.833009223	-4.614441799
1	0.892150021	-1.159440153	-3.737286654
1	1.113012189	0.103050507	-4.544255146
8	-3.717825789	1.908752132	-2.383252798
1	-2.919366018	1.550495124	-2.029710205
1	-4.422184498	1.366025161	-2.066701543
8	-2.372130414	-0.664205491	3.718341074
1	-2.222259314	0.110392277	4.236429295
1	-1.649079998	-0.731373326	3.115377534
8	-0.855671104	-3.134912973	-3.421476542
1	-1.029470382	-2.448095892	-4.045138760
1	-0.741763850	-2.717281457	-2.582734920
8	-1.634332812	1.453323951	5.085869805
1	-0.743314311	1.304974221	5.359652280
1	-1.607480454	2.133046921	4.431550243
8	3.739470000	-2.050128242	4.436526900
1	4.119511170	-1.745071795	3.628202877
1	2.805940500	-2.084294077	4.301494231
8	3.360604255	2.137251921	5.407183276

1	2.727315735	2.618238361	5.915588772
1	3.443416266	1.287833611	5.810307524
8	2.896846873	2.255175657	2.746165226
1	2.988029137	2.137292724	3.678188757
1	3.346706967	1.533774423	2.336183994
8	-1.457423460	-2.733732463	1.468617167
1	-0.871955457	-1.994006059	1.438442370
1	-2.256797329	-2.464476468	1.045083130
8	3.263728199	3.003291843	-3.602724570
1	3.011525595	3.806498341	-4.029493387
1	2.869495590	3.016328977	-2.745234548
8	1.350392669	-3.319333863	-0.569551229
1	0.871735139	-3.954847868	-0.061725105
1	0.792789930	-2.562248868	-0.651891682
8	0.383479936	2.208303829	1.703244780
1	1.261773889	2.186206457	2.048193896
1	0.100990215	1.311309003	1.622756925
8	-0.582847596	3.269179080	-4.053476946
1	-1.415753204	3.065631646	-4.448084529
1	-0.716354984	3.262059387	-3.119130361
8	1.296662081	1.713815243	-4.928301630
1	0.614587853	2.210507933	-4.505277312
1	2.114277892	2.005474782	-4.557737799
8	1.798644497	2.912330814	-1.365292217
1	0.990204567	3.395268237	-1.301458219
1	1.568492151	1.996957789	-1.366051333
8	1.516892826	3.194780758	7.309483531
1	2.019613703	3.253797072	8.106143589
1	1.165133271	2.319597085	7.274882808
8	4.345537119	0.995641388	0.848926514
1	3.861958687	0.633039824	0.123977923
1	4.481265081	1.909261068	0.654618889
8	4.854090900	-1.369280412	2.168198889
1	4.873903781	-0.462832862	1.905827506
1	4.521587605	-1.857566068	1.432062264
8	-1.593822396	3.120435178	3.081594429
1	-2.242717373	2.753672027	2.502544730
1	-0.756785445	2.999107051	2.662634905
8	3.096028507	-0.087444515	-1.217249195
1	3.493138800	0.059052358	-2.060884504
1	2.162631952	-0.023518993	-1.342000362
8	1.722861913	-4.226526791	-3.082823629
1	1.698002390	-3.949566592	-2.180851619
1	0.903087573	-3.963878551	-3.469946849
8	-2.378745880	-2.555063314	5.571548770
1	-2.466631869	-1.895700677	4.901925428
1	-1.867472680	-3.254878926	5.197735611
8	0.371588365	0.944636516	6.900342982
1	0.761014612	0.085795304	6.860125757
1	-0.443937345	0.851170790	7.366240426
8	-3.460085972	-3.306950202	-2.297705848
1	-3.873341415	-2.701307981	-2.892092837
1	-2.611447815	-3.505983787	-2.659751928
8	-0.876932802	-3.991484225	3.715973499
1	-0.797575513	-4.871801978	3.384882077

1	-1.158563255	-3.454078083	2.992953872
8	3.795282952	-2.332763919	-0.116591663
1	3.513662207	-1.498435229	-0.456391380
1	3.041502998	-2.900600884	-0.132573426
8	-4.353160305	-0.412681613	1.998178873
1	-4.135817696	-1.028060519	1.316306857
1	-3.801035790	-0.618581382	2.735499874
8	1.119030316	-1.593798119	7.182349799
1	1.153932963	-2.189020345	6.450659454
1	0.275222115	-1.712200066	7.588363535
8	-4.817219199	3.545927489	0.745525476
1	-4.059255946	3.013675439	0.927398825
1	-4.617862806	4.045973433	-0.029774168
8	3.582157117	-0.312502530	6.528015358
1	2.825968545	-0.667655791	6.967245889
1	3.809432259	-0.921653560	5.843793546
8	-3.599483804	4.375309563	-1.622077872
1	-3.715955781	4.994264433	-2.325076878
1	-3.733371038	3.517048981	-1.991322284
8	1.329529325	-3.197092642	5.068456944
1	1.888890860	-3.956908865	5.094388305
1	0.578180678	-3.431015739	4.547272092
8	1.447380062	5.008614955	-4.460019586
1	1.330966660	5.645104855	-3.772846404
1	0.689781028	4.446017012	-4.439877318
8	4.384394551	0.353434800	-3.463398381
1	4.124269067	-0.140517798	-4.224466064
1	4.276261611	1.265289104	-3.681818729
8	3.630727967	3.661632719	0.504519875
1	3.241626857	3.502120785	1.349525629
1	2.971461423	3.459981745	-0.140137370
8	-2.962299139	2.471036418	-4.857120927
1	-3.028689114	1.714247884	-5.417247644
1	-3.382024365	2.243559414	-4.042895283
8	3.552699399	-1.260935289	-5.373256536
1	3.808794603	-2.136168671	-5.129822299
1	2.613828764	-1.218809565	-5.285930667
8	5.408622447	3.657930869	4.449037706
1	5.181337976	3.688552878	3.533460011
1	4.767605524	3.107236371	4.869408171
8	3.694102979	-4.642849084	4.994543299
1	3.942095521	-3.743989010	4.848157780
1	3.962655749	-5.126363463	4.229708866
8	-1.224193699	3.958155339	7.509705394
1	-1.556749608	4.250913878	6.676292256
1	-0.288020055	3.882027377	7.416636082
8	-1.516919557	-1.474615931	7.861166289
1	-1.902394217	-1.859552664	7.090380033
1	-1.897387424	-0.615921675	7.954797643
8	4.100480118	-3.620125512	-4.244193002
1	4.632123230	-3.290996042	-3.537151386
1	3.284172972	-3.900342565	-3.862094190
8	-0.502908416	-4.985014871	0.634829499
1	-0.970531095	-5.333007867	-0.107537230
1	-0.934906534	-4.180892597	0.874919998

