Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Photolysis of ortho-nitrobenzylic derivatives: the importance of the leaving group.

Tomáš Šolomek,[†] Sébastien Mercier[§], Thomas Bally* and Christian G. Bochet*

Department of Chemistry, University of Fribourg Chemin du Musée 9, CH-1700 Fribourg, Switzerland. Email: Christian.Bochet@unifr.ch, Thomas.Bally@unifr.ch

Supporting Information

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[†] On leave from Masaryk University, Brno, Czech Republic.

[§] Current address: Syngenta Crop Protection AG, Monthey, Switzerland.

Table S1. *DFT calculated total energies and corresponding scaled ZPVE corrections for compounds* ***9****.*

Structure	B2PLYP[a] (in Hartree)	M06-2X[a] (in Hartree)	ZPVE[b] (in Hartree)
9a	-778.821256	-779.0899029	0.176460931
9b	-758.9517582	-759.2204781	0.189203828
9c[c]	-947.4966694	-947.8203991	0.203710825
9d[c]	-872.2875008	-872.5896083	0.19865387
9e	-947.4975063	-947.8211444	0.203187184
9f	-892.1532444	-892.4555293	0.18585606
9g	-967.3604211	-967.6843034	0.191743582
9h[d]	-664.3472461	-664.5756857	0.144014838

[a] With 6-311+G(3df,2p) basis set at B3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688). [b] At B3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688); scaled by 0.9806. [c] Geometries with no intramolecular hydrogen bonding. [d] Parent compound with no leaving group (X) but hydrogen present (see Scheme 3 in the paper; X = H).

Table S2. *DFT calculated total energies and corresponding scaled ZPVE corrections and RSEs for radicals* ***9*****•**.

Structure	UB2PLYP[a] (in Hartree)	UM06-2X[a] (in Hartree)	ZPVE[b] (in Hartree)	RSE[c] (UB2PLYP; kcal mol^{-1})	RSE[c] (UM06-2X; kcal mol^{-1})
9a•	-778.1891053	-778.4558173	0.163671946	11.5	10.9
9b•	-758.3333792	-758.6005234	0.176270695	20.2	19.9
9c•	-946.8626899	-947.184300	0.190862023	9.7	8.9
9d•	-871.6526177	-871.9532207	0.185538345	10.4	9.7
9e•	-946.8573164	-947.1795544	0.190140301	9.1	8.7
9f•	-891.5111326	-891.8124064	0.172526764	10.0	9.7
9g•	-966.7173088	-967.0402162	0.178166195	6.6	6.4
9h•[d]	-663.6964769	-663.9239523	0.130957169	**0.0**	**0.0**

[a] With 6-311+G(3df,2p) basis set at UB3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688). [b] At UB3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688); scaled by 0.9806. [c] Calculated according to Scheme 3 in the paper. [d] Parent compound with no leaving group (X) but hydrogen present (see Scheme 3 in the paper; X = H).

Table S3. *DFT calculated total energies and corresponding scaled ZPVE corrections and $\Delta_r Hs$ for aci-nitro intermediates* ***10***[a].

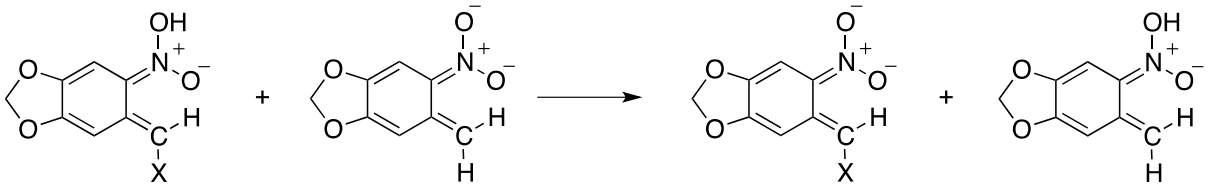
Structure	B2PLYP[b] (in Hartree)	M06-2X[b] (in Hartree)	ZPVE[c] (in Hartree)	$\Delta_r H$[d] (B2PLYP; kcal mol^{-1})	$\Delta_r H$[d] (M06-2X; kcal mol^{-1})
10a	-778.7892087	-779.0600408	0.177713	18.7	17.4
10b	-758.9279833	-759.1993106	0.189981	13.1	11.5
10c	-947.4642984	-947.7899899	0.205444	19.6	17.7
10d	-872.2526297	-872.5572212	0.20041	20.5	19.0
10e	-947.4605672	-947.7864260	0.205008	21.8	20.4
10f	-892.1152995	-892.4200144	0.187258	22.4	20.9
10g	-967.3219240	-967.6482404	0.192993	22.6	21.1
10h	-664.3021503	-664.5331137	0.145129	27.2	25.6

[a] The most stable *EE* diastereomers were considered. [b] With 6-311+G(3df,2p) basis set at B3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688). [c] At B3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688); scaled by 0.9806. [d] Calculated according to Scheme 5 in the paper.

Table S4. *DFT calculated total energies and corresponding scaled ZPVE corrections and $\Delta_r Hs$ for aci-nitro intermediate anions* ***10***$^-$.[a]

Structure	B2PLYP[b] (in Hartree)	M06-2X[b] (in Hartree)	ZPVE[c] (in Hartree)	$\Delta_r H$[d] (B2PLYP; kcal mol^{-1})	$\Delta_r H$[d] (M06-2X; kcal mol^{-1})
10a$^-$	-778.3257649	-778.5959359	0.162445215	-4.5	-4.8
10b$^-$	-758.4583147	-758.7281743	0.174736056	-8.5	-9.4
10c$^-$	-947.0036009	-947.3287877	0.189730410	-2.8	-3.1
10d$^-$	-871.7931116	-872.0967701	0.184630310	-2.0	-2.5
10e$^-$	-947.0016810	-947.3272345	0.189103807	-1.5	-1.7
10f$^-$	-891.6586478	-891.9626411	0.171813868	-0.2	-0.6
10g$^-$	-966.8654810	-967.1915272	0.177263062	0.0	-0.1
10h$^-$	-663.8456712	-664.0765618	0.130345274	**0.0**	**0.0**

[a] The most stable *E* diastereomers were considered. [b] With 6-311+G(3df,2p) basis set at B3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688). [c] At B3LYP/6-31G* geometries with PCM solvation model using acetonitrile (ε = 35.688); scaled by 0.9806. [d] Calculated according to isodesmic reaction shown in Scheme S1 in the Supporting Information.



