Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

CRANAD-1 as a cyanide sensor in aqueous media: A theoretical study

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Optimized geometric parameters for **1** in B3LYP/SDD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.127300	-0.643216	-0.000003
2	6	0	-5.931330	0.076200	-0.000099
3	6	0	-7.103159	-2.064309	0.000306
4	1	0	-5.940458	1.161811	-0.000330
5	6	0	-4.680835	-0.608524	0.000097
6	6	0	-5.878364	-2.750197	0.000511
7	1	0	-5.883830	-3.835502	0.000752
8	6	0	-4.677005	-2.029421	0.000407
9	1	0	-3.739683	-2.576025	0.000584
10	6	0	-3.462906	0.189819	-0.000015
11	1	0	-3.596207	1.271051	-0.000133
12	6	0	-2.170998	-0.272726	0.000009
13	1	0	-1.943432	-1.334107	0.000091
14	6	0	-1.031579	0.610922	-0.000074
15	8	0	-1.271993	1.944940	-0.000165
16	6	0	0.290129	0.131089	-0.000041
17	1	0	0.453917	-0.937120	0.000042
18	6	0	1.381203	1.025084	-0.000090
19	8	0	1.146924	2.360583	-0.000093
20	6	0	2.781135	0.674300	-0.000086
21	1	0	3.451839	1.528782	0.000026
22	6	0	3.265765	-0.610343	-0.000243
23	1	0	2.555039	-1.435620	-0.000406
24	6	0	4.662582	-1.017331	-0.000227
25	6	0	5.742805	-0.084297	0.000093
26	6	0	4.955294	-2.406581	-0.000530
27	1	0	5.545365	0.981429	0.000341
28	1	0	4.138906	-3.123832	-0.000765
29	6	0	7.056395	-0.546930	0.000093
30	6	0	6.279425	-2.871052	-0.000549
31	1	0	6.505343	-3.932259	-0.000787
32	6	0	7.331241	-1.946514	-0.000239
33	8	0	8.213564	0.231025	0.000375
34	6	0	8.091977	1.692692	0.000963
35	1	0	7.566626	2.034160	-0.898629
36	1	0	7.566475	2.033420	0.900748
37	1	0	9.115710	2.068248	0.001199
38	8	0	8.644153	-2.385040	-0.000233
39	1	0	9.260398	-1.616526	0.000038
40	8	0	-8.419307	-0.115410	-0.000188
41	6	0	-8.593932	1.340647	-0.000487
42	1	0	-8.147957	1.781583	0.898760
43	1	0	-8.147898	1.781222	-0.899881
44	1	0	-9.672334	1.503000	-0.000555
45	8	0	-8.293875	-2.773495	0.000416
46	1	0	-9.058909	-2.153342	0.000252
47	5	0	-0.206718	2.975459	-0.000076
48	9	0	-0.346335	3.804823	-1.165328
49	9	0	-0.346366	3.804691	1.165256

Optimized geometric parameters for **1a** in B3LYP/SDD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.534147	-0.233411	-0.024710
2	6	0	-5.310895	0.412595	-0.031260
3	6	0	-6.627440	-1.695373	0.017498
4	1	0	-5.258674	1.498455	-0.061774
5	6	0	-4.069400	-0.318991	0.002411
6	6	0	-5.366300	-2.406845	0.050733
7	1	0	-5.430145	-3.491332	0.081817
8	6	0	-4.148594	-1.752445	0.043333
9	1	0	-3.231570	-2.336278	0.069442
10	6	0	-2.841997	0.397480	-0.005291
11	1	0	-2.902614	1.485872	-0.037903
12	6	0	-1.544165	-0.120880	0.025251
13	1	0	-1.369001	-1.192476	0.060519
14	6	0	-0.392426	0.702704	0.012361
15	8	0	-0.544406	2.043379	-0.053017
16	6	0	0.932263	0.158289	0.048012
17	1	0	1.049797	-0.916450	0.099716
18	6	0	2.041590	0.993850	-0.003487
19	8	0	1.902465	2.339632	-0.060200
20	6	0	3.441286	0.566920	-0.013184
21	1	0	4.130939	1.407907	-0.042013
22	6	0	3.898376	-0.716236	0.008404
23	1	0	3.172815	-1.529503	0.032631
24	6	0	5.302194	-1.145321	0.002406
25	6	0	6.386307	-0.223088	-0.025573
26	6	0	5.599486	-2.529299	0.025287
27	1	0	6.185428	0.842358	-0.042461
28	1	0	4.782539	-3.246830	0.046938
29	6	0	7.700789	-0.689207	-0.030400
30	6	0	6.925842	-2.997020	0.020683
31	1	0	7.153803	-4.058091	0.038315
32	6	0	7.981268	-2.081012	-0.007193
33	8	0	8.861077	0.104568	-0.056998
34	6	0	8.713481	1.553661	-0.085496
35	1	0	8.171545	1.873647	-0.985309
36	1	0	8.188845	1.910922	0.810496
37	1	0	9.729717	1.952584	-0.103517
38	8	0	9.301651	-2.524167	-0.012158
39	1	0	9.904377	-1.747813	-0.032877
40	8	0	-7.779867	0.394596	-0.055939
41	6	0	-7.824771	1.843799	-0.100969
42	1	0	-7.351260	2.286715	0.788188
43	1	0	-7.331707	2.231345	-1.005229
44	1	0	-8.886476	2.098434	-0.120326
45	8	0	-7.759848	-2.321721	0.024778
46	1	0	-9.217020	-1.853219	-0.003596
47	5	0	0.572694	3.037657	0.046955
48	9	0	0.460058	3.975406	-1.014514
49	9	0	0.503597	3.697578	1.312530
50	7	0	-10.264096	-1.646637	-0.020293
51	6	0	-11.434017	-1.424375	-0.038757

Optimized geometric parameters for **1b** in B3LYP/SDD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.927352	-0.794403	-0.000328
2	6	0	-5.863180	0.111108	-0.000391
3	6	0	-6.682232	-2.188016	-0.000071
4	1	0	-6.043115	1.182855	-0.000587
5	6	0	-4.521915	-0.359610	-0.000191
6	6	0	-5.362743	-2.663205	0.000132
7	1	0	-5.194089	-3.735549	0.000342
8	6	0	-4.287036	-1.762443	0.000071
9	1	0	-3.271015	-2.151905	0.000277
10	6	0	-3.432222	0.621212	-0.000255
11	1	0	-3.705541	1.677015	-0.000484
12	6	0	-2.109518	0.294660	-0.000055
13	1	0	-1.776824	-0.744428	0.000165
14	6	0	-1.019286	1.248234	-0.000053
15	8	0	-1.261944	2.572460	-0.000743
16	6	0	0.287223	0.747802	0.000480
17	1	0	0.412892	-0.326233	0.000997
18	6	0	1.388407	1.619356	-0.000040
19	8	0	1.196825	2.949739	-0.000572
20	6	0	2.766892	1.159034	-0.000095
21	1	0	3.518531	1.945563	-0.000262
22	6	0	3.081716	-0.174364	0.000045
23	1	0	2.276778	-0.914954	0.000205
24	6	0	4.408972	-0.782918	0.000046
25	6	0	5.620810	-0.036241	-0.000221
26	6	0	4.468335	-2.201087	0.000338
27	1	0	5.584502	1.048388	-0.000449
28	1	0	3.531124	-2.756900	0.000512
29	6	0	6.842706	-0.706938	-0.000195
30	6	0	5.705656	-2.867411	0.000400
31	1	0	5.765535	-3.951253	0.000622
32	6	0	6.892636	-2.126511	0.000132
33	8	0	8.121210	-0.110697	-0.000377
34	6	0	8.204461	1.341363	-0.001613
35	1	0	7.730379	1.760793	-0.899405
36	1	0	7.730778	1.762308	0.895681
37	1	0	9.271081	1.576918	-0.002028
38	8	0	8.128777	-2.770670	0.000146
39	1	0	8.843034	-2.095110	-0.000061
40	8	0	-8.300917	-0.466429	-0.000497
41	6	0	-8.671337	0.938957	-0.000688
42	1	0	-8.290797	1.446020	0.896669
43	1	0	-8.290694	1.445803	-0.898123
44	1	0	-9.763686	0.957826	-0.000754
45	8	0	-7.754128	-3.082067	-0.000008
46	1	0	-8.595296	-2.573710	-0.000171
47	5	0	-0.168313	3.608536	0.000462
48	9	0	-0.284281	4.409000	-1.170368
49	9	0	-0.283928	4.405951	1.173495
50	6	0	0.682517	-2.656147	0.000625
51	7	0	-0.522540	-2.606279	0.000625

Optimized geometric parameters for **1c** in B3LYP/SDD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.539935	-2.095297	-0.248472
2	6	0	-4.770908	-0.729071	-0.346924
3	6	0	-3.373739	-2.611385	0.460685
4	1	0	-5.627602	-0.359062	-0.905782
5	6	0	-3.873556	0.239330	0.224655
6	6	0	-2.557183	-1.625147	1.125819
7	1	0	-1.738014	-1.994166	1.737693
8	6	0	-2.789158	-0.262456	1.007071
9	1	0	-2.158956	0.434832	1.549706
10	6	0	-4.148730	1.634585	0.009102
11	1	0	-5.187002	1.835084	-0.272932
12	6	0	-3.373125	2.790989	0.084832
13	1	0	-3.909635	3.737549	0.046488
14	6	0	-1.950705	2.984740	0.097620
15	8	0	-1.557534	4.255823	0.334066
16	6	0	-0.952808	2.008554	-0.177430
17	1	0	-1.240630	1.000408	-0.430723
18	6	0	0.403232	2.329980	-0.087237
19	8	0	0.809242	3.586100	0.188592
20	6	0	1.424289	1.304518	-0.224729
21	1	0	1.045747	0.295732	-0.371414
22	6	0	2.762973	1.558569	-0.155810
23	1	0	3.061029	2.600600	-0.044938
24	6	0	3.838702	0.565882	-0.211443
25	6	0	3.586571	-0.835215	-0.144314
26	6	0	5.179658	1.007692	-0.317151
27	1	0	2.570677	-1.198375	-0.035105
28	1	0	5.383375	2.074977	-0.359380
29	6	0	4.646282	-1.740833	-0.190320
30	6	0	6.247900	0.094388	-0.376213
31	1	0	7.277227	0.428320	-0.461621
32	6	0	5.985420	-1.277522	-0.314999
33	8	0	4.553797	-3.133603	-0.115544
34	6	0	3.241494	-3.745000	0.138944
35	1	0	2.818554	-3.384184	1.082180
36	1	0	2.548396	-3.537911	-0.684171
37	1	0	3.415162	-4.817894	0.208439
38	8	0	7.024139	-2.202403	-0.358574
39	1	0	6.643130	-3.107335	-0.286497
40	8	0	-5.356762	-3.079629	-0.815775
41	6	0	-6.528524	-2.648655	-1.551202
42	1	0	-7.225052	-2.085885	-0.910204
43	1	0	-6.255634	-2.027758	-2.418576
44	1	0	-7.009212	-3.567496	-1.895691
45	8	0	-3.102824	-3.889207	0.495659
46	1	0	-1.801927	-4.362495	0.709668
47	5	0	-0.144831	4.750251	0.164638
48	9	0	-0.037123	5.413393	-1.097720
49	9	0	0.169315	5.626564	1.230604
50	6	0	0.397777	-5.036354	0.900105
51	7	0	-0.738748	-4.692316	0.811539

Optimized geometric parameters for **1d** in B3LYP/SDD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.338216	-1.985468	-0.003658
2	6	0	-4.159473	-1.243217	-0.001673
3	6	0	-6.597946	-1.335867	-0.008045
4	1	0	-3.174193	-1.714328	0.001756
5	6	0	-4.220629	0.180395	-0.003948
6	6	0	-6.666117	0.065957	-0.010395
7	1	0	-7.644520	0.536972	-0.013752
8	6	0	-5.483324	0.823635	-0.008305
9	1	0	-5.543064	1.908641	-0.009995
10	6	0	-2.926068	0.850059	-0.001120
11	1	0	-2.105275	0.134652	0.001733
12	6	0	-2.609177	2.181764	-0.002158
13	1	0	-3.350543	2.976584	-0.007412
14	6	0	-1.214370	2.600756	0.002088
15	8	0	-0.967895	3.919644	-0.012025
16	6	0	-0.144607	1.690032	0.016030
17	1	0	-0.305495	0.622411	0.029078
18	6	0	1.182876	2.135860	0.003946
19	8	0	1.481290	3.445030	-0.012138
20	6	0	2.210051	1.118999	0.004338
21	1	0	1.796233	0.113025	0.012690
22	6	0	3.561292	1.300072	-0.006638
23	1	0	3.965299	2.312181	-0.015565
24	6	0	4.511399	0.182993	-0.007683
25	6	0	4.056210	-1.170007	0.001834
26	6	0	5.903984	0.436210	-0.018966
27	1	0	2.992614	-1.399274	0.009684
28	1	0	6.257539	1.464933	-0.026173
29	6	0	4.983979	-2.207798	-0.000187
30	6	0	6.836808	-0.618130	-0.021084
31	1	0	7.906455	-0.432336	-0.029726
32	6	0	6.380149	-1.940130	-0.011790
33	8	0	4.678044	-3.575297	0.007792
34	6	0	3.257347	-3.956114	0.031996
35	1	0	2.762575	-3.566055	0.927502
36	1	0	2.728735	-3.561785	-0.841778
37	1	0	3.255960	-5.048371	0.029689
38	8	0	7.280002	-3.004867	-0.013645
39	1	0	6.767889	-3.845317	-0.005762
40	8	0	-5.421138	-3.387652	-0.001658
41	6	0	-4.160070	-4.134590	0.002739
42	1	0	-3.564988	-3.899211	-0.887495
43	1	0	-3.569527	-3.896435	0.895258
44	1	0	-4.447494	-5.188307	0.003654
45	8	0	-7.765986	-2.095891	-0.009978
46	1	0	-7.522734	-3.049103	-0.007806
47	5	0	0.425338	4.525868	0.004453
48	9	0	0.575635	5.336209	-1.151811
49	9	0	0.566808	5.291568	1.193508
50	6	0	-0.654324	-1.939823	0.008952
51	7	0	0.550387	-1.909928	0.010352

Optimized geometric parameters for **1e** in B3LYP/SDD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.175318	-0.341248	-0.016565
2	6	0	-5.960893	0.334996	-0.019536
3	6	0	-7.241562	-1.794326	0.005809
4	1	0	-5.936040	1.422552	-0.035828
5	6	0	-4.708476	-0.363839	-0.001116
6	6	0	-5.971585	-2.471714	0.023866
7	1	0	-6.007531	-3.558350	0.040542
8	6	0	-4.759016	-1.789526	0.020487
9	1	0	-3.831264	-2.357836	0.035064
10	6	0	-3.484482	0.395580	-0.004498
11	1	0	-3.582815	1.481837	-0.020981
12	6	0	-2.185336	-0.076207	0.011137
13	1	0	-1.972953	-1.142371	0.028560
14	6	0	-1.039123	0.790501	0.006126
15	8	0	-1.259852	2.127169	-0.026083
16	6	0	0.280955	0.294926	0.026394
17	1	0	0.433327	-0.775952	0.051653
18	6	0	1.389948	1.171722	0.002735
19	8	0	1.174379	2.511093	-0.024201
20	6	0	2.776298	0.792041	-0.001951
21	1	0	3.461092	1.635916	-0.017558
22	6	0	3.256684	-0.506813	0.010830
23	1	0	2.522332	-1.314707	0.024501
24	6	0	4.624807	-0.945422	0.008519
25	6	0	5.743598	-0.044532	-0.009023
26	6	0	4.913289	-2.343546	0.024152
27	1	0	5.552180	1.024179	-0.020893
28	1	0	4.079502	-3.046190	0.037626
29	6	0	7.046638	-0.517869	-0.010764
30	6	0	6.217992	-2.826067	0.022799
31	1	0	6.426026	-3.893200	0.034913
32	6	0	7.361340	-1.949047	0.005351
33	8	0	8.189332	0.298469	-0.027757
34	6	0	8.002459	1.735119	-0.046012
35	1	0	7.452660	2.058090	-0.943435
36	1	0	7.463096	2.082326	0.848663
37	1	0	9.009365	2.159723	-0.057595
38	8	0	8.586391	-2.391893	0.003866
39	1	0	10.011036	-1.595428	-0.012731
40	8	0	-8.435826	0.277638	-0.034086
41	6	0	-8.489757	1.723205	-0.058040
42	1	0	-8.014720	2.160950	0.834013
43	1	0	-8.002924	2.131550	-0.957649
44	1	0	-9.553595	1.973459	-0.069093
45	8	0	-8.370497	-2.457880	0.009504
46	1	0	-9.736612	-2.041706	-0.002975
47	5	0	-0.175707	3.154846	0.026285
48	9	0	-0.313016	4.038229	-1.089955
49	9	0	-0.292408	3.900692	1.245319
50	7	0	-10.827244	-1.866647	-0.010028
51	6	0	-12.006040	-1.691406	-0.017342
52	6	0	11.070961	-1.210477	-0.022607
53	7	0	12.184885	-0.810843	-0.032964