8	-5.291789292	0.052467198	-1.358469992
1	-4.678835767	-0.510539206	-0.913284393
1	-5.841745659	0.434500348	-0.693280455
8	-6.288282189	1.214355750	0.841851359
1	-5.765431686	0.732385185	1.462504386
1	-5.943106778	2.092579347	0.820504142
8	-2.212435660	1.369077927	7.663357496
1	-1.998386597	2.249123695	7.929028156
1	-2.358573052	1.395060034	6.731237736
8	5.456741281	-2.270462068	-2.320525009
1	5.017778529	-2.387139907	-1.493133664
1	5.339985063	-1.366158631	-2.564413782
8	-0.774630336	-0.771785783	-6.626500691
1	-0.366423542	-0.063996918	-7.099026448
1	-0.197038653	-0.990079101	-5.912627922
8	-2.199489024	4.761209312	5.073450897
1	-3.136356645	4.859638841	5.014551477
1	-1.929445955	4.274142688	4.311400177
8	0.463588224	1.540588009	-7.430832878
1	-0.150111216	2.255422590	-7.487955310
1	0.924650872	1.643518765	-6.613700729
8	-3.217316959	0.117658213	-6.100305931
1	-3.666216314	-0.421184264	-5.468628318
1	-2.391448598	-0.303380627	-6.277918428

DEP (Reactant)

15	0.071124105	1.050623939	-0.602679211
8	1.342520101	0.224251396	0.001436435
8	-1.074845736	1.071033383	0.381572027
8	0.715369121	2.569593397	-0.564271436
6	1.134041509	-1.175703440	0.407745682
1	0.641911904	-1.157847692	1.373917258
1	0.463029253	-1.663868819	-0.306076309
6	2.478783059	-1.857221741	0.513960452
1	2.331757368	-2.846115928	0.947553789
1	3.148716964	-1.302924715	1.177204453
1	2.958224788	-1.975200717	-0.462838457
6	1.621895381	2.984026050	-1.630225761
1	1.027495812	3.169760234	-2.530972691
1	2.317948040	2.176277132	-1.845277712
6	2.351697293	4.232320431	-1.179158135
1	2.919768166	4.052317974	-0.262827325
1	1.662298319	5.056735563	-0.993047348
1	3.060408710	4.548633020	-1.952636264
8	-0.200862903	0.631822803	-2.034777136
8	-1.523437980	-2.748078163	-0.807312493
1	-1.806032007	-3.366130912	-0.123238467
8	-3.490185007	1.422699048	-0.851572689
1	-2.696630135	1.191523892	-0.395823672
1	-3.249599705	1.585829357	-1.749562482

8	-1.631257522	3.382120218	1.680789788
1	-1.594170240	2.755034159	0.976328247
1	-2.375173278	3.148796663	2.212793473
8	-0.357286649	0.274446286	3.002612796
1	-0.069613122	1.088399206	2.621033131
1	-0.882307719	-0.160555269	2.349922228
8	-4.164952690	-2.337101879	-1.447638906
1	-3.234895683	-2.306897242	-1.289651259
1	-4.377245302	-3.234923474	-1.646954446
8	-1.769313090	-1.440468961	1.561587106
1	-1.684743633	-1.385274372	0.623141573
1	-1.610845216	-2.340987586	1.795750708
8	1.170871008	-3.521046992	3.283401581
1	0.347519914	-3.635699388	2.836382276
1	1.735330168	-4.220814800	2.996017996
8	0.752617208	-4.350895859	-1.117256791
1	0.152236654	-3.635920390	-0.978578307
1	0.827403346	-4.465073341	-2.051199504
8	-1.458482536	-1.231302952	-3.831390045
1	-2.093616218	-0.607068472	-4.144143901
1	-1.161624526	-0.918750395	-2.991708751
8	-3.948676461	-0.186031932	2.368661133
1	-3.162866269	-0.655746030	2.138988621
1	-4.573296257	-0.349191920	1.680106572
8	-1.914808914	-3.768439142	-3.272136628
1	-1.686363850	-3.589519050	-2.373983574
1	-1.944388427	-2.935755015	-3.715578451
8	0.775522607	2.721317208	2.388753620
1	-0.085727710	3.069227598	2.221168695
1	1.206606719	2.649513709	1.552159812
8	5.032490812	2.477143306	0.959994046
1	4.370697103	2.789357689	1.556173313
1	4.592650092	1.930841770	0.328350771
8	-1.216365108	-3.894550076	2.279710773
1	-1.117508237	-4.527138965	1.586214508
1	-1.836360924	-4.257670261	2.891778885
8	4.368704768	-0.261034092	4.082268892
1	4.626345683	-1.021003357	4.579205839
1	3.475044048	-0.402737511	3.813625799
8	1.858048729	5.104033369	3.262771422
1	2.765198749	4.886897763	3.407026139
1	1.400067377	4.287988790	3.139471866
8	-2.000337001	2.305359730	-3.184818890
1	-1.366558593	1.692807094	-2.847205721
1	-1.845813118	3.125864174	-2.744622024
8	5.732777796	-1.147271071	0.256996688
1	6.058918320	-0.663452033	0.998906353
1	5.136380278	-0.575214936	-0.199007954
8	4.013223945	0.674157142	-0.750415504
1	4.035200376	0.809438951	-1.684275410
1	3.123630809	0.448671785	-0.529827973
8	2.038720630	-1.841200049	6.332785862
1	1.423138236	-2.551234023	6.421038484
1	1.950824780	-1.513868825	5.451873242
8	-0.693836318	-5.781001074	0.552952744