10 **10**$^{-}$

a: X = OMe
b: X = NHMe
c: X = NHCOOMe
d: X = NHCOMe
e: X = OC(O)NHMe
f : X = OC(O)Me
g: X = OC(O)OMe
h: X = H

Scheme S1. *Model reaction to evaluate relative acidities of aci-nitro intermediates.*

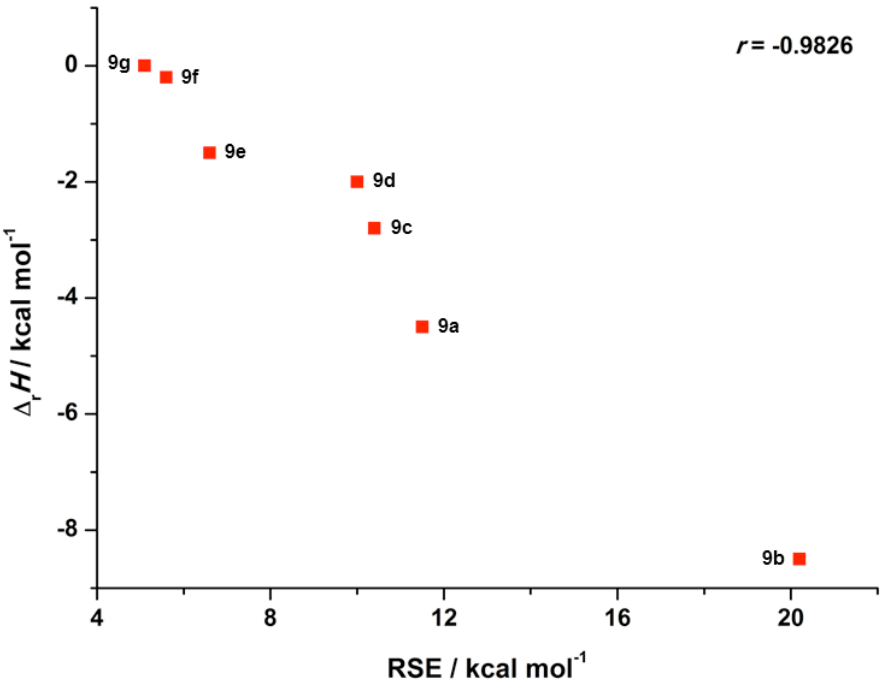


Figure S1. *Linear correlation of computed RSEs of* ***9*** *derivatives with the computed enthalpies according to Scheme S1. Correlation coefficient is shown.*

Table S5. Quantum yields for the disappearance of compounds **1a**-**g** on photolysis at 254 and at 360 nm.

Substrate	Leaving group (LG)	Φ_{254}	Φ_{360}
1a	O-C_8H_{17}	0.16	0.22
1b	NH-$C_{12}H_{25}$	0.16	0.14
1c	NHC(O)O-C_9H_{19}	0.076	0.080
1d	NHC(O)CH_2-$C_{10}H_{21}$	0.054	0.072
1e	OC(O)NH-$C_{12}H_{25}$	0.012	0.019
1f	OC(O)CH_2-$C_{11}H_{23}$	0.0074	0.0081
1g	OC(O)O-$C_{10}H_{21}$	0.011	0.0091

Cartesian Coordinates from B3LYP/6-31G Geometries*

9a

1	0.152017	-2.296729	-0.000005
6	-0.194772	-1.272914	-0.000001
6	-1.139033	1.410442	-0.000019
6	0.738563	-0.218932	0.000017
6	-1.540890	-0.966752	-0.000014
6	-2.006464	0.350370	-0.000014
6	0.242664	1.104701	0.000002
1	-1.470927	2.438881	-0.000033
8	-2.590665	-1.827051	-0.000026
8	-3.373618	0.359365	-0.000034
7	1.133982	2.249912	0.000017
8	0.639008	3.384518	-0.000265
8	2.358259	2.058257	0.000318
6	2.212156	-0.582149	0.000046
1	2.708742	-0.145898	-0.879019
1	2.708612	-0.146217	0.879345
8	2.350372	-1.989569	-0.000197
6	3.710262	-2.390303	-0.000017
1	4.238165	-2.023364	-0.892796
1	3.721251	-3.482672	-0.000222
1	4.237827	-2.023704	0.893103
6	-3.785264	-1.017174	0.000116
1	-4.362016	-1.228835	-0.904149
1	-4.361730	-1.228734	0.904591

9b

1	-0.166111	-2.292555	0.134510
6	0.196890	-1.274004	0.087739
6	1.169564	1.393622	-0.038766
6	-0.729202	-0.212153	0.065511
6	1.546168	-0.985254	0.052032
6	2.026157	0.324369	-0.015611
6	-0.214274	1.103084	0.012949
1	1.512812	2.417540	-0.084652
8	2.587729	-1.857531	0.075574
8	3.393742	0.317971	-0.037804
7	-1.087296	2.264362	0.017353
8	-0.615346	3.355710	-0.328627
8	-2.264306	2.130466	0.377818
6	-2.212815	-0.555741	0.068913
1	-2.630759	-0.318403	1.055196
1	-2.743910	0.104700	-0.633693
7	-2.457517	-1.972138	-0.193394
6	-3.871373	-2.318204	-0.043580
1	-4.165669	-2.202499	1.005902
1	-4.017094	-3.366049	-0.323060
1	-4.552107	-1.699189	-0.653893
6	3.789825	-1.062404	0.008239
1	4.390209	-1.242763	0.903851
1	4.338789	-1.317867	-0.902342
1	-2.172669	-2.181285	-1.149767