Optimized geometric parameters for **1f** in B3LYP/SDD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.455739	-1.843946	-0.703198
2	6	0	-5.340179	-0.486391	-0.976449
3	6	0	-4.578910	-2.500241	0.256491
4	1	0	-6.020660	-0.012773	-1.681441
5	6	0	-4.335462	0.338863	-0.365090
6	6	0	-3.592677	-1.649271	0.871085
7	1	0	-2.938938	-2.110392	1.608094
8	6	0	-3.467124	-0.293700	0.571124
9	1	0	-2.727525	0.298197	1.101101
10	6	0	-4.365848	1.751043	-0.684165
11	1	0	-5.306188	2.038793	-1.166131
12	6	0	-3.530092	2.839420	-0.496170
13	1	0	-3.969875	3.811216	-0.718422
14	6	0	-2.141331	2.994644	-0.116689
15	8	0	-1.827256	4.287392	0.173070
16	6	0	-1.123040	2.025690	-0.137009
17	1	0	-1.350829	1.008198	-0.420218
18	6	0	0.225858	2.383479	0.119336
19	8	0	0.533081	3.661656	0.443254
20	6	0	1.303185	1.443705	0.032585
21	1	0	1.028658	0.421273	-0.213873
22	6	0	2.625261	1.815707	0.226725
23	1	0	2.778332	2.869146	0.462670
24	6	0	3.808927	1.010337	0.143591
25	6	0	3.800698	-0.396110	-0.149152
26	6	0	5.079443	1.629099	0.348433
27	1	0	2.846852	-0.892954	-0.300632
28	1	0	5.105668	2.694462	0.575599
29	6	0	4.982106	-1.118850	-0.237485
30	6	0	6.267423	0.911728	0.259986
31	1	0	7.231381	1.389873	0.413718
32	6	0	6.289841	-0.493830	-0.041703
33	8	0	5.061741	-2.488410	-0.517294
34	6	0	3.828705	-3.225521	-0.711726
35	1	0	3.192542	-3.189509	0.185524
36	1	0	3.260176	-2.839013	-1.571510
37	1	0	4.134563	-4.256201	-0.905268
38	8	0	7.410435	-1.157750	-0.131797
39	1	0	7.747779	-2.527585	-0.456125
40	8	0	-6.417076	-2.686403	-1.292909
41	6	0	-7.335097	-2.096857	-2.240770
42	1	0	-7.950273	-1.307911	-1.777979
43	1	0	-6.808320	-1.670786	-3.110005
44	1	0	-7.980745	-2.915735	-2.570948
45	8	0	-4.713471	-3.771534	0.533600
46	1	0	-4.190994	-4.589847	1.553352
47	5	0	-0.455332	4.779866	0.492347
48	9	0	-0.083073	5.778302	-0.468099
49	9	0	-0.450413	5.357153	1.802222
50	6	0	-3.495246	-6.040116	3.200141
51	7	0	-3.845577	-5.284842	2.345970
52	6	0	8.622396	-4.580920	-0.954843
53	7	0	8.156751	-3.515768	-0.693115

Optimized geometric parameters for **1a-CN**$^-$ in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.534147	-0.233411	-0.024710
2	6	0	-5.310895	0.412595	-0.031260
3	6	0	-6.627440	-1.695373	0.017498
4	1	0	-5.258674	1.498455	-0.061774
5	6	0	-4.069400	-0.318991	0.002411
6	6	0	-5.366300	-2.406845	0.050733
7	1	0	-5.430145	-3.491332	0.081817
8	6	0	-4.148594	-1.752445	0.043333
9	1	0	-3.231570	-2.336278	0.069442
10	6	0	-2.841997	0.397480	-0.005291
11	1	0	-2.902614	1.485872	-0.037903
12	6	0	-1.544165	-0.120880	0.025251
13	1	0	-1.369001	-1.192476	0.060519
14	6	0	-0.392426	0.702704	0.012361
15	8	0	-0.544406	2.043379	-0.053017
16	6	0	0.932263	0.158289	0.048012
17	1	0	1.049797	-0.916450	0.099716
18	6	0	2.041590	0.993850	-0.003487
19	8	0	1.902465	2.339632	-0.060200
20	6	0	3.441286	0.566920	-0.013184
21	1	0	4.130939	1.407907	-0.042013
22	6	0	3.898376	-0.716236	0.008404
23	1	0	3.172815	-1.529503	0.032631
24	6	0	5.302194	-1.145321	0.002406
25	6	0	6.386307	-0.223088	-0.025573
26	6	0	5.599486	-2.529299	0.025287
27	1	0	6.185428	0.842358	-0.042461
28	1	0	4.782539	-3.246830	0.046938
29	6	0	7.700789	-0.689207	-0.030400
30	6	0	6.925842	-2.997020	0.020683
31	1	0	7.153803	-4.058091	0.038315
32	6	0	7.981268	-2.081012	-0.007193
33	8	0	8.861077	0.104568	-0.056998
34	6	0	8.713481	1.553661	-0.085496
35	1	0	8.171545	1.873647	-0.985309
36	1	0	8.188845	1.910922	0.810496
37	1	0	9.729717	1.952584	-0.103517
38	8	0	9.301651	-2.524167	-0.012158
39	1	0	9.904377	-1.747813	-0.032877
40	8	0	-7.779867	0.394596	-0.055939
41	6	0	-7.824771	1.843799	-0.100969
42	1	0	-7.351260	2.286715	0.788188
43	1	0	-7.331707	2.231345	-1.005229
44	1	0	-8.886476	2.098434	-0.120326
45	8	0	-7.759848	-2.321721	0.024778
46	1	0	-9.217020	-1.853219	-0.003596
47	5	0	0.572694	3.037657	0.046955
48	9	0	0.460058	3.975406	-1.014514
49	9	0	0.503597	3.697578	1.312530
50	7	0	-10.264096	-1.646637	-0.020293
51	6	0	-11.434017	-1.424375	-0.038757

Optimized geometric parameters for **1a-CN**$^{-}$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.526316	-0.245512	-0.005604
2	6	0	-5.300140	0.406740	-0.008527
3	6	0	-6.603995	-1.696140	0.013008
4	1	0	-5.255381	1.492245	-0.022060
5	6	0	-4.063869	-0.322856	0.005440
6	6	0	-5.356061	-2.407404	0.026990
7	1	0	-5.407698	-3.492800	0.040840
8	6	0	-4.131799	-1.751332	0.023088
9	1	0	-3.217978	-2.338653	0.034490
10	6	0	-2.832025	0.408397	0.001742
11	1	0	-2.913900	1.495341	-0.007780
12	6	0	-1.541195	-0.106438	0.008716
13	1	0	-1.360981	-1.176879	0.016259
14	6	0	-0.383060	0.719713	0.005852
15	8	0	-0.555149	2.071775	-0.004146
16	6	0	0.934136	0.190014	0.010959
17	1	0	1.056383	-0.884311	0.017862
18	6	0	2.051142	1.030812	0.004013
19	8	0	1.881329	2.385437	-0.002055
20	6	0	3.443783	0.625166	0.001254
21	1	0	4.141957	1.458086	-0.001096
22	6	0	3.888992	-0.669686	0.000579
23	1	0	3.154875	-1.474804	0.001977
24	6	0	5.278671	-1.118144	-0.002286
25	6	0	6.383694	-0.216461	-0.004489
26	6	0	5.535308	-2.512953	-0.003060
27	1	0	6.214852	0.854270	-0.003913
28	1	0	4.700739	-3.209104	-0.001403
29	6	0	7.685803	-0.714052	-0.007374
30	6	0	6.848189	-3.012973	-0.005963
31	1	0	7.044563	-4.080268	-0.006582
32	6	0	7.924536	-2.118586	-0.008128
33	8	0	8.862762	0.036823	-0.009790
34	6	0	8.775425	1.500334	-0.009248
35	1	0	8.256267	1.854762	-0.907535
36	1	0	8.259876	1.854321	0.891288
37	1	0	9.807637	1.852301	-0.011233
38	8	0	9.228724	-2.592973	-0.011029
39	1	0	9.862412	-1.839275	-0.012217
40	8	0	-7.771125	0.390534	-0.019572
41	6	0	-7.804192	1.852484	-0.041459
42	1	0	-7.323502	2.271033	0.852390
43	1	0	-7.313916	2.244170	-0.942245
44	1	0	-8.862255	2.119617	-0.051017
45	8	0	-7.750282	-2.346358	0.017144
46	1	0	-9.044461	-1.902521	0.001801
47	5	0	0.555863	3.045963	0.010589
48	9	0	0.447075	3.909939	-1.139420
49	9	0	0.450139	3.872377	1.189492
50	7	0	-10.154897	-1.703629	-0.009291
51	6	0	-11.330281	-1.508571	-0.020968

Optimized geometric parameters for **1a-CN**$^{-}$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.454246	-0.264321	-0.051800
2	6	0	-5.231251	0.389356	-0.057327
3	6	0	-6.494702	-1.677133	0.056462
4	1	0	-5.196819	1.467910	-0.139050
5	6	0	-4.012704	-0.321314	0.042384
6	6	0	-5.286418	-2.380277	0.156131
7	1	0	-5.334370	-3.459832	0.238284
8	6	0	-4.067922	-1.723430	0.149552
9	1	0	-3.158168	-2.305098	0.229174
10	6	0	-2.778673	0.430687	0.031789
11	1	0	-2.886861	1.508734	-0.047500
12	6	0	-1.511001	-0.053601	0.109883
13	1	0	-1.313606	-1.115512	0.190072
14	6	0	-0.351933	0.795568	0.088085
15	8	0	-0.540022	2.095109	-0.031105
16	6	0	0.938323	0.265484	0.162829
17	1	0	1.059175	-0.802155	0.257104
18	6	0	2.049396	1.102757	0.045581
19	8	0	1.889318	2.407441	-0.058762
20	6	0	3.427101	0.675094	0.001624
21	1	0	4.135537	1.491783	-0.078364
22	6	0	3.847369	-0.612895	0.053643
23	1	0	3.102654	-1.400004	0.127877
24	6	0	5.214975	-1.091321	0.021700
25	6	0	6.330403	-0.225731	-0.075684
26	6	0	5.440935	-2.476314	0.090902
27	1	0	6.183931	0.843645	-0.130485
28	1	0	4.595749	-3.150583	0.164998
29	6	0	7.612004	-0.741525	-0.101100
30	6	0	6.729976	-2.998163	0.067008
31	1	0	6.904061	-4.065877	0.120768
32	6	0	7.818046	-2.140934	-0.028299
33	8	0	8.768567	-0.026793	-0.193400
34	6	0	8.695106	1.401188	-0.285214
35	1	0	8.144529	1.702742	-1.179894
36	1	0	8.222511	1.822422	0.605643
37	1	0	9.724141	1.745863	-0.352963
38	8	0	9.077467	-2.639175	-0.052543
39	1	0	9.697977	-1.897271	-0.121608
40	8	0	-7.669111	0.342784	-0.143528
41	6	0	-7.715800	1.765975	-0.261003
42	1	0	-7.272050	2.248128	0.614875
43	1	0	-7.203895	2.102871	-1.167079
44	1	0	-8.771177	2.022598	-0.322036
45	8	0	-7.635319	-2.378614	0.069602
46	1	0	-8.493902	-1.868877	-0.015635
47	5	0	0.568772	3.061242	0.110822
48	9	0	0.433653	4.049161	-0.866754
49	9	0	0.514610	3.639178	1.391321
50	7	0	-10.221907	-1.642163	-0.130547
51	6	0	-11.380901	-1.503090	-0.230093

Optimized geometric parameters for **1a-F**$^{-}$ in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.750652	-0.311981	-0.027742
2	6	0	-5.532860	0.343764	-0.033556
3	6	0	-6.831456	-1.775829	0.013561
4	1	0	-5.489823	1.430066	-0.063485
5	6	0	-4.284433	-0.376989	0.000194
6	6	0	-5.563207	-2.476282	0.046986
7	1	0	-5.617959	-3.561307	0.077453
8	6	0	-4.351620	-1.811730	0.040437
9	1	0	-3.429555	-2.387643	0.066601
10	6	0	-3.064099	0.349391	-0.006814
11	1	0	-3.133750	1.437238	-0.039341
12	6	0	-1.760749	-0.157784	0.024319
13	1	0	-1.576592	-1.227885	0.059837
14	6	0	-0.616959	0.675168	0.011668
15	8	0	-0.779631	2.015244	-0.054287
16	6	0	0.713062	0.142283	0.047846
17	1	0	0.839729	-0.931448	0.099940
18	6	0	1.814908	0.986905	-0.003625
19	8	0	1.664780	2.332155	-0.060852
20	6	0	3.218240	0.571821	-0.012964
21	1	0	3.900525	1.418867	-0.041996
22	6	0	3.687117	-0.707083	0.009041
23	1	0	2.969124	-1.527024	0.033469
24	6	0	5.095073	-1.122853	0.003212
25	6	0	6.170355	-0.190329	-0.024919
26	6	0	5.405909	-2.503874	0.026356
27	1	0	5.959218	0.873122	-0.042035
28	1	0	4.595958	-3.229281	0.048120
29	6	0	7.489322	-0.643716	-0.029644
30	6	0	6.736812	-2.958685	0.021844
31	1	0	6.974991	-4.017527	0.039682
32	6	0	7.783357	-2.032579	-0.006190
33	8	0	8.641889	0.161632	-0.056382
34	6	0	8.479520	1.609073	-0.084903
35	1	0	7.934230	1.923588	-0.984638
36	1	0	7.951250	1.961055	0.811062
37	1	0	9.491620	2.018446	-0.102993
38	8	0	9.108331	-2.462922	-0.011057
39	1	0	9.703062	-1.680440	-0.031958
40	8	0	-8.000596	0.303464	-0.058734
41	6	0	-8.060372	1.751157	-0.102183
42	1	0	-7.591449	2.198755	0.787353
43	1	0	-7.571310	2.145568	-1.005934
44	1	0	-9.124830	1.993835	-0.121282
45	8	0	-7.955899	-2.414531	0.020018
46	1	0	-9.379159	-1.945933	-0.010143
47	5	0	0.329095	3.017885	0.047258
48	9	0	0.208647	3.957224	-1.012604
49	9	0	0.254429	3.676501	1.313822
50	9	0	-10.368116	-1.813826	-0.026016