1	-0.060589221	-5.505566492	-0.090485178
1	-0.266520374	-6.423654818	1.096345516
8	1.537232497	0.558919209	-4.144900058
1	1.076569775	0.435650839	-3.330361404
1	0.957052019	1.037850901	-4.714894358
8	-3.103575016	-4.504452423	4.031281080
1	-3.835976609	-4.441748027	3.439221523
1	-3.074273441	-3.693535041	4.513394005
8	-3.355099635	-5.734669593	0.054067766
1	-2.419027647	-5.829050448	0.129830166
1	-3.534800692	-5.529293274	-0.849484419
8	5.107333554	-3.641336508	0.857193521
1	5.147578770	-2.707157501	0.728475385
1	5.883406707	-4.003529676	0.460450500
8	1.558991858	6.544040461	1.065632327
1	0.639030153	6.473436363	0.866725375
1	1.696049957	6.088361244	1.880770341
8	-4.608358465	-4.276724484	1.878119299
1	-4.195633116	-4.802310223	1.211564071
1	-4.686225952	-3.404389248	1.526201205
8	1.838930630	-1.050118162	3.783352835
1	1.695259076	-1.906831235	3.414192097
1	1.091606971	-0.524164133	3.547221170
8	-4.129007017	0.746776366	5.000505366
1	-3.251646223	0.613645692	5.322052742
1	-4.227023204	0.193108354	4.242400482
8	-3.807006903	2.410694286	2.757438324
1	-4.010438557	2.495395902	3.675218065
1	-3.790869745	1.486314011	2.567335317
8	4.575453213	-4.365200855	3.474718448
1	4.838783406	-4.064033316	2.619830282
1	3.859506974	-4.965797696	3.342118024
8	-5.266394843	-0.755158657	-3.371910091
1	-5.994695667	-0.350873889	-2.928051792
1	-4.847104590	-1.322051450	-2.744449575
8	0.825194111	-2.043810879	-4.996252549
1	-0.037587632	-1.774261924	-4.724536745
1	1.404199810	-1.320001902	-4.818119400
8	-4.065505240	-4.908591321	-2.445002887
1	-3.344811411	-4.608339056	-2.975405976
1	-4.645367970	-5.383274658	-3.018861231
8	-0.341749415	6.812769247	3.813837011
1	0.475563932	6.342892111	3.859584400
1	-0.689983797	6.667741048	2.948632937
8	-1.307914247	4.329111697	-1.665616285
1	-0.676177424	4.037992523	-1.027622032
1	-1.954581534	4.832245959	-1.197048479
8	-1.125079229	5.948990523	1.229928411
1	-1.875186951	6.208654600	0.719250992
1	-1.247537786	5.038982446	1.448486543
8	4.611663913	-2.496947831	5.412727021
1	4.577992620	-3.225632531	4.813758486
1	3.803338389	-2.508667821	5.899913786
8	6.229466673	0.416196097	2.290586351
1	5.596518066	0.190399425	2.953361107

1	5.978308509	1.260729098	1.952116203
8	-5.218942715	-0.420642047	-0.011280776
1	-4.644457686	0.240337992	-0.363347238
1	-4.973074767	-1.237199529	-0.415831497
8	-1.867987006	-2.312014513	4.809378863
1	-1.543321866	-2.220638123	3.927833994
1	-1.886541099	-1.445374717	5.182835236
8	5.738070963	5.116040469	1.302573331
1	5.170712827	5.694645850	0.818632206
1	5.743654044	4.292824046	0.840878622
8	1.750484577	2.209841202	4.975305110
1	2.688342316	2.306459595	4.930963224
1	1.427521473	2.289257409	4.091978243
8	3.000519094	-5.131323315	0.087606411
1	2.310017876	-4.697544100	-0.387706238
1	3.696393722	-4.501888313	0.189824485
8	3.986454970	1.076180029	-3.384845754
1	3.154215728	0.930505293	-3.805601229
1	4.334431517	1.877558964	-3.742032791
8	4.215763997	3.952398833	3.159757263
1	4.578191660	3.440543287	3.865114296
1	4.930088529	4.443067362	2.785774228
8	-1.101381095	-6.194383621	4.714223745
1	-0.599026975	-5.566380000	5.208319125
1	-1.932035650	-5.788335268	4.524444398
8	3.987713266	6.753609182	0.000276373
1	3.087462840	6.644562204	0.262070911
1	4.178780881	7.675775911	0.063364761
8	-4.648012699	3.497182901	0.432109540
1	-4.544744873	3.254955499	1.338498031
1	-4.334172224	2.769514355	-0.080609776
8	-1.508594746	0.198604214	5.380083898
1	-1.100735319	0.410157376	4.555599573
1	-0.870592039	0.377707154	6.052209731
8	4.488750241	2.123263768	5.043794588
1	4.559304460	1.224550865	4.764123934
1	4.849054238	2.165296340	5.915168645
8	-7.181324796	0.358140914	-1.662438770
1	-6.683063999	0.105792477	-0.901561054
1	-7.331338743	1.287381493	-1.592537293
8	7.289939949	-2.937337707	-0.947741718
1	6.847222817	-2.175817692	-0.608673492
1	7.127201434	-2.954290949	-1.877315393
8	-0.526173122	1.726336357	-5.478834969
1	-1.038490273	1.044975451	-5.883997785
1	-1.079304862	2.132793605	-4.830979864
8	-3.310415071	0.491363659	-4.618062340
1	-3.170519946	1.314120873	-4.177178710
1	-4.114561349	0.133978933	-4.276736433
8	0.668517817	0.594356755	6.825748557
1	1.125337073	1.184745556	6.248136503
1	1.188356570	-0.191810476	6.876613189
8	0.136501862	-3.897562271	5.702962166
1	-0.628252839	-3.353290739	5.603981352
1	0.641728578	-3.802063652	4.911441835

8	2.396224212	-5.700751664	2.516557894
1	2.595322593	-5.663200746	1.594696615
1	1.755981608	-6.385232308	2.628155875
8	0.649754585	-4.491406061	-3.785255323
1	-0.293157577	-4.457872769	-3.811151813
1	0.961040467	-3.724244897	-4.238513861
8	0.177746489	-7.209662611	2.681379694
1	-0.309146546	-6.850397209	3.405770471
1	0.136215253	-8.148827561	2.765776411
8	-3.322955931	5.595128607	-0.372797388
1	-3.848668587	4.895441338	-0.019325488
1	-3.908514820	6.158357635	-0.853185047