9c

1	-0.677963	-1.461206	-0.475657
6	0.220906	-0.885623	-0.296687
6	2.616284	0.572755	0.155463
6	0.162463	0.519325	-0.250725
6	1.438533	-1.511572	-0.117160
6	2.617096	-0.796132	0.103476
6	1.369871	1.219001	-0.021295
1	3.512674	1.152004	0.325019
8	1.700223	-2.842930	-0.122082
8	3.665840	-1.661296	0.245151
7	1.411775	2.670357	0.052239
8	2.515746	3.223878	0.130930
8	0.348945	3.306151	0.039460
6	-1.193398	1.197343	-0.464099
1	-1.488866	1.726479	0.443165
1	-1.107987	1.952413	-1.249159
7	-2.264803	0.283506	-0.803777
6	3.119152	-2.982737	0.104663
1	3.280847	-3.547909	1.026283
1	3.572675	-3.478751	-0.757520
1	-2.376712	-0.022039	-1.760883
6	-3.232224	-0.068583	0.088162
8	-3.272721	0.269849	1.262670
8	-4.154136	-0.860179	-0.513648
6	-5.229938	-1.301280	0.330549
1	-4.848050	-1.889414	1.168870
1	-5.862807	-1.918862	-0.306844
1	-5.796250	-0.448509	0.713560

9d

1	-0.759592	-1.695315	-0.320168
6	0.039559	-0.975136	-0.202670
6	2.181848	0.868426	0.081468
6	-0.247345	0.402450	-0.187989
6	1.350654	-1.387901	-0.072391
6	2.405177	-0.483099	0.064986
6	0.838582	1.296095	-0.040974
1	2.977989	1.591660	0.186572
8	1.827113	-2.658482	-0.058210
8	3.587698	-1.160858	0.170243
7	0.644254	2.736324	-0.000896
8	1.642470	3.465861	-0.054989
8	-0.505254	3.187220	0.093651
6	-1.702643	0.844884	-0.345922
1	-2.058656	1.287117	0.586280
1	-1.772257	1.622255	-1.110191
7	-2.616162	-0.231605	-0.679704
6	3.257160	-2.558016	0.112033
1	3.541236	-3.043260	1.049734
1	3.753591	-3.017646	-0.746393
1	-2.656830	-0.544221	-1.640162
6	-3.512628	-0.741396	0.215313
8	-3.559542	-0.372715	1.389419
6	-4.453208	-1.801361	-0.330058
1	-4.320454	-2.722083	0.246726

1	-4.299460	-2.021856	-1.389738
1	-5.485041	-1.467571	-0.182155

9e

1	0.686368	-1.437815	-0.802025
6	-0.184486	-0.868739	-0.505975
6	-2.507134	0.576353	0.274047
6	-0.116390	0.533169	-0.405530
6	-1.380960	-1.497152	-0.221896
6	-2.521943	-0.789232	0.163506
6	-1.286403	1.225957	-0.022874
1	-3.374400	1.150205	0.568409
8	-1.652985	-2.825485	-0.260486
8	-3.553911	-1.657420	0.383572
7	-1.306008	2.673608	0.086316
8	-2.312625	3.216647	0.556916
8	-0.319875	3.316093	-0.301244
6	1.209662	1.213376	-0.715456
1	1.134912	1.806686	-1.628537
1	1.511079	1.872129	0.097717
6	-3.045179	-2.969588	0.093268
1	-3.587851	-3.395653	-0.755050
1	-3.125995	-3.600005	0.982090
8	2.248090	0.256250	-0.960391
6	3.055016	-0.052399	0.106042
8	2.946302	0.446756	1.216871
7	3.955851	-0.992504	-0.259819
6	5.025620	-1.424946	0.624299
1	4.679202	-1.349671	1.656054
1	5.928443	-0.811849	0.510132
1	5.275371	-2.466009	0.406281
1	3.997181	-1.239275	-1.239064

9f

1	0.390254	-1.937525	0.000030
6	-0.286954	-1.095375	0.000051
6	-2.117622	1.081730	0.000111
6	0.214170	0.220167	-0.000010
6	-1.655059	-1.283668	0.000137
6	-2.555613	-0.216297	0.000167
6	-0.717796	1.283374	0.000021
1	-2.790577	1.927260	0.000132
8	-2.331775	-2.458894	0.000205
8	-3.836824	-0.690286	0.000257
7	-0.287897	2.670508	-0.000041
8	-1.150963	3.556260	-0.000006
8	0.925464	2.921982	-0.000126
6	1.715425	0.427710	-0.000107
1	2.041648	0.990450	-0.877457
1	2.041754	0.990503	0.877169
8	2.355513	-0.862600	-0.000106
6	-3.736076	-2.123911	0.000264
1	-4.200319	-2.525248	-0.904270
1	-4.200241	-2.525233	0.904844
6	3.708487	-0.852092	-0.000221

8	4.364911	0.169461	-0.000321
6	4.258542	-2.255696	-0.000207
1	5.348310	-2.221801	-0.000294
1	3.904340	-2.797544	-0.883026
1	3.904479	-2.797472	0.882713

9g

1	0.647605	-1.467625	-0.849761
6	-0.201308	-0.876220	-0.534127
6	-2.474627	0.622688	0.290948
6	-0.096758	0.522535	-0.423298
6	-1.409834	-1.475558	-0.237129
6	-2.526141	-0.741493	0.170978
6	-1.242592	1.242526	-0.019752
1	-3.322458	1.216690	0.601636
8	-1.716720	-2.795379	-0.283323
8	-3.576877	-1.583812	0.398175
7	-1.222346	2.689750	0.095656
8	-2.197503	3.255145	0.603008
8	-0.234325	3.307934	-0.325632
6	1.238084	1.176740	-0.744300
1	1.180035	1.749120	-1.671190
1	1.558094	1.843994	0.053950
6	-3.105387	-2.907420	0.095740
1	-3.673510	-3.317828	-0.743342
1	-3.184727	-3.537807	0.984711
8	2.261434	0.188681	-0.975438
6	3.050455	-0.111820	0.075618
8	2.984512	0.374548	1.184659
8	3.918860	-1.040990	-0.329992
6	4.860249	-1.480638	0.671430
1	5.478325	-0.644065	1.004773
1	5.471917	-2.234042	0.176955
1	4.333246	-1.913750	1.524369