Optimized geometric parameters for **1a-F**$^{-}$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.740184	-0.332348	-0.028282
2	6	0	-5.519222	0.330047	-0.038016
3	6	0	-6.804435	-1.783272	0.003446
4	1	0	-5.483977	1.415737	-0.058970
5	6	0	-4.276582	-0.388101	-0.021729
6	6	0	-5.550349	-2.483213	0.013588
7	1	0	-5.592809	-3.568923	0.033818
8	6	0	-4.331745	-1.816875	0.001867
9	1	0	-3.412847	-2.396210	0.013398
10	6	0	-3.051448	0.354608	-0.026671
11	1	0	-3.143487	1.440711	-0.037837
12	6	0	-1.755946	-0.147912	-0.016932
13	1	0	-1.565427	-1.216577	-0.008759
14	6	0	-0.605889	0.689755	-0.015183
15	8	0	-0.791531	2.040020	-0.024317
16	6	0	0.716394	0.173235	-0.005427
17	1	0	0.849222	-0.899831	0.000747
18	6	0	1.824993	1.025313	-0.005633
19	8	0	1.641487	2.378081	-0.007189
20	6	0	3.221583	0.633659	-0.004056
21	1	0	3.911517	1.473317	0.008669
22	6	0	3.679441	-0.656690	-0.019681
23	1	0	2.953177	-1.468663	-0.037327
24	6	0	5.073300	-1.091782	-0.017390
25	6	0	6.169535	-0.179900	0.012741
26	6	0	5.343275	-2.483796	-0.046258
27	1	0	5.990519	0.888916	0.036248
28	1	0	4.515426	-3.187588	-0.068754
29	6	0	7.476300	-0.665127	0.012767
30	6	0	6.660848	-2.971264	-0.047017
31	1	0	6.867481	-4.036383	-0.069506
32	6	0	7.728500	-2.066968	-0.017770
33	8	0	8.645939	0.096576	0.041136
34	6	0	8.544259	1.558546	0.083129
35	1	0	8.030560	1.934097	-0.809670
36	1	0	8.016300	1.881135	0.988296
37	1	0	9.572919	1.920279	0.101836
38	8	0	9.037124	-2.528931	-0.017520
39	1	0	9.663610	-1.769576	0.005750
40	8	0	-7.989153	0.294630	-0.047527
41	6	0	-8.032237	1.755974	-0.078379
42	1	0	-7.554759	2.183490	0.812973
43	1	0	-7.544392	2.145719	-0.981363
44	1	0	-9.092067	2.015912	-0.089925
45	8	0	-7.942929	-2.448162	0.021426
46	1	0	-9.206590	-2.011004	0.084681
47	5	0	0.309412	3.025179	0.007059
48	9	0	0.197126	3.901359	-1.132977
49	9	0	0.190122	3.836615	1.195279
50	9	0	-10.248503	-1.877029	0.146325

Optimized geometric parameters for **1a-F**$^{-}$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.680533	-0.344037	-0.077624
2	6	0	-5.470055	0.313306	-0.094148
3	6	0	-6.739897	-1.782833	0.030499
4	1	0	-5.439065	1.392843	-0.172949
5	6	0	-4.232529	-0.386929	-0.008539
6	6	0	-5.488682	-2.462883	0.108930
7	1	0	-5.522347	-3.544146	0.186428
8	6	0	-4.283694	-1.797928	0.091215
9	1	0	-3.365653	-2.370276	0.156436
10	6	0	-3.018748	0.361307	-0.022156
11	1	0	-3.131677	1.439199	-0.103786
12	6	0	-1.730944	-0.108681	0.059421
13	1	0	-1.523809	-1.168273	0.146016
14	6	0	-0.594629	0.744927	0.036128
15	8	0	-0.785407	2.048548	-0.098886
16	6	0	0.713715	0.234228	0.124343
17	1	0	0.848435	-0.830708	0.234193
18	6	0	1.808584	1.077755	0.007780
19	8	0	1.639728	2.387449	-0.110048
20	6	0	3.197072	0.666713	-0.018832
21	1	0	3.894649	1.495779	-0.065236
22	6	0	3.637789	-0.612845	0.003259
23	1	0	2.905186	-1.414464	0.031411
24	6	0	5.016994	-1.068836	-0.011923
25	6	0	6.119514	-0.182715	-0.021319
26	6	0	5.266191	-2.450677	-0.018159
27	1	0	5.956295	0.885671	-0.012760
28	1	0	4.431763	-3.142361	-0.009700
29	6	0	7.411186	-0.675698	-0.038223
30	6	0	6.565513	-2.949647	-0.036075
31	1	0	6.756061	-4.016017	-0.041438
32	6	0	7.640624	-2.072178	-0.046562
33	8	0	8.556954	0.064013	-0.046711
34	6	0	8.458321	1.492907	-0.034177
35	1	0	7.929932	1.852153	-0.920900
36	1	0	7.949887	1.837673	0.869808
37	1	0	9.481906	1.859863	-0.042607
38	8	0	8.911007	-2.548872	-0.062669
39	1	0	9.519297	-1.794076	-0.065637
40	8	0	-7.900168	0.265848	-0.158937
41	6	0	-7.938640	1.686594	-0.271045
42	1	0	-7.484687	2.166517	0.601868
43	1	0	-7.430524	2.027018	-1.178936
44	1	0	-8.992512	1.953623	-0.323788
45	8	0	-7.848224	-2.436507	0.054358
46	1	0	-9.153819	-1.977995	0.061188
47	5	0	0.313604	3.016614	0.069970
48	9	0	0.168647	4.032033	-0.882827
49	9	0	0.246911	3.570939	1.366032
50	9	0	-10.163487	-1.832975	0.084231

Optimized geometric parameters for **1a-Cl**$^-$ in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.372259	-0.043245	0.393216
2	6	0	-5.123332	0.572097	0.333653
3	6	0	-6.462747	-1.480999	0.380406
4	1	0	-5.090838	1.659448	0.368734
5	6	0	-3.903813	-0.167467	0.266231
6	6	0	-5.236310	-2.221888	0.333195
7	1	0	-5.326624	-3.304198	0.335700
8	6	0	-4.001497	-1.595494	0.273493
9	1	0	-3.100519	-2.202046	0.230129
10	6	0	-2.657162	0.541915	0.211724
11	1	0	-2.708969	1.631013	0.219247
12	6	0	-1.382189	0.001723	0.149100
13	1	0	-1.226287	-1.073224	0.136720
14	6	0	-0.205249	0.807659	0.098060
15	8	0	-0.335556	2.144701	0.124502
16	6	0	1.098149	0.232268	0.035157
17	1	0	1.191508	-0.845364	0.014248
18	6	0	2.229095	1.049053	0.022003
19	8	0	2.114782	2.391389	0.042014
20	6	0	3.618527	0.594240	-0.003814
21	1	0	4.326880	1.419267	-0.018645
22	6	0	4.042209	-0.700704	-0.008118
23	1	0	3.295931	-1.495168	0.010083
24	6	0	5.432795	-1.166191	-0.034454
25	6	0	6.540213	-0.271900	-0.059903
26	6	0	5.691015	-2.558040	-0.033837
27	1	0	6.368239	0.798734	-0.061210
28	1	0	4.855054	-3.253340	-0.014733
29	6	0	7.841067	-0.772880	-0.082943
30	6	0	7.003521	-3.061421	-0.057224
31	1	0	7.203156	-4.128149	-0.056817
32	6	0	8.082868	-2.173176	-0.081670
33	8	0	9.021972	-0.013166	-0.109053
34	6	0	8.918410	1.440659	-0.115190
35	1	0	8.379264	1.789715	-1.005702
36	1	0	8.413067	1.799819	0.790987
37	1	0	9.946177	1.808128	-0.136550
38	8	0	9.388028	-2.651447	-0.104818
39	1	0	10.014267	-1.893604	-0.120094
40	8	0	-7.515591	0.742306	0.578035
41	6	0	-8.178765	1.260381	-0.638021
42	1	0	-7.441293	1.764783	-1.280940
43	1	0	-8.695628	0.443951	-1.156428
44	1	0	-8.918242	1.978511	-0.275182
45	8	0	-7.593250	-2.189031	0.448226
46	1	0	-8.541521	-1.807528	0.116931
47	5	0	0.796303	3.126205	-0.010520
48	9	0	0.694379	3.785501	-1.266924
49	9	0	0.744915	4.047564	1.063849
50	17	0	-10.139361	-1.549230	-0.725519

Optimized geometric parameters for **1a-Cl**$^-$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.344256	-0.146457	-0.093758
2	6	0	-5.104337	0.498394	-0.091192
3	6	0	-6.406408	-1.573963	-0.075041
4	1	0	-5.054130	1.583065	-0.101323
5	6	0	-3.886890	-0.243714	-0.077937
6	6	0	-5.199077	-2.309535	-0.070172
7	1	0	-5.265148	-3.393232	-0.060381
8	6	0	-3.960624	-1.663787	-0.071747
9	1	0	-3.055430	-2.262639	-0.063860
10	6	0	-2.634391	0.488242	-0.067857
11	1	0	-2.711234	1.575217	-0.066258
12	6	0	-1.363987	-0.040149	-0.056561
13	1	0	-1.193317	-1.112099	-0.058601
14	6	0	-0.183659	0.779714	-0.036907
15	8	0	-0.349318	2.126474	-0.034362
16	6	0	1.114458	0.230972	-0.021223
17	1	0	1.222777	-0.844373	-0.025252
18	6	0	2.248886	1.063695	-0.004132
19	8	0	2.088596	2.411937	0.007561
20	6	0	3.630419	0.640090	0.002311
21	1	0	4.342474	1.460317	0.023952
22	6	0	4.052039	-0.665373	-0.017905
23	1	0	3.302996	-1.456042	-0.042817
24	6	0	5.429794	-1.137485	-0.011047
25	6	0	6.550942	-0.255333	0.025040
26	6	0	5.660055	-2.537567	-0.041626
27	1	0	6.401145	0.817847	0.049344
28	1	0	4.812642	-3.217244	-0.068644
29	6	0	7.842593	-0.776636	0.029215
30	6	0	6.962327	-3.061521	-0.038010
31	1	0	7.139973	-4.131659	-0.061522
32	6	0	8.054661	-2.186339	-0.002872
33	8	0	9.033200	-0.050845	0.063333
34	6	0	8.976301	1.414050	0.106488
35	1	0	8.478756	1.805570	-0.788504
36	1	0	8.454325	1.751334	1.009661
37	1	0	10.015572	1.743436	0.130424
38	8	0	9.347375	-2.683696	0.001638
39	1	0	9.996189	-1.943116	0.028182
40	8	0	-7.582873	0.490718	-0.116809
41	6	0	-7.623711	1.954122	-0.113379
42	1	0	-7.152267	2.356636	0.791960
43	1	0	-7.129147	2.361788	-1.003931
44	1	0	-8.683069	2.213645	-0.126518
45	8	0	-7.580756	-2.273339	-0.070644
46	1	0	-8.466471	-1.773792	0.021935
47	5	0	0.769882	3.095363	0.024594
48	9	0	0.687794	3.987101	-1.099519
49	9	0	0.660407	3.877773	1.227671
50	17	0	-10.469439	-1.576109	0.276467

Optimized geometric parameters for **1a-Cl**$^-$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.271853	-0.149804	-0.051952
2	6	0	5.043615	0.494214	-0.052978
3	6	0	6.321263	-1.560873	0.029165
4	1	0	4.999378	1.573730	-0.114867
5	6	0	3.833554	-0.232287	0.026405
6	6	0	5.126255	-2.282186	0.108032
7	1	0	5.184352	-3.362506	0.169228
8	6	0	3.901248	-1.635067	0.107079
9	1	0	2.996781	-2.226722	0.169465
10	6	0	2.589701	0.507656	0.022548
11	1	0	2.686299	1.587625	-0.043399
12	6	0	1.329377	0.007262	0.093030
13	1	0	1.144815	-1.057676	0.162357
14	6	0	0.158116	0.842465	0.078452
15	8	0	0.330492	2.144487	-0.030076
16	6	0	-1.123538	0.294386	0.149944
17	1	0	-1.229865	-0.775542	0.234899
18	6	0	-2.246658	1.118385	0.042268
19	8	0	-2.103325	2.424875	-0.054176
20	6	0	-3.618111	0.672714	0.000717
21	1	0	-4.337643	1.479350	-0.081502
22	6	0	-4.020847	-0.620811	0.060606
23	1	0	-3.265469	-1.397094	0.140789
24	6	0	-5.381441	-1.117861	0.032442
25	6	0	-6.508299	-0.268760	-0.078697
26	6	0	-5.588637	-2.504787	0.120544
27	1	0	-6.376035	0.801596	-0.148923
28	1	0	-4.734439	-3.166308	0.205061
29	6	0	-7.782669	-0.802139	-0.098685
30	6	0	-6.870360	-3.044303	0.102844
31	1	0	-7.030125	-4.113389	0.171478
32	6	0	-7.969803	-2.203186	-0.005920
33	8	0	-8.948584	-0.104791	-0.203459
34	6	0	-8.894415	1.322359	-0.319396
35	1	0	-8.430854	1.765235	0.565677
36	1	0	-8.344867	1.616032	-1.217296
37	1	0	-9.927849	1.651558	-0.396403
38	8	0	-9.222095	-2.718589	-0.024838
39	1	0	-9.852434	-1.986186	-0.105644
40	8	0	7.486017	0.461173	-0.124172
41	6	0	7.533223	1.887341	-0.217214
42	1	0	7.026651	2.237632	-1.120860
43	1	0	7.083517	2.352665	0.664348
44	1	0	8.588824	2.144587	-0.267150
45	8	0	7.481023	-2.245412	0.033284
46	1	0	8.288238	-1.685281	-0.027767
47	5	0	-0.790748	3.096892	0.110101
48	9	0	-0.741875	3.679855	1.387867
49	9	0	-0.670731	4.082186	-0.871809
50	17	0	10.552303	-1.577905	-0.107202

Optimized geometric parameters for **1a-Br**$^-$ in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.595540	0.066528	-0.178065
2	6	0	-4.345006	0.679225	-0.146686
3	6	0	-5.700883	-1.368951	-0.172784
4	1	0	-4.270218	1.763735	-0.146370
5	6	0	-3.138973	-0.091574	-0.121476
6	6	0	-4.500716	-2.130441	-0.157030
7	1	0	-4.603645	-3.211118	-0.156772
8	6	0	-3.253603	-1.513601	-0.131916
9	1	0	-2.359522	-2.130638	-0.115553
10	6	0	-1.876886	0.596879	-0.091007
11	1	0	-1.910253	1.686833	-0.087565
12	6	0	-0.610402	0.038746	-0.065025
13	1	0	-0.467365	-1.038005	-0.063616
14	6	0	0.578547	0.831463	-0.037121
15	8	0	0.460201	2.169381	-0.053505
16	6	0	1.874829	0.241866	-0.003824
17	1	0	1.956968	-0.836736	0.009555
18	6	0	3.015593	1.047162	-0.003715
19	8	0	2.914167	2.389808	-0.015936
20	6	0	4.399517	0.577198	0.001977
21	1	0	5.117794	1.393606	0.005301
22	6	0	4.807128	-0.723232	0.003811
23	1	0	4.050570	-1.508109	-0.001199
24	6	0	6.191256	-1.206737	0.012422
25	6	0	7.310720	-0.327121	0.020454
26	6	0	6.430520	-2.602044	0.012947
27	1	0	7.153172	0.745756	0.020657
28	1	0	5.585111	-3.286062	0.007123
29	6	0	8.604815	-0.845458	0.028377
30	6	0	7.736174	-3.123003	0.021016
31	1	0	7.921525	-4.192273	0.021590
32	6	0	8.827579	-2.249161	0.028700
33	8	0	9.796008	-0.102252	0.036829
34	6	0	9.713299	1.353050	0.038940
35	1	0	9.201898	1.716121	-0.862252
36	1	0	9.190537	1.712838	0.934906
37	1	0	10.746415	1.705659	0.046091
38	8	0	10.125790	-2.744880	0.036799
39	1	0	10.762942	-1.996012	0.041805
40	8	0	-6.818723	0.705093	-0.225634
41	6	0	-6.900600	2.147835	-0.094188
42	1	0	-6.442214	2.485536	0.846881
43	1	0	-6.418270	2.652806	-0.944574
44	1	0	-7.970635	2.360092	-0.086717
45	8	0	-6.869156	-2.028395	-0.187325
46	1	0	-7.775214	-1.523831	-0.089114
47	5	0	1.605036	3.140868	0.045069
48	9	0	1.545100	4.042493	-1.045740
49	9	0	1.530515	3.823057	1.289882
50	35	0	-9.812737	-1.042751	0.219215