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15	-0.390519462	0.252469525	-0.412668180
8	0.762000449	-0.875543133	-0.021715307
8	-1.549828665	0.467559028	0.555956970
8	0.516710421	1.614182681	0.111680704
6	1.371609920	-0.899787267	1.288901209
1	1.641467534	0.119101811	1.582172915
1	0.648596658	-1.290926364	2.006827670
6	2.607505217	-1.782221353	1.227454986
1	3.186225220	-1.695082977	2.149618521
1	3.253948344	-1.491231544	0.393059663
1	2.338924585	-2.824483032	1.091395473
6	1.665590730	1.992889293	-0.652215712
1	1.362570513	2.692998853	-1.438560094
1	2.081551244	1.113729302	-1.149092480
6	2.679081169	2.633787949	0.278730944
1	2.966294898	1.933322043	1.072101837
1	2.264389504	3.523173038	0.734549452
1	3.570568058	2.915669016	-0.270310638
8	-0.457660461	0.475736915	-1.913252781
8	-1.548758669	-1.839982965	-0.920012028
1	-1.173569150	-2.437719881	-0.263258798
8	-3.695458620	1.476253925	-0.837585341
1	-2.984022484	1.081538962	-0.359111543
1	-3.372987787	1.652248254	-1.707020221
8	-1.756969447	2.954759687	1.759419405
1	-1.646602172	2.240626040	1.152203914
1	-2.597419309	2.833121250	2.171398257
8	-1.177044610	-0.014973262	3.244373193
1	-0.420125309	0.538358567	3.135858156
1	-1.606216157	-0.055313801	2.404692970
8	-4.242470623	-2.044035200	-1.526227477
1	-3.332163638	-1.893598119	-1.327259307
1	-4.333114227	-2.967252600	-1.700387814
8	-2.853993329	-1.678329746	1.539330569
1	-2.559560519	-1.323479758	0.715759527
1	-2.155061498	-2.222216827	1.865765237
8	1.266011960	-3.225920246	3.590191712
1	0.471768062	-3.237494725	3.080367119
1	1.854654835	-3.845429013	3.189458749

8	1.175855214	-3.503532191	-1.129922631
1	0.903290700	-2.625315490	-0.917031896
1	1.129376809	-3.581778051	-2.069388329
8	-1.473738613	-0.913146550	-4.070495652
1	-2.166645408	-0.338845172	-4.354989158
1	-1.229175070	-0.634017995	-3.202650979
8	-4.734909430	-0.079950141	2.459664001
1	-4.009197626	-0.671667520	2.340956906
1	-5.303018413	-0.194525710	1.714678715
8	-1.741618291	-3.350150595	-3.209452498
1	-1.556282206	-3.026128607	-2.342539157
1	-1.831374874	-2.594618173	-3.768015806
8	0.620905819	2.634540563	2.666069033
1	-0.290602127	2.874699508	2.617536577
1	0.837914476	2.225768435	1.843456703
8	5.667477658	2.359755890	1.069734960
1	5.001236415	2.737002149	1.621718945
1	5.221999147	1.816313829	0.439577776
8	-1.027141866	-3.462626998	2.342283189
1	-0.862205552	-4.001212766	1.584919447
1	-1.599978271	-3.956566444	2.906872181
8	4.874582460	-0.541199209	4.399413600
1	5.353020774	-1.269582942	4.761949629
1	3.975055759	-0.817343990	4.325425566
8	2.153041405	4.840998854	2.675608710
1	3.030071811	4.565912079	2.890139330
1	1.601157552	4.080273236	2.762782103
8	-2.096954945	2.372767633	-2.995138317
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1	-1.941687125	3.245890665	-2.671987380
8	6.385506922	-1.135971136	0.154285619
1	6.568760123	-0.722399719	0.982690956
1	5.918025083	-0.503259846	-0.367265537
8	4.667234155	0.710557025	-0.859510814
1	4.492494035	1.227100838	-1.629917741
1	3.862150581	0.269296659	-0.640403115
8	1.428647003	-1.635686106	7.118449506
1	0.932284037	-2.428080923	6.989559188
1	1.934012463	-1.501302726	6.332685347
8	-0.353205600	-5.040163030	0.389109980
1	0.255117133	-4.648865191	-0.217279258
1	0.116934500	-5.720593379	0.843930034
8	1.536258098	1.120298545	-3.757798875
1	1.015995946	0.823693016	-3.028257301
1	0.947681217	1.561798253	-4.349012641
8	-2.965848445	-4.390154805	3.943709604
1	-3.642684440	-4.307357150	3.291087172
1	-2.949912835	-3.577010692	4.422688897
8	-3.016893415	-5.457293696	-0.040205605
1	-2.081103874	-5.343812264	0.007735529
1	-3.269155634	-5.258479718	-0.927738832
8	5.600616517	-3.629700414	0.493793654
1	5.692795882	-2.692530126	0.429814979
1	6.352646762	-4.006141290	0.065283176
8	1.514819244	5.669756641	0.150974375

1	0.578513559	5.626517999	0.262062347
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8	-4.333359102	-3.970542950	1.750080225
1	-3.968400253	-4.549823152	1.100374185
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8	2.338374364	-1.098155394	4.597207359
1	1.884431732	-1.764216524	4.106109496
1	1.860314037	-0.294283174	4.470218260
8	-4.887871215	1.110356572	5.049588488
1	-4.070089883	0.879496177	5.460460275
1	-5.025662759	0.489733878	4.351935698
8	-4.149680376	2.448169780	2.711806132
1	-4.360870463	2.612606185	3.616923732
1	-4.319864064	1.533034894	2.555460021
8	5.160724217	-4.438052998	3.070021700
1	5.381893635	-4.151205852	2.198424742
1	4.284652395	-4.786630170	3.026771594
8	-5.363801270	-0.574615170	-3.506044395
1	-6.140961272	-0.211676377	-3.112120269
1	-4.947339130	-1.105066236	-2.845696452
8	0.970488095	-1.399725894	-5.031299926
1	0.065456090	-1.195499991	-4.857843004
1	1.479723585	-0.676414407	-4.702091538
8	-3.843645568	-4.619805652	-2.486453756
1	-3.110001070	-4.266786999	-2.963970285
1	-4.359712433	-5.110550090	-3.105907822
8	0.071435020	6.685536719	3.093940859
1	0.897312712	6.230485903	3.135573131
1	-0.404311637	6.318205888	2.366196650
8	-1.589612359	4.774686150	-2.054705932
1	-0.828454911	4.789596887	-1.496767347
1	-2.296974911	5.154923536	-1.558786378
8	-1.076312750	5.364394510	0.921070293
1	-1.871169958	5.723736740	0.560579469
1	-1.283194228	4.492957892	1.218856673
8	5.813396292	-2.902451151	5.118547024
1	5.626232564	-3.464869179	4.384017137
1	5.424746502	-3.308291036	5.876916183
8	6.577408119	0.190109849	2.414442141
1	5.932687676	-0.036560459	3.065467929
1	6.377130597	1.066899983	2.128074493
8	-5.607336348	-0.261665530	-0.128702423
1	-5.008128637	0.410843462	-0.410766648
1	-5.276528886	-1.078703860	-0.466183154
8	-1.960958916	-2.159275548	4.926014128
1	-1.548688706	-1.759303500	4.177058796
1	-2.283187933	-1.455615869	5.466301061
8	5.679943200	4.868683623	-0.351381400
1	4.865894447	4.819206210	-0.826518292
1	5.822631310	4.017914536	0.031646691
8	1.668164556	1.422759236	4.722198222
1	2.545142257	1.736221103	4.875593866
1	1.301482236	1.964672196	4.041938805
8	3.238960601	-4.757517723	-0.042674931
1	2.638069797	-4.226215641	-0.540195578