9h

1	-0.732323	2.671341	-0.000179
6	-0.514150	1.609528	-0.000123
6	-0.010055	-1.183611	-0.000043
6	0.823734	1.161653	-0.000078
6	-1.537025	0.682466	-0.000083
6	-1.288280	-0.691982	-0.000064
6	1.041701	-0.235472	-0.000024
1	0.207755	-2.241930	-0.000032
8	-2.874845	0.910769	-0.000120
8	-2.472700	-1.376860	-0.000124
7	2.382634	-0.801484	0.000060
8	3.362056	-0.046051	0.000583
8	2.496941	-2.035296	-0.000377
6	1.902798	2.218636	-0.000131
1	2.552221	2.132792	-0.875896
1	1.442016	3.210140	-0.000489
1	2.551838	2.133252	0.875965
6	-3.511486	-0.385046	0.000381
1	-4.116978	-0.486270	0.905002

1	-4.118015	-0.486466	-0.903505

9a•

1	0.086791	-2.360937	-0.000056
6	-0.228343	-1.326174	-0.000042
6	-1.082318	1.400784	-0.000005
6	0.767583	-0.281282	-0.000029
6	-1.546148	-0.982922	-0.000032
6	-1.971706	0.362385	-0.000006
6	0.299830	1.087785	-0.000017
1	-1.397336	2.434195	0.000005
8	-2.635822	-1.800965	-0.000045
8	-3.332408	0.412513	-0.000003
7	1.180522	2.208238	-0.000001
8	0.689980	3.359695	0.000040
8	2.419582	2.027048	-0.000029
6	2.113794	-0.677085	-0.000009
1	2.934523	0.023407	0.000003
8	2.399828	-1.983508	0.000011
6	3.797340	-2.323305	0.000043
1	4.283975	-1.928472	-0.896936
1	3.842553	-3.411986	0.000114
1	4.283961	-1.928356	0.896977
6	-3.794393	-0.949624	0.000070
1	-4.380721	-1.133588	-0.903949
1	-4.380517	-1.133573	0.904226

9b•

1	0.040627	-2.382962	-0.000162
6	-0.242673	-1.337573	-0.000105
6	-1.125562	1.372320	-0.000035
6	0.750553	-0.289370	-0.000067
6	-1.563306	-1.012170	-0.000092
6	-2.002253	0.329113	-0.000048
6	0.269179	1.080615	-0.000040
1	-1.448943	2.402759	-0.000022
8	-2.645117	-1.844205	-0.000185
8	-3.366632	0.362133	-0.000109
7	1.113648	2.213514	0.000012
8	0.592521	3.364197	0.000076
8	2.370803	2.078252	-0.000003
6	2.120595	-0.639030	-0.000032
1	2.855493	0.150945	-0.000052
7	2.606723	-1.885464	0.000031
6	4.027436	-2.204746	0.000089
1	4.602976	-1.277820	-0.000013
1	4.288861	-2.786465	-0.890088
1	4.288842	-2.786256	0.890408
6	-3.811719	-1.004232	0.000323
1	-4.397308	-1.195868	-0.903083
1	-4.396352	-1.195619	0.904417
1	1.977104	-2.677638	0.000109

9c•

6	-4.078220	-2.261030	0.000040
8	-2.673445	-2.573136	0.000082
6	-2.008229	-1.386670	0.000037
6	-2.937677	-0.327293	-0.000002
8	-4.202923	-0.827947	0.000007
6	-2.536345	0.979352	-0.000025
6	-1.145683	1.248721	-0.000007
6	-0.159895	0.183486	0.000032
6	-0.663389	-1.169957	0.000052
6	1.226764	0.403589	0.000061
7	2.165662	-0.591271	-0.000116
6	3.527599	-0.313690	0.000093
8	4.211875	-1.468913	-0.000319
6	5.648073	-1.339212	-0.000156
7	-0.806178	2.638470	-0.000073
8	0.392664	2.995042	0.000010
8	-1.732170	3.479018	-0.000216
8	4.006577	0.803830	0.000570
1	0.005696	-2.020734	0.000124
1	-3.239061	1.799554	-0.000058
1	1.634911	1.398948	0.000237
1	-4.539585	-2.665467	-0.904430
1	-4.539629	-2.665426	0.904506
1	1.913613	-1.571473	-0.000507
1	5.980884	-0.806096	-0.893438
1	6.027446	-2.360062	-0.000401
1	5.980726	-0.806578	0.893470

9d•

6	-3.947391	-1.914768	0.000072
8	-2.585638	-2.380656	-0.000067
6	-1.793182	-1.274959	-0.000058
6	-2.599335	-0.119524	0.000040
8	-3.912378	-0.476640	0.000097
6	-2.055036	1.134541	0.000057
6	-0.643288	1.247367	-0.000016
6	0.218857	0.080035	-0.000093
6	-0.432292	-1.208647	-0.000129
6	1.622610	0.147171	-0.000096
7	2.455749	-0.937521	-0.000136
6	3.848485	-0.808624	0.000013
6	4.595373	-2.122839	0.000145
7	-0.152979	2.593059	-0.000007
8	1.076768	2.817205	-0.000100
8	-0.981808	3.529054	0.000088
8	4.384979	0.289294	0.000092
1	0.137449	-2.129059	-0.000203
1	-2.662381	2.027640	0.000121
1	2.135584	1.092581	-0.000037
1	-4.450903	-2.265639	-0.904286
1	-4.450731	-2.265675	0.904513
1	2.083284	-1.878658	-0.000185
1	4.338556	-2.716607	-0.884591
1	4.338632	-2.716331	0.885097
1	5.666935	-1.921592	0.000082