Optimized geometric parameters for **1a-Br**$^-$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.525606	0.157942	-0.051553
2	6	0	-4.266998	0.765131	-0.048749
3	6	0	-5.628171	-1.262432	-0.059179
4	1	0	-4.181500	1.847513	-0.041628
5	6	0	-3.077615	-0.020051	-0.054503
6	6	0	-4.456525	-2.044192	-0.067997
7	1	0	-4.558097	-3.124951	-0.074922
8	6	0	-3.196950	-1.436187	-0.065676
9	1	0	-2.311740	-2.063840	-0.071562
10	6	0	-1.798588	0.671346	-0.045852
11	1	0	-1.840383	1.760071	-0.038834
12	6	0	-0.548635	0.101508	-0.042526
13	1	0	-0.411885	-0.975319	-0.047718
14	6	0	0.660120	0.883768	-0.027348
15	8	0	0.536425	2.234080	-0.025199
16	6	0	1.937611	0.292927	-0.015880
17	1	0	2.011075	-0.785317	-0.019255
18	6	0	3.099883	1.089462	-0.004663
19	8	0	2.982413	2.440931	0.001846
20	6	0	4.465466	0.620237	-0.000569
21	1	0	5.205633	1.415300	0.005698
22	6	0	4.841800	-0.699687	-0.001957
23	1	0	4.065444	-1.463940	-0.006798
24	6	0	6.202280	-1.217452	0.003799
25	6	0	7.352105	-0.372027	0.006994
26	6	0	6.385890	-2.624833	0.006564
27	1	0	7.237366	0.705754	0.004519
28	1	0	5.516418	-3.276533	0.004087
29	6	0	8.625786	-0.935117	0.012867
30	6	0	7.670116	-3.191162	0.012870
31	1	0	7.812505	-4.266786	0.015267
32	6	0	8.790906	-2.351742	0.016083
33	8	0	9.839850	-0.248997	0.016161
34	6	0	9.832861	1.217829	0.012093
35	1	0	9.339216	1.596879	-0.890415
36	1	0	9.332452	1.601889	0.908729
37	1	0	10.882896	1.512005	0.015226
38	8	0	10.066177	-2.891006	0.022194
39	1	0	10.739182	-2.171782	0.023568
40	8	0	-6.751838	0.819535	-0.047022
41	6	0	-6.765941	2.285027	-0.032398
42	1	0	-6.274416	2.668882	0.869829
43	1	0	-6.276644	2.686808	-0.928003
44	1	0	-7.820671	2.562710	-0.028398
45	8	0	-6.845606	-1.907368	-0.059543
46	1	0	-7.646700	-1.316976	-0.031587
47	5	0	1.686276	3.168000	0.021319
48	9	0	1.627274	4.053214	-1.108495
49	9	0	1.609071	3.959874	1.219567
50	35	0	-10.131336	-1.200838	0.075541

Optimized geometric parameters for **1a-Br**$^-$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.476781	0.136687	-0.053321
2	6	0	-4.230873	0.745246	-0.060102
3	6	0	-5.566946	-1.269302	0.057485
4	1	0	-4.154749	1.821614	-0.142779
5	6	0	-3.043827	-0.015964	0.039283
6	6	0	-4.396841	-2.025824	0.155686
7	1	0	-4.487065	-3.102381	0.239339
8	6	0	-3.153169	-1.414213	0.146656
9	1	0	-2.266929	-2.030849	0.225964
10	6	0	-1.777906	0.686979	0.029081
11	1	0	-1.842669	1.768818	-0.044415
12	6	0	-0.533556	0.149574	0.101691
13	1	0	-0.380588	-0.920115	0.174377
14	6	0	0.663181	0.948639	0.084070
15	8	0	0.530892	2.255095	-0.024882
16	6	0	1.926666	0.360712	0.154017
17	1	0	1.999225	-0.712039	0.239323
18	6	0	3.075230	1.149296	0.044934
19	8	0	2.972646	2.459378	-0.050789
20	6	0	4.431429	0.659753	0.001585
21	1	0	5.177665	1.441998	-0.077902
22	6	0	4.790080	-0.647024	0.054968
23	1	0	4.008126	-1.396911	0.130234
24	6	0	6.132467	-1.190559	0.024043
25	6	0	7.288277	-0.379883	-0.076212
26	6	0	6.290932	-2.584713	0.097307
27	1	0	7.193328	0.695249	-0.133900
28	1	0	5.414000	-3.216812	0.174061
29	6	0	8.543273	-0.957035	-0.100954
30	6	0	7.553074	-3.168369	0.074247
31	1	0	7.675415	-4.243076	0.131033
32	6	0	8.681281	-2.364825	-0.024232
33	8	0	9.732925	-0.299661	-0.196169
34	6	0	9.728880	1.130233	-0.289722
35	1	0	9.190173	1.457197	-1.182684
36	1	0	9.280867	1.575030	0.602401
37	1	0	10.773241	1.424145	-0.361855
38	8	0	9.914874	-2.923096	-0.047961
39	1	0	10.570268	-2.211930	-0.118752
40	8	0	-6.674866	0.776596	-0.146127
41	6	0	-6.686373	2.202088	-0.264517
42	1	0	-6.230494	2.671014	0.611806
43	1	0	-6.165616	2.522854	-1.170928
44	1	0	-7.735046	2.484054	-0.325763
45	8	0	-6.752891	-1.912090	0.071117
46	1	0	-7.523085	-1.309461	0.004161
47	5	0	1.681460	3.172673	0.111511
48	9	0	1.591744	4.157751	-0.873752
49	9	0	1.651511	3.760892	1.387225
50	35	0	-10.037494	-1.188809	-0.062000

Optimized geometric parameters for **1a-AcO$^-$** in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-8.506508	-0.804723	0.150210
2	6	0	-7.335666	-0.043276	0.121916
3	6	0	-8.435962	-2.222019	0.103748
4	1	0	-7.382991	1.040952	0.156381
5	6	0	-6.064059	-0.680935	0.047118
6	6	0	-7.189898	-2.862103	0.029072
7	1	0	-7.157119	-3.946582	-0.006145
8	6	0	-6.013457	-2.098929	0.001015
9	1	0	-5.059242	-2.612620	-0.058046
10	6	0	-4.871982	0.163895	0.020762
11	1	0	-5.044884	1.238843	0.053715
12	6	0	-3.568841	-0.249962	-0.039793
13	1	0	-3.304996	-1.303037	-0.073664
14	6	0	-2.452919	0.672407	-0.062429
15	8	0	-2.748852	2.002891	-0.025457
16	6	0	-1.127055	0.241938	-0.119853
17	1	0	-0.927755	-0.820245	-0.146833
18	6	0	-0.050884	1.174668	-0.143138
19	8	0	-0.345850	2.506276	-0.108570
20	6	0	1.337096	0.868149	-0.199672
21	1	0	1.993345	1.733844	-0.208045
22	6	0	1.862025	-0.420005	-0.239655
23	1	0	1.162986	-1.255916	-0.228779
24	6	0	3.241828	-0.793199	-0.291840
25	6	0	4.319178	0.157057	-0.313364
26	6	0	3.575476	-2.183410	-0.321913
27	1	0	4.092968	1.217388	-0.292219
28	1	0	2.772297	-2.917429	-0.306591
29	6	0	5.639621	-0.263767	-0.361006
30	6	0	4.897191	-2.610033	-0.368789
31	1	0	5.143887	-3.667748	-0.391949
32	6	0	5.988469	-1.680193	-0.390961
33	8	0	6.746165	0.587744	-0.381502
34	6	0	6.514082	2.032754	-0.380538
35	1	0	5.940904	2.337009	-1.265735
36	1	0	5.986377	2.345653	0.529527
37	1	0	7.506016	2.486510	-0.407679
38	8	0	7.235271	-2.097689	-0.434545
39	1	0	8.439761	-1.402542	-0.434998
40	8	0	-9.814469	-0.318549	0.222259
41	6	0	-10.031213	1.130204	0.277759
42	1	0	-9.561835	1.555784	1.172650
43	1	0	-9.635034	1.613484	-0.623152
44	1	0	-11.113007	1.260303	0.326145
45	8	0	-9.603814	-2.974049	0.131913
46	1	0	-10.386610	-2.379466	0.185705
47	5	0	-1.716787	3.060466	-0.035719
48	9	0	-1.936055	3.929680	-1.166239
49	9	0	-1.840483	3.860183	1.159580
50	8	0	9.457397	-1.054987	-0.500684
51	8	0	11.188934	-0.066951	0.579351
52	6	0	10.016004	-0.522751	0.605277
53	6	0	9.155337	-0.514564	1.860572
54	1	0	8.894391	-1.541625	2.144067
55	1	0	9.688917	-0.036317	2.684412
56	1	0	8.218967	0.017963	1.660642

Optimized geometric parameters for **1a-AcO**$^{-}$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-8.506508	-0.804723	0.150210
2	6	0	-7.335666	-0.043276	0.121916
3	6	0	-8.435962	-2.222019	0.103748
4	1	0	-7.382991	1.040952	0.156381
5	6	0	-6.064059	-0.680935	0.047118
6	6	0	-7.189898	-2.862103	0.029072
7	1	0	-7.157119	-3.946582	-0.006145
8	6	0	-6.013457	-2.098929	0.001015
9	1	0	-5.059242	-2.612620	-0.058046
10	6	0	-4.871982	0.163895	0.020762
11	1	0	-5.044884	1.238843	0.053715
12	6	0	-3.568841	-0.249962	-0.039793
13	1	0	-3.304996	-1.303037	-0.073664
14	6	0	-2.452919	0.672407	-0.062429
15	8	0	-2.748852	2.002891	-0.025457
16	6	0	-1.127055	0.241938	-0.119853
17	1	0	-0.927755	-0.820245	-0.146833
18	6	0	-0.050884	1.174668	-0.143138
19	8	0	-0.345850	2.506276	-0.108570
20	6	0	1.337096	0.868149	-0.199672
21	1	0	1.993345	1.733844	-0.208045
22	6	0	1.862025	-0.420005	-0.239655
23	1	0	1.162986	-1.255916	-0.228779
24	6	0	3.241828	-0.793199	-0.291840
25	6	0	4.319178	0.157057	-0.313364
26	6	0	3.575476	-2.183410	-0.321913
27	1	0	4.092968	1.217388	-0.292219
28	1	0	2.772297	-2.917429	-0.306591
29	6	0	5.639621	-0.263767	-0.361006
30	6	0	4.897191	-2.610033	-0.368789
31	1	0	5.143887	-3.667748	-0.391949
32	6	0	5.988469	-1.680193	-0.390961
33	8	0	6.746165	0.587744	-0.381502
34	6	0	6.514082	2.032754	-0.380538
35	1	0	5.940904	2.337009	-1.265735
36	1	0	5.986377	2.345653	0.529527
37	1	0	7.506016	2.486510	-0.407679
38	8	0	7.235271	-2.097689	-0.434545
39	1	0	8.439761	-1.402542	-0.434998
40	8	0	-9.814469	-0.318549	0.222259
41	6	0	-10.031213	1.130204	0.277759
42	1	0	-9.561835	1.555784	1.172650
43	1	0	-9.635034	1.613484	-0.623152
44	1	0	-11.113007	1.260303	0.326145
45	8	0	-9.603814	-2.974049	0.131913
46	1	0	-10.386610	-2.379466	0.185705
47	5	0	-1.716787	3.060466	-0.035719
48	9	0	-1.936055	3.929680	-1.166239
49	9	0	-1.840483	3.860183	1.159580
50	8	0	9.457397	-1.054987	-0.500684
51	8	0	11.188934	-0.066951	0.579351
52	6	0	10.016004	-0.522751	0.605277
53	6	0	9.155337	-0.514564	1.860572
54	1	0	8.894391	-1.541625	2.144067
55	1	0	9.688917	-0.036317	2.684412
56	1	0	8.218967	0.017963	1.660642

Optimized geometric parameters for **1a-AcO**$^{-}$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-8.506508	-0.804723	0.150210
2	6	0	-7.335666	-0.043276	0.121916
3	6	0	-8.435962	-2.222019	0.103748
4	1	0	-7.382991	1.040952	0.156381
5	6	0	-6.064059	-0.680935	0.047118
6	6	0	-7.189898	-2.862103	0.029072
7	1	0	-7.157119	-3.946582	-0.006145
8	6	0	-6.013457	-2.098929	0.001015
9	1	0	-5.059242	-2.612620	-0.058046
10	6	0	-4.871982	0.163895	0.020762
11	1	0	-5.044884	1.238843	0.053715
12	6	0	-3.568841	-0.249962	-0.039793
13	1	0	-3.304996	-1.303037	-0.073664
14	6	0	-2.452919	0.672407	-0.062429
15	8	0	-2.748852	2.002891	-0.025457
16	6	0	-1.127055	0.241938	-0.119853
17	1	0	-0.927755	-0.820245	-0.146833
18	6	0	-0.050884	1.174668	-0.143138
19	8	0	-0.345850	2.506276	-0.108570
20	6	0	1.337096	0.868149	-0.199672
21	1	0	1.993345	1.733844	-0.208045
22	6	0	1.862025	-0.420005	-0.239655
23	1	0	1.162986	-1.255916	-0.228779
24	6	0	3.241828	-0.793199	-0.291840
25	6	0	4.319178	0.157057	-0.313364
26	6	0	3.575476	-2.183410	-0.321913
27	1	0	4.092968	1.217388	-0.292219
28	1	0	2.772297	-2.917429	-0.306591
29	6	0	5.639621	-0.263767	-0.361006
30	6	0	4.897191	-2.610033	-0.368789
31	1	0	5.143887	-3.667748	-0.391949
32	6	0	5.988469	-1.680193	-0.390961
33	8	0	6.746165	0.587744	-0.381502
34	6	0	6.514082	2.032754	-0.380538
35	1	0	5.940904	2.337009	-1.265735
36	1	0	5.986377	2.345653	0.529527
37	1	0	7.506016	2.486510	-0.407679
38	8	0	7.235271	-2.097689	-0.434545
39	1	0	8.439761	-1.402542	-0.434998
40	8	0	-9.814469	-0.318549	0.222259
41	6	0	-10.031213	1.130204	0.277759
42	1	0	-9.561835	1.555784	1.172650
43	1	0	-9.635034	1.613484	-0.623152
44	1	0	-11.113007	1.260303	0.326145
45	8	0	-9.603814	-2.974049	0.131913
46	1	0	-10.386610	-2.379466	0.185705
47	5	0	-1.716787	3.060466	-0.035719
48	9	0	-1.936055	3.929680	-1.166239
49	9	0	-1.840483	3.860183	1.159580
50	8	0	9.457397	-1.054987	-0.500684
51	8	0	11.188934	-0.066951	0.579351
52	6	0	10.016004	-0.522751	0.605277
53	6	0	9.155337	-0.514564	1.860572
54	1	0	8.894391	-1.541625	2.144067
55	1	0	9.688917	-0.036317	2.684412
56	1	0	8.218967	0.017963	1.660642

Optimized geometric parameters for **1a-SCN**$^-$ in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.694638	-0.043239	-0.013924
2	6	0	-4.454750	0.574206	-0.021201
3	6	0	-5.817358	-1.497642	0.027422
4	1	0	-4.378314	1.658497	-0.051029
5	6	0	-3.233314	-0.186234	0.010465
6	6	0	-4.580195	-2.240053	0.058738
7	1	0	-4.670990	-3.322325	0.089180
8	6	0	-3.345010	-1.615162	0.050370
9	1	0	-2.443163	-2.221966	0.075053
10	6	0	-1.987172	0.504251	0.001822
11	1	0	-2.024968	1.593732	-0.028823
12	6	0	-0.704137	-0.041876	0.028917
13	1	0	-0.551112	-1.116903	0.061228
14	6	0	0.466882	0.759456	0.016121
15	8	0	0.339304	2.101020	-0.043541
16	6	0	1.778433	0.188362	0.047781
17	1	0	1.874870	-0.888555	0.094912
18	6	0	2.904893	1.003338	-0.001170
19	8	0	2.791014	2.349788	-0.053156
20	6	0	4.295967	0.549939	-0.012264
21	1	0	5.001653	1.377291	-0.041496
22	6	0	4.727006	-0.742184	0.009237
23	1	0	3.985258	-1.540684	0.034776
24	6	0	6.121538	-1.199590	0.001814
25	6	0	7.223936	-0.299395	-0.029006
26	6	0	6.390004	-2.589341	0.026248
27	1	0	7.044876	0.769923	-0.047206
28	1	0	5.558565	-3.289956	0.050058
29	6	0	8.528478	-0.792231	-0.034964
30	6	0	7.706338	-3.084204	0.020559
31	1	0	7.912646	-4.149617	0.039381
32	6	0	8.780177	-2.189829	-0.010064
33	8	0	9.704635	-0.023219	-0.064396
34	6	0	9.588325	1.428848	-0.095921
35	1	0	9.052308	1.758298	-0.995828
36	1	0	9.072973	1.799212	0.800102
37	1	0	10.612931	1.805463	-0.116219
38	8	0	10.090386	-2.659864	-0.016217
39	1	0	10.709740	-1.896709	-0.038813
40	8	0	-6.924668	0.614125	-0.043721
41	6	0	-6.937372	2.064809	-0.088782
42	1	0	-6.454409	2.496334	0.800636
43	1	0	-6.436643	2.440305	-0.993677
44	1	0	-7.993112	2.342613	-0.107771
45	8	0	-6.966167	-2.109071	0.036116
46	1	0	-8.279438	-1.628368	0.011075
47	5	0	1.475188	3.076931	0.046503
48	9	0	1.380855	4.003089	-1.025338
49	9	0	1.418583	3.747818	1.304830
50	6	0	-10.523348	-1.124538	-0.020532
51	7	0	-9.364197	-1.386244	-0.004762
52	16	0	-12.143706	-0.760879	-0.043801