1	4.064576111	-4.300131510	-0.036730494
8	3.764153042	2.293112506	-2.776007296
1	3.004044415	1.949149000	-3.217371584
1	3.540286389	3.163970082	-2.489006845
8	4.542645738	3.644779121	3.193841892
1	4.543718372	3.060551653	3.935162045
1	5.302561387	4.197474673	3.282916512
8	-0.954047345	-6.042798771	4.501282905
1	-0.522610858	-5.470517299	5.115477441
1	-1.796868039	-5.659057273	4.318870746
8	3.209850205	4.864800183	-1.758941421
1	2.543437655	5.086701819	-1.128439691
1	3.222202491	5.560397252	-2.396805508
8	-4.765006420	3.606063282	0.378243013
1	-4.706407872	3.364093340	1.288679837
1	-4.443500407	2.871061849	-0.119034808
8	-2.317685030	0.414817792	5.644426330
1	-1.988118471	0.480750703	4.762430191
1	-1.603436960	0.640953266	6.218526405
8	4.338684170	1.866901581	5.164864059
1	4.683590125	1.005672280	4.991075599
1	4.542581077	2.064214564	6.065070753
8	-7.451167533	0.431492617	-1.931511443
1	-6.985229004	0.185967926	-1.148250715
1	-7.604370347	1.361175382	-1.875857986
8	8.001194807	-2.958683162	-0.933965437
1	7.586020962	-2.180216316	-0.598557474
1	8.089274415	-2.839026521	-1.866061314
8	-0.507677529	2.103877185	-5.253520247
1	-0.865452590	1.413448078	-5.788481094
1	-1.168304327	2.323136337	-4.616043886
8	-3.421016350	0.773752791	-4.671655717
1	-3.234645533	1.517200592	-4.120811147
1	-4.214547097	0.383644163	-4.341500199
8	0.061023257	0.730064403	6.815372209
1	0.632392837	1.088259349	6.154984719
1	0.439474147	-0.091521012	7.084910301
8	0.010785755	-3.764657407	5.871675079
1	-0.758240374	-3.247831528	5.691763215
1	0.606953943	-3.622908318	5.153782927
8	2.605403396	-5.161277119	2.424505434
1	2.790627577	-5.068024148	1.503704511
1	2.005689349	-5.885256009	2.508624893
8	0.890294223	-3.776173649	-3.721091392
1	-0.050439559	-3.852524181	-3.729398043
1	1.105378696	-3.016391341	-4.238148418
8	0.451447912	-6.722827288	2.403810275
1	-0.082410444	-6.476779874	3.142277864
1	0.398808613	-7.662489910	2.332104526
8	-3.446727325	5.695614725	-0.344309739
1	-3.990535285	4.981588707	-0.052216941
1	-4.016573206	6.437942369	-0.467207242

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15	-0.517139711	0.026425890	-0.445535718
8	0.722671326	-1.017120433	0.086217770
8	-1.644976292	0.409304900	0.557811765
8	0.440121239	1.463929976	0.145395147
6	1.556388969	-0.826643996	1.240157821
1	1.892656682	0.207728494	1.296431330
1	0.968505000	-1.042302034	2.135164330
6	2.742119147	-1.774271296	1.146283976
1	3.437555923	-1.594060812	1.971741437
1	3.283219267	-1.634542740	0.203856800
1	2.424552139	-2.811503069	1.190481002
6	1.547923350	1.883467559	-0.632486550
1	1.216128422	2.530045239	-1.456136588
1	2.031167212	1.017617703	-1.102457739
6	2.535573391	2.645716785	0.244365074
1	2.863150555	2.030355914	1.091109933
1	2.073980441	3.543146157	0.635269346
1	3.416253481	2.932331576	-0.320072655
8	-0.468547414	0.458854345	-1.924911118
8	-1.349808096	-1.568272225	-0.909811066
1	-1.232583499	-2.153507721	-0.150310709
8	-3.653638337	1.660046285	-0.835770818
1	-2.957925717	1.253509453	-0.344252550
1	-3.310212393	1.836201131	-1.697110789
8	-1.645726057	2.969801021	1.656532576
1	-1.492211327	2.255277273	1.059232405
1	-2.495415708	2.824295314	2.040894438
8	-1.050981010	0.080435676	3.249553142
1	-0.249927190	0.579613863	3.253070240
1	-1.412501466	0.153758149	2.380757868
8	-4.096554959	-1.763088643	-1.532088067
1	-3.194820587	-1.551745577	-1.350187859
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8	-3.028885678	-1.640337927	1.595976765
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8	1.257474446	-3.148277953	3.544566184
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1	1.826053401	-3.791058865	3.151591472
8	1.282806615	-3.521302089	-1.112265520
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8	-1.399803486	-0.748381733	-4.214752209
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8	-4.864249450	0.035954308	2.524179071
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1	-0.219977130	2.877162948	2.597599752