9e•

1	-0.191781	-1.909342	-0.003116
6	0.554266	-1.126400	-0.001535
6	2.547710	0.921697	0.002189
6	0.137684	0.255860	-0.000661
6	1.885861	-1.415453	-0.000711
6	2.873068	-0.408421	0.001061
6	1.176485	1.264300	0.001386
1	3.296240	1.700695	0.003638
8	2.487350	-2.636490	-0.001457
8	4.108196	-0.976359	0.001391
7	0.896371	2.668562	0.002768
8	1.854809	3.467909	0.005550
8	-0.287018	3.065024	0.001177
6	-1.234052	0.526476	-0.001997
1	-1.675902	1.506347	-0.002981
6	3.906083	-2.401361	-0.000608
1	4.345473	-2.830420	0.903461
1	4.346154	-2.827977	-0.905517
8	-2.089071	-0.526490	-0.002844
6	-3.459312	-0.235019	-0.008167
8	-3.899118	0.898984	-0.014977
7	-4.144352	-1.389806	-0.017623
6	-5.598019	-1.438454	0.022954
1	-5.987496	-0.473993	-0.304289
1	-5.963183	-1.646144	1.035156
1	-5.955835	-2.219216	-0.652535
1	-3.617620	-2.251207	0.035975

9f•

1	-0.305907	-2.038182	0.000000
6	0.334459	-1.166804	-0.000007
6	2.049984	1.118844	-0.000026
6	-0.254511	0.150817	-0.000006
6	1.692463	-1.283805	-0.000014
6	2.542911	-0.159823	-0.000026
6	0.647681	1.282336	-0.000012
1	2.693408	1.986696	-0.000038
8	2.443897	-2.417991	-0.000026
8	3.839577	-0.564584	-0.000045
7	0.189534	2.642786	0.000000
8	1.038043	3.555212	0.000018
8	-1.033127	2.883884	-0.000006
6	-1.649802	0.244597	0.000006
1	-2.215233	1.158469	0.000022
8	-2.361831	-0.917181	-0.000003
6	3.821471	-2.004278	0.000087
1	4.311995	-2.372037	0.904739
1	4.312191	-2.372205	-0.904386
6	-3.746952	-0.837291	0.000012
8	-4.335846	0.215637	0.000052
6	-4.340313	-2.215183	-0.000033
1	-5.427870	-2.143239	0.000011
1	-4.002645	-2.767687	0.882828
1	-4.002714	-2.767592	-0.882980

9g•

1	-0.192066	-1.911994	-0.000068
6	0.549583	-1.124995	-0.000047
6	2.532534	0.934121	0.000011
6	0.127346	0.255095	-0.000035
6	1.883270	-1.407088	-0.000024
6	2.865165	-0.395545	0.000008
6	1.161246	1.267720	-0.000012
1	3.277307	1.716769	0.000032
8	2.490095	-2.624313	-0.000030
8	4.102122	-0.955892	0.000022
7	0.871528	2.673769	-0.000005
8	1.824200	3.476288	0.000018
8	-0.313117	3.060343	-0.000024
6	-1.243986	0.521781	-0.000037
1	-1.697509	1.495939	-0.000022
8	-2.091012	-0.551135	-0.000053
6	3.907939	-2.382684	0.000062
1	4.349587	-2.807557	0.904814
1	4.349714	-2.807624	-0.904595
6	-3.435078	-0.291325	0.000010
8	-3.935291	0.808080	0.000090
8	-4.049935	-1.465803	-0.000032
6	-5.495363	-1.404407	0.000032
1	-5.822555	-2.442602	-0.000011
1	-5.848838	-0.887902	-0.894491
1	-5.848763	-0.888001	0.894642

9h•

1	-0.809008	2.697666	-0.000123
6	-0.563630	1.641976	-0.000094
6	0.062868	-1.141535	-0.000085
6	0.826659	1.243620	0.000053
6	-1.538331	0.688922	-0.000195
6	-1.232447	-0.686259	-0.000187
6	1.094178	-0.181304	0.000047
1	0.301717	-2.195189	-0.000092
8	-2.889899	0.850752	-0.000411
8	-2.378849	-1.412660	-0.000373
7	2.431648	-0.722916	0.000190
8	3.410691	0.041364	0.000482
8	2.564706	-1.960247	0.000020
6	1.768900	2.271685	0.000186
1	2.830687	2.094003	0.000305
1	1.413323	3.297052	0.000157
6	-3.465722	-0.466844	0.000186
1	-4.062554	-0.604035	0.905264
1	-4.063750	-0.604324	-0.904051

10a

6	0.751467	-0.362254	-0.003942
6	-0.290099	-1.385932	-0.010686
6	-1.581423	-1.004772	-0.013519
6	-1.972213	0.374172	-0.008270
6	-1.084549	1.393171	-0.002935
6	0.324014	1.051612	-0.002519
7	1.218716	2.032461	0.000891
8	2.486996	1.965517	0.004170
6	2.065016	-0.759096	0.001998
8	2.370432	-2.072953	0.001381
6	3.770270	-2.379618	0.008724
8	0.689537	3.352514	0.001258
1	0.001601	-2.428027	-0.015283
8	-2.710585	-1.781620	-0.034550
8	-3.331865	0.449903	-0.019864
1	-1.397482	2.426757	0.000143
1	2.885762	-0.056186	0.007729
1	1.520529	3.866899	0.005881
1	3.844230	-3.467512	0.007937
1	4.249989	-1.977542	0.907752
1	4.259938	-1.975523	-0.884008
6	-3.830217	-0.895584	0.051946
1	-4.503835	-1.074059	-0.789665
1	-4.341463	-1.039112	1.009343