Optimized geometric parameters for **1a-SCN**$^-$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.672501	-0.035907	-0.000271
2	6	0	-4.422520	0.587697	-0.000617
3	6	0	-5.761692	-1.465153	0.001157
4	1	0	-4.354739	1.671486	-0.001669
5	6	0	-3.215212	-0.172259	0.000377
6	6	0	-4.560421	-2.216163	0.002162
7	1	0	-4.643609	-3.298786	0.003245
8	6	0	-3.312388	-1.591565	0.001775
9	1	0	-2.416774	-2.204945	0.002618
10	6	0	-1.953735	0.539778	0.000046
11	1	0	-2.014621	1.627818	-0.000598
12	6	0	-0.688928	-0.005632	0.000532
13	1	0	-0.532267	-1.079734	0.001078
14	6	0	0.500218	0.798850	0.000475
15	8	0	0.351748	2.148100	-0.000548
16	6	0	1.793286	0.235255	0.001185
17	1	0	1.889269	-0.841326	0.001805
18	6	0	2.936558	1.054160	0.000513
19	8	0	2.793195	2.405107	-0.000014
20	6	0	4.313804	0.614631	0.000097
21	1	0	5.034914	1.427246	-0.000715
22	6	0	4.721443	-0.695041	0.000769
23	1	0	3.964046	-1.478178	0.001761
24	6	0	6.094917	-1.180998	0.000415
25	6	0	7.224676	-0.309361	-0.001435
26	6	0	6.311701	-2.583376	0.001983
27	1	0	7.085237	0.765502	-0.002713
28	1	0	5.457764	-3.255373	0.003357
29	6	0	8.511471	-0.842762	-0.001639
30	6	0	7.609128	-3.119668	0.001841
31	1	0	7.776340	-4.191762	0.003062
32	6	0	8.710010	-2.254666	0.000045
33	8	0	9.709060	-0.127476	-0.003402
34	6	0	9.666082	1.338511	-0.006140
35	1	0	9.159053	1.706116	-0.905977
36	1	0	9.160514	1.709538	0.893111
37	1	0	10.708547	1.658576	-0.007584
38	8	0	9.998251	-2.764358	-0.000168
39	1	0	10.653999	-2.029479	-0.001569
40	8	0	-6.898296	0.628635	-0.001206
41	6	0	-6.903432	2.092808	-0.003358
42	1	0	-6.411605	2.487771	0.894507
43	1	0	-6.411060	2.485099	-0.902096
44	1	0	-7.956638	2.377284	-0.004087
45	8	0	-6.937421	-2.144324	0.001625
46	1	0	-7.861651	-1.662215	0.000668
47	5	0	1.482980	3.103911	0.002215
48	9	0	1.397118	3.947237	-1.160136
49	9	0	1.397318	3.940301	1.169802
50	6	0	-10.553099	-1.159976	-0.001158
51	7	0	-9.377680	-1.373769	-0.000368
52	16	0	-12.214766	-0.856632	-0.002282

Optimized geometric parameters for **1a-SCN**$^-$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.604367	-0.090552	0.011275
2	6	0	-4.368863	0.538902	-0.003314
3	6	0	-5.671244	-1.500374	0.127676
4	1	0	-4.313044	1.616047	-0.091539
5	6	0	-3.165395	-0.196797	0.095121
6	6	0	-4.480046	-2.229337	0.226819
7	1	0	-4.549710	-3.307126	0.315732
8	6	0	-3.248282	-1.596632	0.211026
9	1	0	-2.350212	-2.196146	0.290423
10	6	0	-1.915822	0.530596	0.073873
11	1	0	-2.003334	1.610267	-0.008367
12	6	0	-0.658123	0.021554	0.144657
13	1	0	-0.480755	-1.043752	0.226172
14	6	0	0.517721	0.848223	0.112022
15	8	0	0.353423	2.150559	-0.009275
16	6	0	1.797443	0.293291	0.178327
17	1	0	1.898366	-0.776317	0.274041
18	6	0	2.923877	1.108842	0.049446
19	8	0	2.787891	2.415674	-0.058337
20	6	0	4.292361	0.654489	-0.004406
21	1	0	5.015575	1.456473	-0.099032
22	6	0	4.688522	-0.640790	0.056931
23	1	0	3.929701	-1.412493	0.148164
24	6	0	6.046328	-1.145193	0.015969
25	6	0	7.176334	-0.302143	-0.107992
26	6	0	6.247379	-2.532944	0.103915
27	1	0	7.048947	0.768835	-0.177917
28	1	0	5.390768	-3.189987	0.198371
29	6	0	8.447725	-0.842059	-0.140642
30	6	0	7.526140	-3.079095	0.073287
31	1	0	7.681076	-4.148916	0.141638
32	6	0	8.628695	-2.243874	-0.048217
33	8	0	9.615995	-0.150594	-0.258240
34	6	0	9.567702	1.276701	-0.374765
35	1	0	9.010150	1.572469	-1.267032
36	1	0	9.115742	1.722610	0.514788
37	1	0	10.601885	1.600714	-0.462967
38	8	0	9.878216	-2.765735	-0.079636
39	1	0	10.511268	-2.036532	-0.167683
40	8	0	-6.809139	0.536523	-0.078631
41	6	0	-6.832815	1.959769	-0.207620
42	1	0	-6.377585	2.441061	0.662693
43	1	0	-6.318894	2.279929	-1.118482
44	1	0	-7.884028	2.233134	-0.266626
45	8	0	-6.831441	-2.174488	0.148382
46	1	0	-7.657410	-1.629849	0.063677
47	5	0	1.481684	3.095778	0.120133
48	9	0	1.357480	4.082782	-0.859557
49	9	0	1.449669	3.678300	1.399082
50	6	0	-10.573183	-1.102154	-0.139762
51	7	0	-9.431170	-1.357727	-0.046009
52	16	0	-12.183447	-0.741438	-0.271640

Optimized geometric parameters for **1a- NO_3^-** in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.815330	-0.179467	0.521717
2	6	0	-4.587160	0.462765	0.410638
3	6	0	-5.882893	-1.621267	0.590838
4	1	0	-4.545920	1.547275	0.343464
5	6	0	-3.355383	-0.269517	0.395954
6	6	0	-4.649553	-2.342326	0.601634
7	1	0	-4.718074	-3.424226	0.664046
8	6	0	-3.426036	-1.693163	0.504996
9	1	0	-2.512653	-2.282029	0.502612
10	6	0	-2.120417	0.450610	0.291959
11	1	0	-2.186440	1.536805	0.221403
12	6	0	-0.834241	-0.070614	0.275026
13	1	0	-0.659490	-1.140949	0.336019
14	6	0	0.326828	0.750703	0.179674
15	8	0	0.172513	2.083869	0.090517
16	6	0	1.642077	0.197085	0.163668
17	1	0	1.755769	-0.876512	0.234831
18	6	0	2.755170	1.027309	0.038208
19	8	0	2.616730	2.366239	-0.042645
20	6	0	4.149774	0.592115	-0.027732
21	1	0	4.843179	1.425962	-0.109496
22	6	0	4.594477	-0.695306	0.004434
23	1	0	3.862425	-1.499367	0.081774
24	6	0	5.990686	-1.141112	-0.054507
25	6	0	7.082447	-0.232647	-0.151990
26	6	0	6.270848	-2.528091	-0.011944
27	1	0	6.893919	0.834691	-0.184915
28	1	0	5.447066	-3.234147	0.062298
29	6	0	8.389436	-0.715523	-0.203268
30	6	0	7.589518	-3.013058	-0.063482
31	1	0	7.805742	-4.076079	-0.031020
32	6	0	8.653243	-2.110977	-0.159034
33	8	0	9.556767	0.059815	-0.299405
34	6	0	9.429522	1.510352	-0.361414
35	1	0	8.854516	1.814099	-1.246142
36	1	0	8.949666	1.899565	0.546225
37	1	0	10.449859	1.891869	-0.433626
38	8	0	9.964573	-2.570897	-0.210781
39	1	0	10.577379	-1.804827	-0.276475
40	8	0	-7.045360	0.456451	0.610182
41	6	0	-7.189732	1.796580	0.060170
42	1	0	-6.667796	2.540520	0.680417
43	1	0	-6.817488	1.830960	-0.971638
44	1	0	-8.263126	1.994080	0.068233
45	8	0	-7.024072	-2.296463	0.645247
46	1	0	-8.009025	-1.836364	0.389730
47	5	0	1.295795	3.082939	0.098728
48	9	0	1.138180	3.971094	-0.993315
49	9	0	1.289494	3.781444	1.339929
50	7	0	-9.469159	-0.762901	-0.956126
51	8	0	-9.281054	-1.510821	0.149739
52	8	0	-10.612878	-0.199295	-1.119345
53	8	0	-8.495109	-0.643307	-1.802422

Optimized geometric parameters for **1a- NO_3^-** in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.717769	-0.011653	0.321551
2	6	0	-4.469145	0.612141	0.258298
3	6	0	-5.802492	-1.437313	0.379964
4	1	0	-4.402299	1.695061	0.214695
5	6	0	-3.263592	-0.149478	0.251098
6	6	0	-4.606714	-2.191770	0.374991
7	1	0	-4.689301	-3.273429	0.420226
8	6	0	-3.359165	-1.567066	0.312068
9	1	0	-2.463549	-2.180231	0.309838
10	6	0	-2.001323	0.561742	0.182264
11	1	0	-2.062695	1.649017	0.143333
12	6	0	-0.738674	0.015064	0.159626
13	1	0	-0.581784	-1.058481	0.192576
14	6	0	0.451164	0.817951	0.088313
15	8	0	0.302312	2.166187	0.050749
16	6	0	1.741960	0.252392	0.059808
17	1	0	1.837418	-0.823729	0.092767
18	6	0	2.885750	1.069843	-0.002786
19	8	0	2.742094	2.419493	-0.043995
20	6	0	4.261623	0.628728	-0.026702
21	1	0	4.983361	1.439657	-0.068400
22	6	0	4.667487	-0.681595	-0.003446
23	1	0	3.909172	-1.462873	0.034881
24	6	0	6.039525	-1.169776	-0.026103
25	6	0	7.170121	-0.300212	-0.070991
26	6	0	6.254309	-2.572365	-0.001738
27	1	0	7.032028	0.774655	-0.089343
28	1	0	5.399678	-3.242585	0.032380
29	6	0	8.455740	-0.835811	-0.089865
30	6	0	7.550538	-3.110867	-0.021162
31	1	0	7.716370	-4.183003	-0.002947
32	6	0	8.652252	-2.247918	-0.065024
33	8	0	9.653981	-0.123166	-0.132811
34	6	0	9.613266	1.342583	-0.165246
35	1	0	9.086656	1.692182	-1.061004
36	1	0	9.128687	1.733397	0.737162
37	1	0	10.655940	1.660374	-0.196779
38	8	0	9.939224	-2.759682	-0.084534
39	1	0	10.595863	-2.026167	-0.114487
40	8	0	-6.946414	0.646178	0.337160
41	6	0	-6.963454	2.108584	0.262079
42	1	0	-6.446888	2.550365	1.123295
43	1	0	-6.502342	2.457340	-0.670383
44	1	0	-8.018334	2.385883	0.280569
45	8	0	-6.986500	-2.111777	0.442798
46	1	0	-7.869940	-1.597174	0.413175
47	5	0	1.431852	3.118896	-0.055383
48	9	0	1.308984	3.870009	-1.277002
49	9	0	1.381742	4.041754	1.045317
50	7	0	-10.112280	-1.084081	-0.563596
51	8	0	-9.428900	-1.294938	0.555662
52	8	0	-11.370366	-0.777771	-0.482247
53	8	0	-9.508721	-1.189684	-1.711066

Optimized geometric parameters for **1a- NO_3^-** in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-8.466589	-0.794333	-0.240174
2	6	0	-7.303515	-0.042141	-0.212896
3	6	0	-8.397951	-2.195764	-0.097846
4	1	0	-7.347577	1.033916	-0.319987
5	6	0	-6.045265	-0.664391	-0.044925
6	6	0	-7.163633	-2.818202	0.068531
7	1	0	-7.132600	-3.895834	0.175821
8	6	0	-5.999344	-2.062805	0.094641
9	1	0	-5.051960	-2.569930	0.225684
10	6	0	-4.864656	0.178782	-0.023336
11	1	0	-5.047215	1.243466	-0.135880
12	6	0	-3.574615	-0.211504	0.120479
13	1	0	-3.305636	-1.254158	0.237493
14	6	0	-2.473607	0.719528	0.124687
15	8	0	-2.750634	1.998340	-0.038255
16	6	0	-1.159374	0.283057	0.268664
17	1	0	-0.970976	-0.770882	0.398910
18	6	0	-0.099867	1.194688	0.172192
19	8	0	-0.349910	2.480397	0.025694
20	6	0	1.299191	0.861827	0.192761
21	1	0	1.957416	1.720072	0.120270
22	6	0	1.799412	-0.398419	0.289580
23	1	0	1.101017	-1.227988	0.349654
24	6	0	3.188606	-0.791429	0.320047
25	6	0	4.255834	0.136709	0.263747
26	6	0	3.498173	-2.160379	0.407907
27	1	0	4.045046	1.194682	0.200181
28	1	0	2.695173	-2.887225	0.452790
29	6	0	5.571011	-0.290313	0.291504
30	6	0	4.815784	-2.593957	0.435488
31	1	0	5.055248	-3.648513	0.501226
32	6	0	5.867943	-1.678897	0.376551
33	8	0	6.662871	0.517960	0.246535
34	6	0	6.467796	1.930452	0.140942
35	1	0	5.933779	2.183897	-0.779238
36	1	0	5.920335	2.316175	1.005518
37	1	0	7.464552	2.365127	0.116573
38	8	0	7.125110	-2.143043	0.406890
39	1	0	7.837286	-1.456364	0.325927
40	8	0	-9.735231	-0.317180	-0.396278
41	6	0	-9.926952	1.093139	-0.558684
42	1	0	-9.570872	1.636149	0.320470
43	1	0	-9.413659	1.453041	-1.454015
44	1	0	-10.999512	1.234984	-0.668275
45	8	0	-9.532855	-2.938511	-0.122857
46	1	0	-10.285502	-2.340469	-0.248128
47	5	0	-1.718996	3.043192	0.127050
48	9	0	-1.880489	4.000004	-0.876628
49	9	0	-1.866570	3.639898	1.391373
50	7	0	10.014455	-0.489628	-0.698924
51	8	0	9.472702	-0.842128	0.393402
52	8	0	11.093142	0.141913	-0.672226
53	8	0	9.465144	-0.779214	-1.785361