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8	-1.054469864	-3.337835747	2.275888511
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1	3.383809500	3.095355480	-2.413198793
8	4.547332243	3.759011402	3.386248082
1	4.443807858	3.142310992	4.093242962
1	5.370679896	4.198263267	3.527792761
8	0.110727103	-6.343295393	4.476567318
1	0.746178151	-5.651387274	4.385224149
1	-0.735965701	-5.929169284	4.526460354
8	3.144011085	4.839722655	-1.833964600
1	2.555878692	5.149996117	-1.164107061
1	3.124233652	5.477846234	-2.529152061
8	-4.543056989	4.173873309	0.148375179
1	-4.513382034	3.986680607	1.073013889
1	-4.292262047	3.380505448	-0.297211836
8	-2.320926952	0.363069635	5.451441123
1	-1.911880602	0.545262049	4.620558783
1	-1.752267956	0.716041104	6.116960877
8	4.208924237	1.894846436	5.273223652
1	4.448787682	1.021285130	5.008205491
1	4.553028216	2.018455078	6.143391342
8	-7.486004815	1.018969160	-2.445298176
1	-7.046316651	0.803826740	-1.638287326
1	-7.670483628	1.944146847	-2.415427306
8	7.839841053	-2.612347438	-1.048001767
1	7.396130416	-1.887587855	-0.637242871
1	7.860906698	-2.428219771	-1.973491743
8	-0.325310820	2.246001936	-5.035898314

1	-0.803918770	1.719979642	-5.656473395
1	-0.941869406	2.510517147	-4.371996464
8	-3.170229848	1.193916722	-4.645945708
1	-2.936635636	1.801922904	-3.962834677
1	-4.047641011	0.900277732	-4.459386740
8	-0.359323631	1.227669883	7.018162013
1	0.284820746	1.676383384	6.494127024
1	0.091268935	0.525332200	7.459259025
8	0.387312398	-2.666663000	6.095302187
1	-0.424487313	-2.496407853	5.644888081
1	0.469713883	-3.604644759	6.160713719
8	3.158571779	-6.067225380	2.047480298
1	3.203953948	-5.750378694	1.159546128
1	2.536155496	-6.776778137	2.050843116
8	0.834643320	-3.692686090	-3.633072984
1	-0.100724315	-3.778384092	-3.725926063
1	1.094203801	-2.959091603	-4.167250800
8	0.761558977	-7.399823299	2.055676328
1	0.451899507	-7.208060670	2.926432643
1	0.344947028	-6.781190495	1.477224608
8	-2.991706874	6.079673503	-0.652769839
1	-3.609422029	5.432467913	-0.352051756
1	-3.496215835	6.775892156	-1.042165204

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15	-1.029761548	-1.204368873	-0.827896226
8	0.498222527	-1.772576518	-0.590813221
8	-1.727927982	-0.972336238	0.479935468
8	-0.243708307	2.295907997	1.565961951
6	1.422161103	-0.972018105	0.183172111
1	1.666161498	-0.081928857	-0.406254135
1	0.924671719	-0.635275409	1.095885192
6	2.649254241	-1.816926400	0.476003082
1	3.325732960	-1.294407026	1.159054604
1	3.199635275	-2.040484697	-0.442400728
1	2.362957189	-2.761182474	0.942998104
6	0.645377185	2.551623172	0.544545478
1	0.446685848	3.519188070	0.042148407
1	0.583257817	1.800609772	-0.280506728
6	2.110313699	2.591870066	1.007254544
1	2.383845354	1.635917691	1.478550745
1	2.251333860	3.371850816	1.755207206
1	2.792268743	2.793599119	0.177734425
8	-1.007521454	-0.086126807	-1.869172302
8	-1.636218187	-2.514172460	-1.584415097
1	-2.083185696	-3.145704305	-0.992863679
8	-2.301120504	1.735089838	-0.143705809
1	-1.687807996	1.827294949	0.567788701
1	-1.857706091	1.253056318	-0.823342329
8	-1.865639901	4.326451800	2.353134330
1	-1.351638264	3.644013357	1.951937940
1	-2.722340615	3.963312755	2.511476919
8	-0.799772979	0.307159053	3.269512210

1	-0.102014043	-0.327355259	3.306962295
1	-0.516819268	0.987007177	2.679069851
8	-4.194335555	-1.528315303	-2.135778891
1	-3.270838447	-1.471346514	-2.322289220
1	-4.448115753	-2.423723154	-2.293001172
8	-1.580710603	-2.565590112	2.660890119
1	-1.626033471	-1.894133521	1.999096845
1	-0.679023058	-2.840774533	2.706841843
8	0.855479194	-4.085314712	2.583050500
1	0.262498130	-4.623110175	2.083022548
1	1.708566923	-4.482687811	2.510839699
8	1.142640400	-4.264997986	-1.647803410
1	0.926160588	-3.430176401	-1.264283050
1	1.150181703	-4.139977011	-2.583320026
8	-1.658563276	-0.885893195	-4.457013649
1	-2.254547595	-0.207282390	-4.731182430
1	-1.381170866	-0.666082827	-3.582019188
8	-3.405035421	0.324898703	2.612242923
1	-2.482966984	0.141975972	2.697140068
1	-3.692744566	-0.094591748	1.817177100
8	-2.019007776	-3.476126459	-4.095363413
1	-1.613757550	-3.402453006	-3.246114962
1	-2.014484759	-2.611562366	-4.474028074
8	0.404960817	3.886784978	3.721200149
1	-0.455198209	4.274239832	3.691474084
1	0.407849552	3.184003104	3.091146384
8	5.373482231	2.598971935	1.372031104
1	4.734732508	3.085490576	1.868193233
1	4.893815944	2.086149163	0.741308097
8	-0.753457385	-5.962453781	1.649401398
1	-0.735972505	-6.109903634	0.717290206
1	-1.629936561	-5.685559573	1.863859565
8	3.578672280	-0.397319378	4.195477322
1	3.986486587	-1.187514442	4.511954343
1	2.753206811	-0.651691950	3.814977902
8	2.171258299	5.631509964	2.802673168
1	3.021265042	5.278081943	3.011133297
1	1.534760927	5.062951934	3.205775283
8	-1.473408558	2.534957333	-3.234633237
1	-1.279773380	1.844653072	-2.620740820
1	-1.347042714	3.349790061	-2.775331862
8	5.969223707	-1.062808784	0.441227077
1	6.067769728	-0.704825703	1.308991589
1	5.500270106	-0.419581750	-0.065941492
8	4.338165367	0.859925202	-0.408548438
1	4.134271441	1.284961198	-1.226258730
1	3.518718769	0.565992891	-0.043871150
8	1.989495386	-0.747084080	6.892624491
1	1.462340287	-1.486662405	6.635700657
1	2.508983075	-0.510065855	6.141070531
8	-0.654623711	-6.009572237	-1.009225006
1	0.036498832	-5.413348729	-1.249528173
1	-0.498582864	-6.810859618	-1.483005801
8	1.359832784	0.616150707	-3.367061610
1	0.703897674	0.396818579	-2.724783631