10b

6	0.733886	-0.365434	0.000425
6	-0.297847	-1.392250	0.021376
6	-1.598411	-1.034217	0.027864
6	-2.003129	0.334272	0.014112
6	-1.124993	1.362496	0.002229
6	0.290702	1.042943	0.003035
7	1.158175	2.049476	0.004303
8	0.591235	3.362703	-0.008760
6	2.077608	-0.721971	-0.033561
7	2.575296	-1.974745	-0.092280
6	3.991859	-2.276225	0.041761
8	2.439103	2.031299	0.008009
1	-0.030918	-2.442742	0.038579
8	-2.720290	-1.828776	0.077937
8	-3.366722	0.394617	0.038493
1	-1.451385	2.391820	-0.003529
1	2.818670	0.065549	-0.037113
1	1.414065	3.888772	0.009021
1	4.260871	-2.540561	1.073118
1	4.575851	-1.402504	-0.257224
1	4.256399	-3.111796	-0.612579
1	1.947810	-2.765887	-0.044491
6	-3.840261	-0.956068	-0.090181
1	-4.577316	-1.153554	0.690948
1	-4.271428	-1.092230	-1.088684

10c

6	0.134782	0.124379	-0.000007
6	0.660481	-1.238839	-0.000010
6	1.992826	-1.437182	-0.000014
6	2.928735	-0.353406	-0.000018
6	2.549133	0.942307	-0.000019
6	1.127182	1.225063	-0.000016
7	0.741444	2.497239	-0.000019
8	1.789069	3.457797	-0.000023
6	-1.219385	0.356305	0.000006
7	-2.186921	-0.627541	0.000025
6	-3.534851	-0.328864	0.000028
8	-4.003725	0.795626	0.000009
8	-0.426755	2.990001	-0.000018
8	-4.245958	-1.473819	0.000054
6	-5.676741	-1.312405	0.000059
1	-0.008092	-2.090837	-0.000012
8	2.683221	-2.616955	-0.000020
8	4.192665	-0.858872	-0.000023
1	3.266514	1.749093	-0.000024
1	-1.615240	1.358291	0.000002
1	1.262757	4.281547	-0.000027
1	-1.947767	-1.610284	0.000045
1	-6.000547	-0.772542	-0.892847
1	-6.000537	-0.772518	0.892954
1	-6.079979	-2.324442	0.000076
6	4.077749	-2.290257	-0.000012
1	4.546821	-2.689517	-0.903490
1	4.546808	-2.689502	0.903480

10d

6	-0.235456	-0.038879	-0.000019
6	0.509826	-1.294338	0.000153
6	1.856933	-1.266606	0.000286
6	2.598444	-0.041922	0.000263
6	2.007194	1.172153	0.000102
6	0.558310	1.212242	-0.000049
7	-0.034709	2.402762	-0.000213
8	0.836395	3.524169	-0.000213
6	-1.611577	-0.032781	-0.000144
7	-2.405433	-1.160642	-0.000105
6	-3.791439	-1.210448	-0.000252
8	-4.351168	-2.302143	-0.000190
8	-1.269810	2.693779	-0.000369
6	-4.539343	0.104446	-0.000485
1	-0.005584	-2.246811	0.000173
8	2.734438	-2.314299	0.000466
8	3.928759	-0.328722	0.000427
1	2.579507	2.087584	0.000082
1	-2.138785	0.905825	-0.000280
1	-1.984053	-2.082735	0.000045
1	-5.607844	-0.112703	-0.000576
1	-4.293674	0.702426	-0.885102
1	-4.293867	0.702631	0.884046
1	0.180449	4.248970	-0.000359
6	4.055030	-1.759399	0.000503

1	4.584247	-2.074590	-0.902933
1	4.584157	-2.074501	0.904022

10e

6	0.110314	0.191766	-0.001906
6	0.554429	-1.200969	-0.003208
6	1.874514	-1.464921	-0.001226
6	2.867770	-0.429362	0.002112
6	2.559600	0.885703	0.003429
6	1.155121	1.240039	0.001385
7	0.820291	2.525433	0.002364
8	-0.328435	3.054289	0.000840
6	-1.226348	0.471115	-0.003638
8	-2.114563	-0.571455	-0.005826
6	-3.466078	-0.252729	-0.010669
8	-3.891497	0.889567	-0.013869
8	1.902977	3.442192	0.005670
7	-4.184962	-1.391204	-0.026556
6	-5.637825	-1.399445	0.031211
1	-0.186630	-1.989084	-0.005843
8	2.505598	-2.677804	-0.001891
8	4.102817	-1.000034	0.003496
1	3.318367	1.653949	0.005840
1	-1.654556	1.457860	-0.003674
1	1.412918	4.288144	0.005455
1	-3.681587	-2.265526	0.036401
1	-6.001236	-1.562947	1.052709
1	-6.006036	-0.436625	-0.324828
1	-6.023892	-2.192264	-0.614151
6	3.914313	-2.423684	0.000666
1	4.361308	-2.847723	0.904052
1	4.364013	-2.844493	-0.902898

10f

6	-0.274588	0.089065	-0.000007
6	0.340618	-1.236959	0.000089
6	1.683521	-1.332573	0.000084
6	2.540484	-0.181371	-0.000012
6	2.070348	1.084486	-0.000104
6	0.632541	1.258951	-0.000103
7	0.138216	2.492628	-0.000187
8	-1.065921	2.871434	-0.000202
6	-1.634937	0.199353	-0.000004
8	-2.382145	-0.956708	0.000094
6	-3.752200	-0.845440	0.000100
8	-4.328112	0.218438	0.000016
8	1.096733	3.535349	-0.000273
6	-4.383588	-2.209484	0.000229
1	-0.295408	-2.111823	0.000161
8	2.459682	-2.456352	0.000164
8	3.836472	-0.593900	0.000008
1	2.726813	1.941765	-0.000175
1	-2.187691	1.121555	-0.000074
1	0.507618	4.315816	-0.000318
1	-5.469051	-2.109268	0.000196