Optimized geometric parameters for **1e- CN^-** in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.175318	-0.341248	-0.016565
2	6	0	-5.960893	0.334996	-0.019536
3	6	0	-7.241562	-1.794326	0.005809
4	1	0	-5.936040	1.422552	-0.035828
5	6	0	-4.708476	-0.363839	-0.001116
6	6	0	-5.971585	-2.471714	0.023866
7	1	0	-6.007531	-3.558350	0.040542
8	6	0	-4.759016	-1.789526	0.020487
9	1	0	-3.831264	-2.357836	0.035064
10	6	0	-3.484482	0.395580	-0.004498
11	1	0	-3.582815	1.481837	-0.020981
12	6	0	-2.185336	-0.076207	0.011137
13	1	0	-1.972953	-1.142371	0.028560
14	6	0	-1.039123	0.790501	0.006126
15	8	0	-1.259852	2.127169	-0.026083
16	6	0	0.280955	0.294926	0.026394
17	1	0	0.433327	-0.775952	0.051653
18	6	0	1.389948	1.171722	0.002735
19	8	0	1.174379	2.511093	-0.024201
20	6	0	2.776298	0.792041	-0.001951
21	1	0	3.461092	1.635916	-0.017558
22	6	0	3.256684	-0.506813	0.010830
23	1	0	2.522332	-1.314707	0.024501
24	6	0	4.624807	-0.945422	0.008519
25	6	0	5.743598	-0.044532	-0.009023
26	6	0	4.913289	-2.343546	0.024152
27	1	0	5.552180	1.024179	-0.020893
28	1	0	4.079502	-3.046190	0.037626
29	6	0	7.046638	-0.517869	-0.010764
30	6	0	6.217992	-2.826067	0.022799
31	1	0	6.426026	-3.893200	0.034913
32	6	0	7.361340	-1.949047	0.005351
33	8	0	8.189332	0.298469	-0.027757
34	6	0	8.002459	1.735119	-0.046012
35	1	0	7.452660	2.058090	-0.943435
36	1	0	7.463096	2.082326	0.848663
37	1	0	9.009365	2.159723	-0.057595
38	8	0	8.586391	-2.391893	0.003866
39	1	0	10.011036	-1.595428	-0.012731
40	8	0	-8.435826	0.277638	-0.034086
41	6	0	-8.489757	1.723205	-0.058040
42	1	0	-8.014720	2.160950	0.834013
43	1	0	-8.002924	2.131550	-0.957649
44	1	0	-9.553595	1.973459	-0.069093
45	8	0	-8.370497	-2.457880	0.009504
46	1	0	-9.736612	-2.041706	-0.002975
47	5	0	-0.175707	3.154846	0.026285
48	9	0	-0.313016	4.038229	-1.089955
49	9	0	-0.292408	3.900692	1.245319
50	7	0	-10.827244	-1.866647	-0.010028
51	6	0	-12.006040	-1.691406	-0.017342
52	6	0	11.070961	-1.210477	-0.022607
53	7	0	12.184885	-0.810843	-0.032964

Optimized geometric parameters for **1e- CN**$^{-}$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.169386	-0.341948	0.000578
2	6	0	5.947041	0.335321	0.000529
3	6	0	7.208308	-1.776947	-0.000128
4	1	0	5.926923	1.421388	0.001080
5	6	0	4.706199	-0.368144	-0.000189
6	6	0	5.966776	-2.467517	-0.000889
7	1	0	6.000001	-3.553492	-0.001452
8	6	0	4.745500	-1.789025	-0.000918
9	1	0	3.823674	-2.363489	-0.001531
10	6	0	3.474423	0.401821	-0.000160
11	1	0	3.586489	1.485813	0.000184
12	6	0	2.187540	-0.080751	-0.000473
13	1	0	1.981112	-1.147283	-0.000740
14	6	0	1.029444	0.778668	-0.000417
15	8	0	1.254942	2.127108	-0.000026
16	6	0	-0.278921	0.284195	-0.000635
17	1	0	-0.426454	-0.786959	-0.000881
18	6	0	-1.399589	1.158843	-0.000382
19	8	0	-1.171812	2.508699	-0.000045
20	6	0	-2.772365	0.786998	-0.000266
21	1	0	-3.466762	1.622685	-0.000036
22	6	0	-3.244347	-0.523827	-0.000377
23	1	0	-2.510360	-1.329822	-0.000590
24	6	0	-4.606726	-0.953470	-0.000215
25	6	0	-5.723940	-0.046686	0.000063
26	6	0	-4.887829	-2.357175	-0.000271
27	1	0	-5.538390	1.021885	0.000119
28	1	0	-4.054693	-3.057783	-0.000474
29	6	0	-7.025489	-0.520163	0.000246
30	6	0	-6.190636	-2.837973	-0.000085
31	1	0	-6.392456	-3.905930	-0.000115
32	6	0	-7.326873	-1.953869	0.000159
33	8	0	-8.167444	0.286944	0.000483
34	6	0	-7.989677	1.739024	0.000774
35	1	0	-7.450349	2.068737	0.898320
36	1	0	-7.450664	2.069151	-0.896810
37	1	0	-8.997940	2.156567	0.001036
38	8	0	-8.557150	-2.398142	0.000422
39	1	0	-9.954028	-1.578813	0.000504
40	8	0	8.421644	0.280131	0.001294
41	6	0	8.476126	1.741376	0.002333
42	1	0	7.997893	2.154950	-0.895046
43	1	0	7.997152	2.153688	0.899897
44	1	0	9.538243	1.991988	0.002941
45	8	0	8.351582	-2.494241	-0.000086
46	1	0	9.384580	-2.073445	0.000000
47	5	0	0.169883	3.126726	-0.000610
48	9	0	0.301964	3.975390	1.163117
49	9	0	0.301727	3.973818	-1.165561
50	7	0	10.740619	-1.843106	-0.000065
51	6	0	11.924208	-1.663031	-0.000161
52	6	0	-11.008201	-1.178238	0.000576
53	7	0	-12.113883	-0.759067	0.000657

Optimized geometric parameters for **1e- CN**$^{-}$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.090443	-0.354062	-0.052524
2	6	0	-5.884364	0.334347	-0.064816
3	6	0	-7.092865	-1.764413	0.065046
4	1	0	-5.881210	1.412991	-0.154016
5	6	0	-4.647267	-0.339347	0.038292
6	6	0	-5.866769	-2.431194	0.168210
7	1	0	-5.883065	-3.511319	0.257802
8	6	0	-4.665068	-1.739772	0.155679
9	1	0	-3.739867	-2.296505	0.238135
10	6	0	-3.428770	0.450313	0.019931
11	1	0	-3.567504	1.523717	-0.072599
12	6	0	-2.153194	0.001403	0.105146
13	1	0	-1.931499	-1.055229	0.199660
14	6	0	-1.004086	0.875597	0.071866
15	8	0	-1.231562	2.175927	-0.071030
16	6	0	0.284805	0.379763	0.158998
17	1	0	0.426078	-0.683505	0.275185
18	6	0	1.398816	1.240017	0.029212
19	8	0	1.187803	2.545889	-0.099025
20	6	0	2.757239	0.841698	-0.006026
21	1	0	3.462688	1.660241	-0.094203
22	6	0	3.204961	-0.461860	0.059246
23	1	0	2.459773	-1.249595	0.132078
24	6	0	4.544762	-0.924148	0.041880
25	6	0	5.677939	-0.056523	-0.041602
26	6	0	4.790325	-2.320390	0.109530
27	1	0	5.517963	1.011833	-0.092133
28	1	0	3.942212	-2.995184	0.173582
29	6	0	6.955896	-0.554048	-0.055491
30	6	0	6.066737	-2.831089	0.095659
31	1	0	6.238714	-3.900652	0.147717
32	6	0	7.220989	-1.988930	0.012654
33	8	0	8.088881	0.203666	-0.131211
34	6	0	7.949243	1.621423	-0.206093
35	1	0	7.392021	1.916951	-1.100640
36	1	0	7.447892	2.017030	0.682790
37	1	0	8.960657	2.019723	-0.260044
38	8	0	8.406189	-2.445376	-0.001057
39	1	0	9.912811	-1.576397	-0.088672
40	8	0	-8.322366	0.222169	-0.146070
41	6	0	-8.405444	1.642527	-0.270635
42	1	0	-7.971485	2.140730	0.601246
43	1	0	-7.904893	1.988437	-1.179754
44	1	0	-9.467138	1.872611	-0.329939
45	8	0	-8.218005	-2.499690	0.085208
46	1	0	-9.082996	-2.011088	-0.012705
47	5	0	-0.142743	3.152053	0.103545
48	9	0	-0.308893	4.184164	-0.830578
49	9	0	-0.206044	3.689037	1.410350
50	7	0	-10.843135	-1.848167	-0.149067
51	6	0	-12.004290	-1.743660	-0.265582
52	6	0	10.953566	-1.199243	-0.136545
53	7	0	12.036441	-0.808264	-0.186062

Optimized geometric parameters for **1e- F^-** in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.160968	-0.425791	-0.000380
2	6	0	-5.952194	0.258908	-0.000408
3	6	0	-7.216740	-1.882481	-0.000023
4	1	0	-5.935508	1.346829	-0.000638
5	6	0	-4.692228	-0.429063	-0.000121
6	6	0	-5.937235	-2.548097	0.000268
7	1	0	-5.964145	-3.635259	0.000528
8	6	0	-4.731467	-1.856464	0.000230
9	1	0	-3.798678	-2.416883	0.000456
10	6	0	-3.476846	0.339346	-0.000123
11	1	0	-3.584299	1.424922	-0.000313
12	6	0	-2.171163	-0.120503	0.000221
13	1	0	-1.948976	-1.184793	0.000497
14	6	0	-1.035040	0.755918	0.000282
15	8	0	-1.266812	2.091628	-0.000296
16	6	0	0.291804	0.273023	0.000725
17	1	0	0.454446	-0.796681	0.001160
18	6	0	1.390859	1.159649	0.000349
19	8	0	1.164288	2.498092	-0.000105
20	6	0	2.782638	0.793454	0.000273
21	1	0	3.458686	1.644563	0.000035
22	6	0	3.276152	-0.499266	0.000482
23	1	0	2.550464	-1.315124	0.000699
24	6	0	4.650365	-0.924196	0.000479
25	6	0	5.759604	-0.012985	0.000202
26	6	0	4.952602	-2.318435	0.000780
27	1	0	5.558751	1.054087	0.000001
28	1	0	4.126970	-3.030709	0.000986
29	6	0	7.069411	-0.471681	0.000215
30	6	0	6.263475	-2.786309	0.000826
31	1	0	6.484120	-3.850804	0.001064
32	6	0	7.395180	-1.898033	0.000549
33	8	0	8.200637	0.354118	-0.000066
34	6	0	8.004587	1.787640	-0.000800
35	1	0	7.457689	2.120537	-0.896894
36	1	0	7.457976	2.121492	0.895115
37	1	0	9.009544	2.216826	-0.001193
38	8	0	8.620676	-2.345737	0.000642
39	1	0	9.907267	-1.690240	-0.001222
40	8	0	-8.424904	0.184256	-0.000722
41	6	0	-8.486988	1.628680	-0.000664
42	1	0	-8.008618	2.055684	0.895183
43	1	0	-8.008391	2.055787	-0.896341
44	1	0	-9.552448	1.872696	-0.000813
45	8	0	-8.334950	-2.556589	0.000159
46	1	0	-9.718594	-2.155692	-0.002281
47	5	0	-0.191992	3.129454	0.001056
48	9	0	-0.327225	3.947819	-1.167091
49	9	0	-0.326832	3.944429	1.171719
50	9	0	-10.729902	-2.061942	-0.004095
51	9	0	10.882557	-1.411477	-0.002575

Optimized geometric parameters for **1e- F^-** in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.151474	-0.427963	-0.024524
2	6	0	-5.943721	0.264457	-0.027971
3	6	0	-7.183204	-1.876407	-0.011694
4	1	0	-5.935689	1.351035	-0.035300
5	6	0	-4.686763	-0.422281	-0.022791
6	6	0	-5.915413	-2.544022	-0.011816
7	1	0	-5.930791	-3.630898	-0.005272
8	6	0	-4.709254	-1.848263	-0.016718
9	1	0	-3.777658	-2.407603	-0.014003
10	6	0	-3.472789	0.354692	-0.021917
11	1	0	-3.593830	1.437998	-0.022475
12	6	0	-2.172053	-0.114096	-0.018924
13	1	0	-1.955488	-1.178380	-0.019813
14	6	0	-1.031524	0.752240	-0.013163
15	8	0	-1.259895	2.100138	-0.009060
16	6	0	0.290684	0.269334	-0.010925
17	1	0	0.447283	-0.800582	-0.014363
18	6	0	1.394687	1.149168	-0.003630
19	8	0	1.164637	2.498604	0.002968
20	6	0	2.781292	0.789137	-0.001729
21	1	0	3.464012	1.634534	0.008817
22	6	0	3.264141	-0.508592	-0.013319
23	1	0	2.540562	-1.323927	-0.026386
24	6	0	4.639993	-0.928662	-0.011198
25	6	0	5.744390	-0.014247	0.008596
26	6	0	4.931943	-2.324335	-0.029555
27	1	0	5.550946	1.052772	0.023403
28	1	0	4.108440	-3.035766	-0.044345
29	6	0	7.055039	-0.475365	0.009603
30	6	0	6.244898	-2.790971	-0.029470
31	1	0	6.458277	-3.856259	-0.044093
32	6	0	7.361501	-1.897688	-0.010287
33	8	0	8.185546	0.346499	0.029162
34	6	0	7.992254	1.795440	0.056484
35	1	0	7.455284	2.138490	-0.837540
36	1	0	7.444412	2.102931	0.956871
37	1	0	8.996210	2.223158	0.070981
38	8	0	8.600546	-2.359316	-0.010597
39	1	0	9.754633	-1.708129	0.004227
40	8	0	-8.414610	0.176756	-0.033627
41	6	0	-8.484593	1.636501	-0.043089
42	1	0	-8.013364	2.060977	0.853244
43	1	0	-8.006205	2.049750	-0.940878
44	1	0	-9.549089	1.877662	-0.048880
45	8	0	-8.309438	-2.574390	-0.002038
46	1	0	-9.559432	-2.173594	0.077414
47	5	0	-0.181910	3.107161	0.004639
48	9	0	-0.315951	3.965591	-1.151469
49	9	0	-0.323480	3.942228	1.177120
50	9	0	-10.616326	-2.063513	0.149975
51	9	0	10.764262	-1.387059	0.014258

Optimized geometric parameters for **1e- F^-** in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.088130	-0.441193	-0.088040
2	6	0	-5.891163	0.246465	-0.096327
3	6	0	-7.114312	-1.877823	0.007496
4	1	0	-5.887657	1.327142	-0.166615
5	6	0	-4.639474	-0.422172	-0.013208
6	6	0	-5.850114	-2.525614	0.084789
7	1	0	-5.856552	-3.608185	0.153782
8	6	0	-4.657808	-1.831103	0.075809
9	1	0	-3.727312	-2.383631	0.139169
10	6	0	-3.438047	0.361333	-0.019966
11	1	0	-3.580279	1.435975	-0.098666
12	6	0	-2.145133	-0.074357	0.063509
13	1	0	-1.911802	-1.129106	0.148712
14	6	0	-1.020285	0.808954	0.043205
15	8	0	-1.252906	2.109632	-0.095619
16	6	0	0.288711	0.333568	0.136858
17	1	0	0.446916	-0.727870	0.249682
18	6	0	1.378228	1.204983	0.015159
19	8	0	1.160758	2.511168	-0.107587
20	6	0	2.757088	0.828560	-0.015770
21	1	0	3.444091	1.664625	-0.086367
22	6	0	3.226546	-0.456681	0.033057
23	1	0	2.498696	-1.262091	0.088077
24	6	0	4.587165	-0.896892	0.018954
25	6	0	5.698328	-0.009294	-0.039661
26	6	0	4.858457	-2.282230	0.063929
27	1	0	5.519689	1.056606	-0.073204
28	1	0	4.027922	-2.979626	0.109204
29	6	0	6.992594	-0.479352	-0.051788
30	6	0	6.152650	-2.762997	0.051774
31	1	0	6.347936	-3.829076	0.087016
32	6	0	7.277734	-1.898703	-0.006289
33	8	0	8.104014	0.311040	-0.105276
34	6	0	7.928626	1.725175	-0.151363
35	1	0	7.371702	2.027052	-1.044136
36	1	0	7.410841	2.090010	0.741411
37	1	0	8.930384	2.149278	-0.188336
38	8	0	8.478785	-2.367362	-0.016415
39	1	0	9.685668	-1.715429	-0.056429
40	8	0	-8.321344	0.146022	-0.167743
41	6	0	-8.388181	1.565892	-0.266958
42	1	0	-7.945704	2.047825	0.610904
43	1	0	-7.885729	1.926045	-1.170569
44	1	0	-9.447155	1.812605	-0.319362
45	8	0	-8.210484	-2.564603	0.021158
46	1	0	-9.497199	-2.143561	0.030883
47	5	0	-0.178296	3.096524	0.097669
48	9	0	-0.354985	4.140252	-0.822212
49	9	0	-0.253820	3.615031	1.412147
50	9	0	-10.523667	-2.019560	0.053736
51	9	0	10.665313	-1.414334	-0.081744