1	0.924104410	1.112817228	-4.041110276
8	-2.563522874	-4.765029141	4.988939489
1	-3.002568263	-4.873490077	4.160474748
1	-2.647845714	-3.854675667	5.223512857
8	-2.874928057	-4.560668212	-0.713594293
1	-2.212356502	-5.210462685	-0.885770165
1	-3.495134533	-4.610966773	-1.423307219
8	5.378681617	-3.631813773	0.432416643
1	5.383095150	-2.687965208	0.435393468
1	6.189581733	-3.905635660	0.034495759
8	1.450937514	5.884230871	0.217536423
1	0.540489557	6.098734129	0.343834969
1	1.827460090	5.782581757	1.077057605
8	-3.017001947	-4.663979720	2.047145020
1	-3.347610363	-4.587175022	1.166419429
1	-2.627821815	-3.831967643	2.264338902
8	1.237562072	-1.561200266	3.582586203
1	1.282102320	-2.293607831	2.988891181
1	0.982476871	-1.907993250	4.422553238
8	-4.455121013	1.135631833	4.992732494
1	-3.645601301	1.083094009	5.475221942
1	-4.325567214	0.652835014	4.192106802
8	-4.095897809	2.885564930	2.592421531
1	-4.592160341	2.974710421	3.390328189
1	-3.807418935	1.987810859	2.551238749
8	4.950458935	-4.383383298	3.027427879
1	5.218201613	-4.088114640	2.171852791
1	4.233892084	-4.983365881	2.895400217
8	-5.382999385	0.574665126	-3.413420627
1	-5.689727193	1.161360298	-2.740676038
1	-5.082421117	-0.205960143	-2.976207466
8	0.911403088	-1.544827722	-5.099187904
1	0.007263241	-1.274068615	-5.109142635
1	1.375919531	-0.919753773	-4.565909847
8	-4.255408736	-4.179155031	-2.973422428
1	-3.565862709	-4.022908859	-3.598715851
1	-4.951304347	-4.613846191	-3.439953614
8	0.472097248	7.943779002	2.710028729
1	1.179604445	7.326976053	2.809357187
1	-0.125539043	7.572101785	2.081088856
8	-0.953021893	4.825809525	-2.054407309
1	-0.242871249	4.802851354	-1.433088196
1	-1.673689207	5.260136587	-1.626766012
8	-1.114251842	6.406133436	0.933980201
1	-1.793535392	6.560974990	0.297209908
1	-1.431445752	5.728830202	1.509763847
8	4.619547045	-2.658538343	4.976674566
1	4.784283649	-3.276045042	4.282105792
1	4.191447755	-3.136607798	5.668815483
8	5.836759825	0.273666034	2.717930190
1	5.037850906	0.114590439	3.194708911
1	5.797587189	1.166052474	2.412986915
8	-4.439604947	0.092483928	0.079543072
1	-3.643407476	0.595736978	0.018843742
1	-4.353361181	-0.625865959	-0.526603699

8	-2.095850833	-2.059767342	5.226278220
1	-2.034597825	-2.024288029	4.285072748
1	-2.270724833	-1.180016189	5.520107163
8	5.541679749	4.717109931	-0.634063888
1	4.657790963	4.656128091	-0.959487125
1	5.642998879	4.030997324	0.006141063
8	1.511938932	3.161156798	6.034296363
1	2.332783831	2.796028315	5.744860194
1	1.068792281	3.477384223	5.263258287
8	3.301352640	-5.254019944	-0.265494271
1	2.630618073	-4.879103082	-0.813610081
1	3.972531369	-4.597239893	-0.170428335
8	3.392190018	2.127147677	-2.434567503
1	2.653022629	1.677546778	-2.811885746
1	3.098404494	2.997454222	-2.217461451
8	4.327195616	4.021462556	3.447062149
1	4.138329116	3.368580250	4.102006875
1	5.156601860	4.407199472	3.679808296
8	0.091384598	-5.195637083	4.998906884
1	0.335506088	-4.802869978	4.176096363
1	-0.851915215	-5.193125864	5.031427821
8	2.899652961	4.701220137	-1.658665634
1	2.323314239	5.040025482	-0.992390114
1	2.888815625	5.323129167	-2.368588281
8	-4.131315411	3.644556599	-0.023744984
1	-4.312568022	3.540184610	0.896652991
1	-3.453575320	3.023854368	-0.238862544
8	-1.880757224	0.553037949	5.678675622
1	-1.451728737	0.679311861	4.847490979
1	-1.269588106	0.826843475	6.343793129
8	3.877207929	2.019240290	5.213556863
1	3.758567804	1.158626553	4.844575872
1	4.458936542	1.920704576	5.950280005
8	-6.018389365	1.921577997	-1.145140015
1	-5.676578058	1.241087547	-0.587487585
1	-5.560140202	2.714680094	-0.917378689
8	7.825215579	-2.604502713	-0.669855328
1	7.312758301	-1.907275798	-0.292839915
1	8.078026847	-2.319052929	-1.533269097
8	0.056251279	1.975565537	-5.278102579
1	-0.421144346	1.479402115	-5.923698219
1	-0.585061601	2.354137427	-4.698206408
8	-3.204127224	1.207512768	-4.777921518
1	-2.780739132	1.872283468	-4.258594169
1	-4.057967471	1.070625881	-4.399639524
8	0.125314748	1.238663307	7.276891358
1	0.559549732	2.001983404	6.930971047
1	0.764477532	0.544224052	7.287065382
8	0.388956617	-2.616027257	5.849982627
1	-0.531565309	-2.410739532	5.812904495
1	0.457270937	-3.557412418	5.847618788
8	2.828190663	-5.769221041	2.235152047
1	2.944826618	-5.848971080	1.301924080
1	2.362843180	-6.540415401	2.517268039
8	0.815652386	-4.037667163	-4.238326054