1	-4.062000	-2.771576	0.883072
1	-4.061959	-2.771768	-0.882475
6	3.826737	-2.029718	0.000101
1	4.323415	-2.393585	-0.903426
1	4.323460	-2.393467	0.903652

10g

6	-0.099585	0.191263	-0.000035
6	-0.550385	-1.199245	-0.000094
6	-1.872311	-1.454639	-0.000081
6	-2.861613	-0.414246	-0.000002
6	-2.546520	0.898877	0.000056
6	-1.140328	1.244025	0.000018
7	-0.795826	2.527452	0.000003
8	-1.870225	3.449514	-0.000166
6	1.235814	0.466702	-0.000052
8	2.115659	-0.596962	-0.000159
6	3.443107	-0.308271	0.000033
8	3.927773	0.800686	0.000310
8	0.355417	3.044871	0.000031
8	4.092693	-1.469381	-0.000138
6	5.533586	-1.366804	0.000028
1	0.185446	-1.992028	-0.000137
8	-2.507810	-2.662920	-0.000216
8	-4.098374	-0.979552	-0.000124
1	-3.300493	1.671785	0.000097
1	1.677074	1.447070	0.000018
1	-1.377367	4.294083	0.000379
1	5.891665	-2.395078	-0.000215
1	5.874660	-0.840901	0.894208
1	5.874835	-0.840414	-0.893798
6	-3.916078	-2.403881	0.000383
1	-4.364644	-2.824322	0.904468
1	-4.365576	-2.825094	-0.902861

10h

6	0.768825	1.309771	0.000015
6	-0.653052	1.665658	-0.000034
6	-1.582957	0.693491	-0.000031
6	-1.238350	-0.701053	0.000015
6	0.037184	-1.143216	0.000049
6	1.085296	-0.142639	0.000037
7	2.351882	-0.548178	0.000015
8	2.538092	-1.954114	-0.000062
6	1.687649	2.313122	0.000037
8	3.413557	0.125824	-0.000016
1	-0.923584	2.715465	-0.000057
8	-2.944240	0.807764	-0.000054
8	-2.381249	-1.438838	0.000013
1	0.279275	-2.195399	0.000084
1	2.750304	2.135336	0.000074
1	1.338512	3.341814	0.000019
1	3.514878	-2.001481	-0.000035
6	-3.483256	-0.518695	0.000021

1	-4.079902	-0.671073	0.903542
1	-4.079966	-0.671136	-0.903446

10a⁻

6	-0.805915	-0.275713	-0.038646
6	0.220637	-1.327122	-0.008907
6	1.525029	-0.986071	0.028527
6	1.970844	0.370001	0.040757
6	1.101980	1.404563	0.024364
6	-0.312583	1.120785	-0.007441
7	-1.149328	2.204679	-0.003794
8	-2.421497	2.041389	-0.011362
6	-2.116505	-0.667082	-0.109845
8	-2.423559	-2.014017	-0.215700
6	-3.745994	-2.332712	0.188644
8	-0.674230	3.400025	0.008938
1	-0.095845	-2.362403	-0.017122
8	2.628525	-1.811864	0.091495
8	3.355030	0.383022	0.123011
1	1.415427	2.439072	0.045467
1	-2.945508	0.022055	-0.147969
1	-3.892659	-3.397812	-0.007674
1	-4.488543	-1.757045	-0.382841
1	-3.899870	-2.136474	1.259198
6	3.760573	-0.961665	-0.130770
1	4.559418	-1.237230	0.560763
1	4.090338	-1.061259	-1.174417

10b⁻

6	0.789847	-0.282792	-0.070047
6	-0.234649	-1.337640	-0.086488
6	-1.541924	-1.013795	-0.003025
6	-1.995733	0.335517	0.087743
6	-1.136292	1.377672	0.071875
6	0.280616	1.114015	-0.018640
7	1.092004	2.214452	-0.028929
8	0.593843	3.402673	0.058316
6	2.114060	-0.653464	-0.095279
7	2.569623	-1.986522	-0.110485
6	3.986810	-2.182281	0.173291
8	2.369214	2.087585	-0.120670
1	0.059957	-2.374383	-0.204760
8	-2.639314	-1.850636	0.015104
8	-3.379103	0.332449	0.198678
1	-1.458906	2.407962	0.126807
1	2.880902	0.102942	-0.154067
1	4.296572	-1.827655	1.171414
1	4.586061	-1.647140	-0.571659
1	4.227479	-3.247157	0.096820
1	1.998770	-2.615477	0.446279
6	-3.778411	-0.994487	-0.141741
1	-4.570520	-1.320885	0.535189
1	-4.114757	-1.026754	-1.187695

10c⁻

6	-0.133775	0.247415	-0.003562
6	-0.609356	-1.141870	0.040600
6	-1.933872	-1.405721	0.006297
6	-2.923371	-0.383919	-0.056118
6	-2.587290	0.925130	-0.060974
6	-1.192223	1.284721	-0.021335
7	-0.923325	2.634016	-0.015204
8	-1.879627	3.486863	-0.075401
6	1.216297	0.499406	-0.039375
7	2.188763	-0.517969	-0.126619
6	3.517899	-0.286848	0.048093
8	4.026639	0.774229	0.390210
8	0.281141	3.058216	0.049709
8	4.224519	-1.422584	-0.218656
6	5.644335	-1.309560	-0.054566
1	0.094046	-1.961048	0.135175
8	-2.560883	-2.629587	0.019421
8	-4.174440	-0.977255	-0.119246
1	-3.319238	1.719777	-0.093784
1	1.611896	1.497811	-0.016189
1	1.941936	-1.438864	-0.463433
1	5.899004	-1.055096	0.978102
1	6.055247	-0.549020	-0.724147
1	6.045767	-2.290960	-0.309193
6	-3.957866	-2.351139	0.199326
1	-4.230639	-2.540900	1.246391
1	-4.539536	-2.978772	-0.478777