Optimized geometric parameters for **1e- Cl^-** in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.159240	-0.203631	-0.421673
2	6	0	5.938237	0.473970	-0.348575
3	6	0	7.185349	-1.636999	-0.383471
4	1	0	5.960988	1.560976	-0.400560
5	6	0	4.690676	-0.201761	-0.244030
6	6	0	5.930711	-2.314125	-0.291110
7	1	0	5.967144	-3.399736	-0.272672
8	6	0	4.723362	-1.627744	-0.220962
9	1	0	3.796944	-2.191944	-0.145878
10	6	0	3.469946	0.575411	-0.180111
11	1	0	3.579001	1.659909	-0.207376
12	6	0	2.179697	0.105809	-0.087470
13	1	0	1.966052	-0.959392	-0.055730
14	6	0	1.033178	0.978063	-0.026860
15	8	0	1.251893	2.306296	-0.069659
16	6	0	-0.282481	0.477905	0.065170
17	1	0	-0.432554	-0.592615	0.097077
18	6	0	-1.386161	1.357729	0.101034
19	8	0	-1.178172	2.688503	0.068064
20	6	0	-2.779789	0.974645	0.165475
21	1	0	-3.465462	1.817156	0.193847
22	6	0	-3.246358	-0.318422	0.188451
23	1	0	-2.511951	-1.125191	0.152360
24	6	0	-4.623881	-0.765066	0.253080
25	6	0	-5.739417	0.116818	0.321615
26	6	0	-4.897330	-2.163172	0.264728
27	1	0	-5.595290	1.193631	0.352652
28	1	0	-4.066573	-2.866440	0.219580
29	6	0	-7.052720	-0.351702	0.387614
30	6	0	-6.202858	-2.644485	0.330146
31	1	0	-6.415508	-3.709484	0.337571
32	6	0	-7.322513	-1.765303	0.382176
33	8	0	-8.090535	0.575479	0.562990
34	6	0	-8.720266	1.107148	-0.663768
35	1	0	-7.944261	1.475573	-1.352483
36	1	0	-9.355915	0.339492	-1.122128
37	1	0	-9.350283	1.934480	-0.326567
38	8	0	-8.541181	-2.331719	0.468036
39	1	0	-9.421281	-1.830241	0.174682
40	8	0	8.330242	0.541123	-0.633977
41	6	0	9.078540	0.955157	0.570765
42	1	0	8.398388	1.447797	1.283004
43	1	0	9.590554	0.091111	1.012052
44	1	0	9.828754	1.665035	0.211868
45	8	0	8.284002	-2.412636	-0.467684
46	1	0	9.247279	-2.061205	-0.228364
47	5	0	0.175508	3.346212	0.051343
48	9	0	0.354751	4.062809	1.270647
49	9	0	0.248396	4.223651	-1.064548
50	17	0	11.004043	-1.884291	0.456285
51	17	0	-11.083033	-1.379002	-0.599229

Optimized geometric parameters for **1e- Cl^-** in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.158781	-0.267130	-0.053555
2	6	0	5.938659	0.415181	-0.050839
3	6	0	7.178394	-1.695306	-0.068796
4	1	0	5.921457	1.500820	-0.036261
5	6	0	4.699699	-0.289272	-0.068239
6	6	0	5.949753	-2.393484	-0.092688
7	1	0	5.982859	-3.478715	-0.107553
8	6	0	4.730810	-1.710188	-0.092493
9	1	0	3.807715	-2.281026	-0.108890
10	6	0	3.469425	0.482348	-0.058512
11	1	0	3.581406	1.566072	-0.041348
12	6	0	2.183276	-0.003163	-0.065631
13	1	0	1.976297	-1.068780	-0.081521
14	6	0	1.029928	0.857902	-0.048711
15	8	0	1.246923	2.198755	-0.028095
16	6	0	-0.284541	0.357472	-0.050496
17	1	0	-0.431096	-0.713260	-0.066306
18	6	0	-1.391997	1.231282	-0.028300
19	8	0	-1.178902	2.573435	-0.006021
20	6	0	-2.783123	0.858055	-0.023594
21	1	0	-3.468412	1.700617	0.002835
22	6	0	-3.250487	-0.435740	-0.049947
23	1	0	-2.526243	-1.249146	-0.080039
24	6	0	-4.636816	-0.863221	-0.043062
25	6	0	-5.734013	0.047925	0.002848
26	6	0	-4.915844	-2.255432	-0.082895
27	1	0	-5.548411	1.115343	0.033789
28	1	0	-4.093068	-2.965087	-0.117651
29	6	0	-7.048196	-0.419990	0.009007
30	6	0	-6.233409	-2.726327	-0.078052
31	1	0	-6.449091	-3.789664	-0.108459
32	6	0	-7.318866	-1.827455	-0.031713
33	8	0	-8.184678	0.382230	0.052766
34	6	0	-8.024415	1.836153	0.112439
35	1	0	-7.476603	2.131767	1.015990
36	1	0	-7.504038	2.208984	-0.778568
37	1	0	-9.038467	2.236734	0.144998
38	8	0	-8.583247	-2.344312	-0.028814
39	1	0	-9.389144	-1.719231	0.021457
40	8	0	8.416078	0.333665	-0.045040
41	6	0	8.499529	1.794440	-0.002609
42	1	0	8.031116	2.239648	-0.889334
43	1	0	8.025776	2.187238	0.905819
44	1	0	9.566008	2.023216	0.006877
45	8	0	8.332529	-2.430040	-0.068941
46	1	0	9.231178	-1.956329	0.024871
47	5	0	0.163374	3.206847	-0.003509
48	9	0	0.297447	4.021992	1.175323
49	9	0	0.282582	4.063405	-1.154201
50	17	0	11.249592	-1.821899	0.253175
51	17	0	-11.362844	-1.246700	0.115939

Optimized geometric parameters for **1e- Cl^-** in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.089512	-0.271354	-0.055654
2	6	0	5.882704	0.412318	-0.060743
3	6	0	7.093397	-1.682816	0.028699
4	1	0	5.873578	1.492597	-0.124549
5	6	0	4.649755	-0.274229	0.017572
6	6	0	5.875593	-2.364753	0.105823
7	1	0	5.898307	-3.446299	0.169198
8	6	0	4.671942	-1.678099	0.100879
9	1	0	3.748469	-2.239825	0.162266
10	6	0	3.430516	0.506894	0.010383
11	1	0	3.563441	1.582609	-0.060830
12	6	0	2.154338	0.050500	0.084197
13	1	0	1.932990	-1.007112	0.159879
14	6	0	1.012222	0.926743	0.066503
15	8	0	1.232113	2.221816	-0.050793
16	6	0	-0.286614	0.425992	0.144582
17	1	0	-0.430432	-0.638790	0.238196
18	6	0	-1.381950	1.289298	0.034316
19	8	0	-1.189706	2.589733	-0.068414
20	6	0	-2.765816	0.892846	-0.002003
21	1	0	-3.458621	1.723364	-0.076050
22	6	0	-3.212405	-0.388729	0.051561
23	1	0	-2.481418	-1.189293	0.118815
24	6	0	-4.585107	-0.841804	0.030992
25	6	0	-5.688690	0.039939	-0.053341
26	6	0	-4.837239	-2.223105	0.099464
27	1	0	-5.522265	1.106302	-0.108216
28	1	0	-4.005278	-2.915000	0.163324
29	6	0	-6.984216	-0.444836	-0.066433
30	6	0	-6.135530	-2.714090	0.088760
31	1	0	-6.330732	-3.778311	0.143344
32	6	0	-7.221446	-1.843554	0.008176
33	8	0	-8.110631	0.311719	-0.147378
34	6	0	-7.981069	1.733342	-0.233337
35	1	0	-7.485957	2.135420	0.654896
36	1	0	-7.426148	2.021464	-1.130530
37	1	0	-8.996655	2.118223	-0.291868
38	8	0	-8.462017	-2.361402	0.001518
39	1	0	-9.187698	-1.695078	-0.037360
40	8	0	8.322942	0.300386	-0.126517
41	6	0	8.415572	1.724272	-0.218850
42	1	0	7.922476	2.090941	-1.123456
43	1	0	7.978585	2.203042	0.661883
44	1	0	9.478796	1.948419	-0.266300
45	8	0	8.231276	-2.404340	0.037554
46	1	0	9.055384	-1.869631	-0.020139
47	5	0	0.146307	3.212678	0.095785
48	9	0	0.218933	3.789258	1.376183
49	9	0	0.299725	4.197972	-0.882017
50	17	0	11.330492	-1.836547	-0.085216
51	17	0	-11.382898	-1.251891	-0.056899

Optimized geometric parameters for **1e- Br^-** in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.161450	-0.073280	0.005859
2	6	0	-5.938249	0.599907	0.003127
3	6	0	-7.201406	-1.505767	-0.010901
4	1	0	-5.915445	1.686759	0.016152
5	6	0	-4.700278	-0.111165	-0.017380
6	6	0	-5.971649	-2.208063	-0.031930
7	1	0	-6.021144	-3.292714	-0.044515
8	6	0	-4.749603	-1.532038	-0.035193
9	1	0	-3.828035	-2.107670	-0.051142
10	6	0	-3.464087	0.646328	-0.019074
11	1	0	-3.556568	1.732710	-0.003493
12	6	0	-2.177779	0.160015	-0.037881
13	1	0	-1.974013	-0.907323	-0.054375
14	6	0	-1.021509	1.022529	-0.036242
15	8	0	-1.232835	2.351858	-0.014450
16	6	0	0.292885	0.511984	-0.054770
17	1	0	0.437097	-0.559671	-0.071123
18	6	0	1.402437	1.384849	-0.047537
19	8	0	1.203610	2.716563	-0.024969
20	6	0	2.795103	0.992989	-0.059939
21	1	0	3.483801	1.833325	-0.044411
22	6	0	3.256807	-0.301255	-0.089719
23	1	0	2.520437	-1.106304	-0.107195
24	6	0	4.635636	-0.750096	-0.102557
25	6	0	5.750429	0.142598	-0.081148
26	6	0	4.899776	-2.145228	-0.140168
27	1	0	5.580972	1.214290	-0.056752
28	1	0	4.063899	-2.842590	-0.157530
29	6	0	7.055893	-0.346301	-0.095234
30	6	0	6.208559	-2.639007	-0.151939
31	1	0	6.415093	-3.704416	-0.175577
32	6	0	7.314846	-1.760979	-0.125755
33	8	0	8.210272	0.415670	-0.088037
34	6	0	8.138138	1.857691	0.039850
35	1	0	7.625994	2.309219	-0.823176
36	1	0	7.623635	2.147971	0.967997
37	1	0	9.179917	2.180544	0.071384
38	8	0	8.559768	-2.287974	-0.133902
39	1	0	9.378616	-1.675161	-0.051664
40	8	0	-8.416543	0.513189	0.022858
41	6	0	-8.546672	1.955747	0.053489
42	1	0	-8.080968	2.378916	0.956401
43	1	0	-8.099435	2.415562	-0.840868
44	1	0	-9.623208	2.133412	0.068332
45	8	0	-8.348986	-2.222738	-0.008287
46	1	0	-9.253496	-1.741725	0.015669
47	5	0	-0.144534	3.386990	-0.015005
48	9	0	-0.267872	4.191220	-1.182501
49	9	0	-0.256164	4.180036	1.160585
50	35	0	-11.445001	-1.362184	0.072169
51	35	0	11.467076	-0.971321	0.180479

Optimized geometric parameters for **1e- Br^-** in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.157612	0.014351	0.004152
2	6	0	5.933918	0.689863	-0.000305
3	6	0	7.183042	-1.407973	0.066870
4	1	0	5.907406	1.774259	-0.047692
5	6	0	4.703953	-0.027359	0.055163
6	6	0	5.970579	-2.122540	0.124144
7	1	0	6.013088	-3.206224	0.172177
8	6	0	4.746062	-1.446375	0.118068
9	1	0	3.827966	-2.023092	0.164014
10	6	0	3.464125	0.733351	0.044521
11	1	0	3.565094	1.817686	0.011357
12	6	0	2.185445	0.233161	0.068832
13	1	0	1.990664	-0.834392	0.096834
14	6	0	1.020576	1.080970	0.053881
15	8	0	1.220501	2.422610	0.025826
16	6	0	-0.286638	0.562653	0.065376
17	1	0	-0.419371	-0.509671	0.086882
18	6	0	-1.404641	1.422689	0.045967
19	8	0	-1.210018	2.765675	0.020877
20	6	0	-2.792275	1.030764	0.047613
21	1	0	-3.487966	1.864959	0.032038
22	6	0	-3.240949	-0.268127	0.062687
23	1	0	-2.506620	-1.072734	0.076769
24	6	0	-4.624006	-0.714065	0.059153
25	6	0	-5.731395	0.185194	0.041568
26	6	0	-4.881244	-2.110396	0.071445
27	1	0	-5.561233	1.255560	0.033714
28	1	0	-4.047693	-2.807653	0.085430
29	6	0	-7.036872	-0.305395	0.034786
30	6	0	-6.192509	-2.603575	0.064145
31	1	0	-6.392553	-3.670147	0.072012
32	6	0	-7.279808	-1.713800	0.044200
33	8	0	-8.196372	0.464725	0.018852
34	6	0	-8.078788	1.925425	0.000732
35	1	0	-7.562122	2.283665	0.899377
36	1	0	-7.548079	2.260167	-0.898823
37	1	0	-9.104483	2.295888	-0.012023
38	8	0	-8.555229	-2.230098	0.035570
39	1	0	-9.294265	-1.561923	0.002297
40	8	0	8.417321	0.607986	-0.048570
41	6	0	8.507674	2.068810	-0.123395
42	1	0	8.016080	2.441989	-1.030080
43	1	0	8.060626	2.531215	0.765023
44	1	0	9.574905	2.290580	-0.160870
45	8	0	8.362927	-2.120144	0.075087
46	1	0	9.196499	-1.578496	0.019122
47	5	0	0.124329	3.418813	0.008815
48	9	0	0.239768	4.274707	1.158781
49	9	0	0.239035	4.232872	-1.171109
50	35	0	11.676233	-1.587093	-0.087984
51	35	0	-11.716663	-1.151927	-0.112571