1	-0.089443246	-4.208352521	-4.444594955
1	1.020826369	-3.189838001	-4.598836528
8	0.914524145	-7.346701276	3.253474698
1	0.765773775	-6.958568665	4.100885377
1	0.222437831	-7.040355361	2.689517990
8	-3.122020762	5.894871448	-0.859830168
1	-3.584792630	5.147197480	-0.516749580
1	-3.740830067	6.381341176	-1.380695507

Table S1: Numerical values of the various terms appearing in the EDA analysis along the reaction coordinate involving the attack of the OH⁻ to phosphorus atom in Monoethyl phosphate dianion (MEP). (Energy values in kcal.mol⁻¹)

P-OH Distance (Å)	ELECTROSTATIC ENERGY	EXCHANGE ENERGY	REPULSION ENERGY	POLARIZATION ENERGY	DFT DISPERSION ENERGY
5.085	113.61	-18.84	39.58	-7.01	-2.15
5.063	114.13	-18.80	39.50	-7.04	-2.14
5.043	114.60	-18.76	39.43	-7.06	-2.14
5.022	115.08	-18.72	39.35	-7.09	-2.13
5.001	115.58	-18.68	39.26	-7.12	-2.13
4.983	116.00	-18.64	39.19	-7.15	-2.12
4.962	116.51	-18.60	39.10	-7.18	-2.12
4.933	117.20	-37.37	38.96	-7.23	-2.11
4.900	118.04	-18.45	38.80	-7.28	-2.10
4.900	118.04	-18.45	38.80	-7.28	-2.10
4.862	119.01	-18.35	38.59	-7.35	-2.09
4.820	121.26	-16.11	33.99	-6.62	-1.95
4.775	121.46	-18.07	38.02	-7.52	-2.04
4.727	122.90	-17.91	37.65	-7.62	-2.02
4.681	124.37	-17.73	37.27	-7.73	-1.99
4.637	125.82	-17.54	36.85	-7.84	-1.96
4.585	127.53	-17.33	36.38	-7.98	-1.93

4.514	130.06	-17.00	35.65	-8.20	-1.89
4.435	132.72	-16.70	35.00	-8.46	-1.86
4.353	135.04	-16.50	34.60	-8.76	-1.85
4.270	136.91	-16.46	34.58	-9.07	-1.87
4.195	138.40	-16.49	34.76	-9.37	-1.90
4.127	139.75	-16.56	35.03	-9.66	-1.94
3.992	142.77	-16.67	35.52	-10.29	-2.04
3.921	144.58	-16.72	35.75	-10.65	-2.09
3.853	146.46	-16.77	35.95	-11.02	-2.15
3.784	148.51	-16.82	36.16	-11.43	-2.22
3.710	150.84	-16.90	36.42	-11.90	-2.29
3.630	153.60	-17.01	36.78	-12.49	-2.38
3.539	156.89	-17.18	37.29	-13.22	-2.48
3.437	160.71	-17.48	38.22	-14.18	-2.60
3.322	164.29	-18.72	41.49	-15.42	-2.83
3.203	167.15	-21.49	48.40	-16.99	-3.12
3.073	169.51	-24.99	57.38	-18.90	-3.47
2.934	169.53	-29.46	69.25	-21.14	-4.02
2.785	167.68	-35.01	84.55	-24.12	-4.68
2.627	161.80	-42.51	106.18	-28.42	-5.65

2.451	149.76	-53.16	138.54	-35.74	-7.00
2.264	128.43	-68.26	187.23	-48.95	-8.74
2.089	96.58	-87.75	254.03	-69.58	-10.62

Table S2: Numerical values of the various terms appearing in the EDA analysis along the reaction coordinate involving the attack of the OH⁻ to phosphorus atom in Diethyl Phosphate Monoanion (DEP). (Energy values in kcal.mol⁻¹)

P-OH Distance (Å)	ELECTROSTATIC ENERGY	EXCHANGE ENERGY	REPULSION ENERGY	POLARIZATION ENERGY	DFT DISPERSION ENERGY
4.125	70.41	-8.01	20.44	-11.16	-2.31
4.123	65.47	-15.11	36.38	-13.5	-3.03
4.114	65.39	-15.36	36.98	-13.56	-3.06
4.103	64.94	-16.06	38.56	13.71	-3.13
4.106	64.83	-16.05	38.54	-13.77	-3.13
4.087	64.66	-16.22	39.05	-14.16	-3.18
4.079	64.15	-16.47	39.7	-14.53	-3.23
4.061	64.12	-16.61	40.12	-14.76	-3.27
4.03	64.21	-16.81	40.72	-15.07	-3.32

4.006	64.4	-16.94	41.11	-15.32	-3.36
4.002	64.44	-16.96	41.18	-15.36	-3.36
3.952	64.89	-17.16	41.79	-15.82	-3.41
3.904	65.61	-17.04	41.52	-15.95	-3.38
3.823	67.71	-16.14	39.25	-15.39	-3.21
3.803	68.45	-15.75	38.25	-15.06	-3.14
3.746	70.57	-14.68	35.57	-13.99	-2.92
3.716	71.27	-14.44	35.11	-13.61	-2.86
3.702	71.6	-14.37	34.99	-13.48	-2.84
3.653	73.04	-14.15	34.48	-13.01	-2.77
3.6	74.33	-14.27	34.74	-12.71	-2.73
3.558	74.45	-14.98	36.77	-12.64	-2.78
3.399	79.84	-16.56	39.66	-11.9	-2.6
3.462	78.81	-15.32	36.71	-11.55	-2.53
3.248	79.54	-19.87	48.48	-13.42	-3.11
3.219	79.27	-20.62	50.47	-13.75	-3.24
3.131	78.27	-22.73	56.23	-14.8	-3.62
3.043	76.91	-24.86	62.24	-16.02	-4.02
2.894	73.3	-29.19	74.66	-18.77	-4.8

2.759	68.04	-34.11	89.11	-22.32	-5.62
2.594	58.21	-41.7	112.18	-28.77	-6.73
2.484	48.89	-48.06	132.15	-34.97	-7.59