10d⁻

6	-0.268871	0.107790	-0.058546
6	0.405335	-1.194132	0.001876
6	1.755674	-1.256948	0.006779
6	2.582302	-0.099408	-0.026957
6	2.054056	1.144954	-0.040948
6	0.620797	1.289405	-0.042348
7	0.151164	2.585246	-0.043220
8	0.968712	3.569994	-0.084914
6	-1.642722	0.150691	-0.143690
7	-2.432132	-1.009117	-0.302305
6	-3.762679	-1.154366	-0.030339
8	-4.361928	-2.196263	-0.327750
8	-1.103408	2.822017	-0.002701
6	-4.454884	0.017778	0.637806
1	-0.175064	-2.105980	0.078462
8	2.556958	-2.373169	0.042519
8	3.909077	-0.497660	-0.050048
1	2.658798	2.040668	-0.050081
1	-2.167342	1.088888	-0.152199
1	-2.030773	-1.822461	-0.757194
1	-5.439495	-0.307854	0.977399
1	-4.584831	0.846855	-0.068890
1	-3.875792	0.400304	1.484679
6	3.891914	-1.890553	0.259765
1	4.578109	-2.420302	-0.403984
1	4.162339	-2.043656	1.313237

10e⁻

6	-0.116000	0.290744	-0.003158
6	-0.537712	-1.116265	-0.011877
6	-1.853459	-1.418601	-0.028658
6	-2.877926	-0.427328	-0.035526
6	-2.586427	0.892408	-0.024478
6	-1.202453	1.293509	-0.007926
7	-0.961838	2.646831	0.002010
8	0.236859	3.088820	0.017807
6	1.222211	0.573492	0.012708
8	2.118497	-0.507697	0.012634
6	3.449600	-0.229972	0.033568
8	3.931742	0.896057	0.046772
8	-1.935814	3.479799	-0.005076
7	4.162267	-1.387553	0.065647
6	5.607691	-1.395326	-0.077432
1	0.216840	-1.892094	-0.005950
8	-2.443063	-2.661941	-0.067781
8	-4.110106	-1.058523	-0.099153
1	-3.343950	1.663679	-0.034347
1	1.668402	1.547584	0.025507
1	3.652224	-2.246344	-0.087848
1	5.926287	-1.318403	-1.125732
1	6.025581	-0.551068	0.474131
1	6.001776	-2.323611	0.342475
6	-3.843252	-2.437787	0.150878
1	-4.418662	-3.052043	-0.544770
1	-4.090070	-2.684028	1.192742

10f⁻

6	-0.280691	0.183133	-0.014270
6	0.315644	-1.157720	-0.020714
6	1.659925	-1.290453	-0.028651
6	2.549865	-0.178453	-0.028616
6	2.091933	1.093414	-0.019871
6	0.668388	1.312936	-0.011818
7	0.256090	2.627699	-0.000726
8	-0.987139	2.911395	0.006248
6	-1.646364	0.294621	-0.005868
8	-2.393687	-0.895104	-0.013265
6	-3.739212	-0.819972	0.029998
8	-4.363614	0.225170	0.095561
8	1.115592	3.574910	0.002268
6	-4.360303	-2.193826	-0.050536
1	-0.333907	-2.023235	-0.020324
8	2.401108	-2.448725	-0.063193
8	3.852210	-0.647237	-0.083258
1	2.744537	1.955107	-0.025474
1	-2.213733	1.203071	0.005869
1	-5.376117	-2.158827	0.347135
1	-3.766328	-2.931170	0.495178
1	-4.409083	-2.512246	-1.099026
6	3.761120	-2.050218	0.162582
1	4.412534	-2.584833	-0.531690
1	4.031872	-2.265813	1.205122

10g$^-$

6	0.106362	0.290280	-0.009954
6	0.534145	-1.113603	-0.021709
6	1.852466	-1.408475	-0.031168
6	2.871696	-0.413144	-0.027697
6	2.572193	0.905068	-0.013900
6	1.186198	1.295977	-0.004566
7	0.935034	2.649996	0.008240
8	1.901787	3.487216	0.010890
6	-1.233257	0.569441	-0.000292
8	-2.119277	-0.530344	-0.008229
6	-3.429921	-0.278317	0.004382
8	-3.964884	0.813938	0.022854
8	-0.265565	3.080611	0.016815
8	-4.069178	-1.461037	-0.007223
6	-5.505340	-1.376068	0.003263
1	-0.215389	-1.894109	-0.023838
8	2.446362	-2.648069	-0.070501
8	4.106964	-1.037084	-0.085366
1	3.324920	1.680974	-0.016474
1	-1.693342	1.536789	0.013507
1	-5.854862	-2.408178	-0.007189
1	-5.865605	-0.843503	-0.880372
1	-5.853963	-0.865435	0.904335
6	3.846319	-2.420544	0.149148
1	4.423253	-3.024367	-0.554292
1	4.094894	-2.677677	1.187700

10h$^-$

6	-0.857080	1.262527	-0.004480
6	0.564500	1.641101	-0.014635
6	1.525038	0.693182	-0.030912
6	1.228853	-0.701220	-0.036784
6	-0.044184	-1.154258	-0.023832
6	-1.119590	-0.192568	-0.005641
7	-2.395000	-0.719051	0.011822
8	-2.566734	-1.987636	0.010358
6	-1.774090	2.280873	0.010044
8	-3.414741	0.043105	0.029740
1	0.817472	2.696824	-0.010220
8	2.892700	0.853909	-0.070688
8	2.419264	-1.409730	-0.102518
1	-0.293294	-2.206024	-0.032292
1	-2.836396	2.106632	0.023152
1	-1.413511	3.307371	0.009386
6	3.443129	-0.450901	0.158391
1	4.278207	-0.614421	-0.525853
1	3.769157	-0.526609	1.205029