Optimized geometric parameters for **1e- Br^-** in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.097453	-0.008801	-0.014704
2	6	0	-5.886019	0.666497	-0.010473
3	6	0	-7.110294	-1.420607	-0.075726
4	1	0	-5.868979	1.747569	0.035979
5	6	0	-4.658349	-0.031682	-0.065107
6	6	0	-5.899362	-2.114621	-0.132598
7	1	0	-5.929841	-3.196756	-0.179830
8	6	0	-4.690600	-1.436311	-0.127358
9	1	0	-3.770995	-2.005738	-0.173026
10	6	0	-3.431921	0.739158	-0.053205
11	1	0	-3.556030	1.817668	-0.017134
12	6	0	-2.159533	0.268368	-0.078594
13	1	0	-1.947749	-0.793366	-0.110439
14	6	0	-1.007763	1.132928	-0.059715
15	8	0	-1.217388	2.433107	-0.026780
16	6	0	0.285731	0.613824	-0.073212
17	1	0	0.418194	-0.456114	-0.099671
18	6	0	1.389784	1.471593	-0.048317
19	8	0	1.213647	2.776838	-0.017082
20	6	0	2.771830	1.064269	-0.051141
21	1	0	3.472897	1.890907	-0.030838
22	6	0	3.206203	-0.221916	-0.072235
23	1	0	2.467761	-1.018240	-0.090973
24	6	0	4.575958	-0.686505	-0.070338
25	6	0	5.688143	0.187991	-0.046408
26	6	0	4.813992	-2.071648	-0.090791
27	1	0	5.532367	1.257326	-0.031980
28	1	0	3.974560	-2.757099	-0.109406
29	6	0	6.978731	-0.309585	-0.041649
30	6	0	6.107877	-2.575561	-0.085735
31	1	0	6.292175	-3.642977	-0.099882
32	6	0	7.200354	-1.711737	-0.059788
33	8	0	8.116175	0.434907	-0.020441
34	6	0	8.007659	1.861011	0.007639
35	1	0	7.495511	2.230973	-0.884723
36	1	0	7.479551	2.194358	0.905144
37	1	0	9.029572	2.232841	0.024230
38	8	0	8.441088	-2.235374	-0.055044
39	1	0	9.153249	-1.561095	-0.011583
40	8	0	-8.329113	0.569500	0.035386
41	6	0	-8.416279	1.995279	0.109657
42	1	0	-7.928600	2.370126	1.013720
43	1	0	-7.969965	2.460864	-0.773352
44	1	0	-9.478769	2.224846	0.145774
45	8	0	-8.258847	-2.128842	-0.083338
46	1	0	-9.063563	-1.571893	-0.021007
47	5	0	-0.121175	3.423048	-0.002966
48	9	0	-0.228843	4.247820	-1.131343
49	9	0	-0.230637	4.193508	1.163018
50	35	0	-11.560873	-1.573139	0.108965
51	35	0	11.595250	-1.163550	0.131490

Optimized geometric parameters for **1e- AcO**$^{-}$ in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.164030	-0.142392	0.197372
2	6	0	5.946394	0.526785	0.160945
3	6	0	7.237554	-1.592832	0.276414
4	1	0	5.916313	1.612828	0.105377
5	6	0	4.698117	-0.177488	0.191376
6	6	0	5.970699	-2.276326	0.297759
7	1	0	6.012511	-3.361214	0.355982
8	6	0	4.755195	-1.601799	0.258698
9	1	0	3.830405	-2.174308	0.283625
10	6	0	3.470962	0.574880	0.150010
11	1	0	3.563715	1.660663	0.102196
12	6	0	2.174490	0.095709	0.162028
13	1	0	1.967224	-0.970487	0.207486
14	6	0	1.025472	0.956455	0.115539
15	8	0	1.239249	2.292241	0.070046
16	6	0	-0.293556	0.454140	0.124090
17	1	0	-0.441446	-0.616951	0.160437
18	6	0	-1.403628	1.326534	0.099839
19	8	0	-1.196457	2.664684	0.050116
20	6	0	-2.791467	0.941384	0.129289
21	1	0	-3.478762	1.782899	0.101310
22	6	0	-3.264191	-0.355695	0.186014
23	1	0	-2.527171	-1.160628	0.212979
24	6	0	-4.633760	-0.800947	0.213186
25	6	0	-5.754870	0.092387	0.182166
26	6	0	-4.913153	-2.197758	0.270253
27	1	0	-5.571126	1.161307	0.132762
28	1	0	-4.077208	-2.897088	0.293391
29	6	0	-7.057457	-0.387138	0.210027
30	6	0	-6.217276	-2.684871	0.300780
31	1	0	-6.421872	-3.751110	0.351510
32	6	0	-7.358957	-1.813945	0.279860
33	8	0	-8.201284	0.426560	0.165885
34	6	0	-8.026313	1.864022	0.244881
35	1	0	-7.490524	2.149710	1.162235
36	1	0	-7.480082	2.253829	-0.627780
37	1	0	-9.036813	2.279318	0.263009
38	8	0	-8.581231	-2.281670	0.318087
39	1	0	-9.880827	-1.658128	0.492916
40	8	0	8.420346	0.489551	0.152499
41	6	0	8.464435	1.935283	0.243826
42	1	0	7.988051	2.412065	-0.626998
43	1	0	7.973636	2.292270	1.161662
44	1	0	9.526253	2.192859	0.269059
45	8	0	8.368933	-2.252849	0.322599
46	1	0	9.741684	-1.834140	0.497557
47	5	0	0.151192	3.311874	-0.051198
48	9	0	0.287756	4.269027	0.999457
49	9	0	0.259694	3.966082	-1.320866
50	8	0	10.782949	-1.693432	0.632407
51	8	0	12.724402	-1.135197	-0.424452
52	6	0	11.489522	-1.351950	-0.463992
53	6	0	10.683295	-1.244106	-1.760915
54	1	0	9.908398	-0.477899	-1.642069
55	1	0	11.348016	-0.993534	-2.591863
56	1	0	10.163618	-2.189017	-1.961884
57	8	0	-10.887656	-1.365421	0.624022
58	8	0	-12.724597	-0.540889	-0.444752
59	6	0	-11.533103	-0.930168	-0.477649
60	6	0	-10.712052	-0.939966	-1.769687
61	1	0	-10.325374	-1.947898	-1.963800
62	1	0	-11.331014	-0.603886	-2.605681
63	1	0	-9.840142	-0.286608	-1.649061

Optimized geometric parameters for **1e- AcO**$^{-}$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.154100	-0.146291	-0.263577
2	6	0	-5.935760	0.526144	-0.218297
3	6	0	-7.208711	-1.586842	-0.394287
4	1	0	-5.910835	1.608004	-0.120640
5	6	0	-4.690878	-0.176634	-0.297613
6	6	0	-5.953475	-2.271384	-0.471704
7	1	0	-5.986167	-3.353306	-0.570752
8	6	0	-4.735990	-1.596112	-0.426006
9	1	0	-3.813651	-2.166833	-0.490676
10	6	0	-3.464340	0.580029	-0.242328
11	1	0	-3.569337	1.661090	-0.150249
12	6	0	-2.171639	0.093802	-0.289613
13	1	0	-1.970910	-0.969914	-0.377661
14	6	0	-1.017699	0.940562	-0.221089
15	8	0	-1.226017	2.287652	-0.120089
16	6	0	0.296669	0.438583	-0.255075
17	1	0	0.437627	-0.630453	-0.336066
18	6	0	1.413873	1.299390	-0.188478
19	8	0	1.204190	2.647232	-0.079441
20	6	0	2.795015	0.920728	-0.221707
21	1	0	3.489058	1.754111	-0.154141
22	6	0	3.260546	-0.378944	-0.325987
23	1	0	2.526732	-1.182524	-0.391796
24	6	0	4.631610	-0.814408	-0.356910
25	6	0	5.746193	0.084266	-0.282509
26	6	0	4.907366	-2.209258	-0.464935
27	1	0	5.565006	1.150387	-0.201030
28	1	0	4.075781	-2.908983	-0.521934
29	6	0	7.051333	-0.391053	-0.314543
30	6	0	6.215009	-2.689814	-0.497344
31	1	0	6.416498	-3.754209	-0.580577
32	6	0	7.341580	-1.812158	-0.425150
33	8	0	8.190780	0.416835	-0.243353
34	6	0	8.012867	1.865786	-0.151290
35	1	0	7.481596	2.252402	-1.030611
36	1	0	7.466719	2.138628	0.760990
37	1	0	9.021335	2.281378	-0.116550
38	8	0	8.576030	-2.286757	-0.457470
39	1	0	9.765337	-1.656842	-0.358194
40	8	0	-8.407941	0.474040	-0.185583
41	6	0	-8.455829	1.931271	-0.075340
42	1	0	-7.959975	2.274902	0.841853
43	1	0	-7.989737	2.407369	-0.947897
44	1	0	-9.516517	2.185996	-0.038933
45	8	0	-8.349133	-2.264226	-0.440166
46	1	0	-9.597589	-1.830610	-0.374757
47	5	0	-0.132762	3.270803	0.007856
48	9	0	-0.259388	4.264393	-1.032769
49	9	0	-0.254252	3.958824	1.275249
50	8	0	-10.699226	-1.673170	-0.406597
51	8	0	-12.579714	-1.089557	0.722829
52	6	0	-11.339156	-1.322815	0.719930
53	6	0	-10.490965	-1.230805	1.982448
54	1	0	-9.660543	-0.535829	1.816431
55	1	0	-11.097461	-0.894944	2.826332
56	1	0	-10.057470	-2.211352	2.215642
57	8	0	10.816016	-1.337785	-0.354341
58	8	0	12.536493	-0.479603	0.850516
59	6	0	11.347835	-0.896921	0.799335
60	6	0	10.441042	-0.936893	2.022360

61	1	0	10.135494	-1.969739	2.230210
62	1	0	10.958140	-0.530449	2.894066
63	1	0	9.531252	-0.359911	1.823148

Optimized geometric parameters for **1e-AcO**$^{-}$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.086664	-0.164440	0.321039
2	6	0	5.885581	0.510862	0.275331
3	6	0	7.132412	-1.608047	0.317433
4	1	0	5.870383	1.593941	0.279168
5	6	0	4.639377	-0.175124	0.223926
6	6	0	5.870542	-2.271026	0.265271
7	1	0	5.885983	-3.355916	0.263115
8	6	0	4.673529	-1.587820	0.220990
9	1	0	3.748164	-2.151589	0.183602
10	6	0	3.430685	0.591709	0.178346
11	1	0	3.559358	1.670995	0.188834
12	6	0	2.141228	0.136025	0.123614
13	1	0	1.921867	-0.925084	0.108430
14	6	0	1.005598	1.002158	0.090346
15	8	0	1.219127	2.314250	0.142094
16	6	0	-0.298043	0.504449	0.037102
17	1	0	-0.441682	-0.564312	-0.004422
18	6	0	-1.399742	1.365517	0.117503
19	8	0	-1.198021	2.681536	0.156888
20	6	0	-2.770975	0.973030	0.190923
21	1	0	-3.469237	1.801923	0.228872
22	6	0	-3.224075	-0.320654	0.212834
23	1	0	-2.485179	-1.117490	0.183514
24	6	0	-4.575470	-0.778270	0.270366
25	6	0	-5.700203	0.095848	0.310695
26	6	0	-4.827906	-2.169074	0.289974
27	1	0	-5.535869	1.164684	0.297020
28	1	0	-3.986739	-2.854788	0.259577
29	6	0	-6.984885	-0.392502	0.366098
30	6	0	-6.112633	-2.669047	0.345951
31	1	0	-6.290484	-3.738843	0.360635
32	6	0	-7.254605	-1.819802	0.387159
33	8	0	-8.109649	0.382810	0.407618
34	6	0	-7.954557	1.800154	0.401860
35	1	0	-7.384726	2.139914	1.272523
36	1	0	-7.459422	2.141463	-0.512840
37	1	0	-8.961342	2.211769	0.444295
38	8	0	-8.447300	-2.288011	0.440302
39	1	0	-9.800723	-1.600857	0.407968
40	8	0	8.316841	0.436418	0.375318
41	6	0	8.371403	1.860140	0.399086
42	1	0	7.934358	2.291220	-0.507564
43	1	0	7.856258	2.263422	1.276921
44	1	0	9.427715	2.118864	0.449059
45	8	0	8.237432	-2.264940	0.359912
46	1	0	9.660938	-1.790036	0.395478
47	5	0	0.127102	3.261317	-0.130897
48	9	0	0.302923	4.396669	0.673824
49	9	0	0.173650	3.644286	-1.494189
50	8	0	10.680322	-1.668571	0.515629
51	8	0	12.535661	-1.114885	-0.552243
52	6	0	11.328580	-1.309498	-0.580256
53	6	0	10.506706	-1.159636	-1.841419
54	1	0	9.718221	-0.421510	-1.680587
55	1	0	11.145688	-0.852735	-2.667098
56	1	0	10.019970	-2.107030	-2.085700
57	8	0	-10.790266	-1.329953	0.479812

58	8	0	-12.496506	-0.551376	-0.690984
59	6	0	-11.330749	-0.916759	-0.656507
60	6	0	-10.439343	-0.926398	-1.878328
61	1	0	-10.084579	-1.941054	-2.074861
62	1	0	-10.988943	-0.556936	-2.741735
63	1	0	-9.560487	-0.304172	-1.697225

Optimized geometric parameters for **1e- SCN**$^{-}$ in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.160458	-0.167544	-0.012207
2	6	0	-5.936108	0.499419	-0.014917
3	6	0	-7.219562	-1.608226	0.007810
4	1	0	-5.906462	1.586245	-0.029566
5	6	0	-4.695464	-0.210846	0.001660
6	6	0	-5.974258	-2.303507	0.024012
7	1	0	-6.024618	-3.388578	0.038910
8	6	0	-4.752346	-1.632955	0.021047
9	1	0	-3.831635	-2.211041	0.034118
10	6	0	-3.460897	0.542183	-0.001302
11	1	0	-3.550575	1.628956	-0.016536
12	6	0	-2.172170	0.055258	0.013505
13	1	0	-1.970209	-1.012619	0.029834
14	6	0	-1.015635	0.913970	0.009431
15	8	0	-1.224371	2.246944	-0.020904
16	6	0	0.298174	0.402782	0.029309
17	1	0	0.440290	-0.669203	0.052898
18	6	0	1.411878	1.271772	0.007390
19	8	0	1.212891	2.607197	-0.018012
20	6	0	2.799769	0.877497	0.003418
21	1	0	3.491263	1.715647	-0.012367
22	6	0	3.261725	-0.421274	0.017755
23	1	0	2.521577	-1.223265	0.032446
24	6	0	4.633129	-0.874398	0.016203
25	6	0	5.755184	0.013609	-0.003239
26	6	0	4.899955	-2.271948	0.034752
27	1	0	5.581361	1.084844	-0.017502
28	1	0	4.061931	-2.967909	0.049681
29	6	0	7.058164	-0.474352	-0.004025
30	6	0	6.204428	-2.766088	0.034486
31	1	0	6.407056	-3.832981	0.048804
32	6	0	7.334181	-1.897526	0.015296
33	8	0	8.207173	0.316721	-0.022823
34	6	0	8.064736	1.759433	-0.045965
35	1	0	7.527260	2.094142	-0.946065
36	1	0	7.537942	2.124207	0.848728
37	1	0	9.085372	2.147078	-0.058492
38	8	0	8.558528	-2.404631	0.015513
39	1	0	9.587709	-1.825280	0.001305
40	8	0	-8.411604	0.452270	-0.027680
41	6	0	-8.476969	1.899668	-0.049349
42	1	0	-8.005909	2.336610	0.844418
43	1	0	-7.995637	2.310099	-0.950186
44	1	0	-9.542975	2.136236	-0.058897
45	8	0	-8.353704	-2.305300	0.011686
46	1	0	-9.413307	-1.883231	0.001481
47	5	0	-0.132809	3.273595	0.026870
48	9	0	-0.258112	4.140151	-1.096541
49	9	0	-0.241643	4.015387	1.241960
50	7	0	-10.720082	-1.616144	-0.007609
51	6	0	-11.887464	-1.374201	-0.015722
52	6	0	11.915689	-1.000185	-0.023968
53	7	0	10.791916	-1.395413	-0.011811
54	16	0	13.496919	-0.441828	-0.041137

55	16	0	-13.532345	-1.029280	-0.027281

Optimized geometric parameters for **1e- SCN**$^{-}$ in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.155981	-0.130627	0.000779
2	6	0	-5.928691	0.538014	0.000747
3	6	0	-7.194339	-1.561171	0.001063
4	1	0	-5.900132	1.623553	0.000544
5	6	0	-4.695545	-0.177764	0.000939
6	6	0	-5.967735	-2.268312	0.001305
7	1	0	-6.011836	-3.353331	0.001534
8	6	0	-4.742165	-1.598855	0.001246
9	1	0	-3.825062	-2.179710	0.001467
10	6	0	-3.458413	0.580449	0.000827
11	1	0	-3.558713	1.665532	0.000933
12	6	0	-2.176643	0.081101	0.000531
13	1	0	-1.982177	-0.987027	0.000292
14	6	0	-1.013593	0.927671	0.000414
15	8	0	-1.213625	2.272282	0.000994
16	6	0	0.294787	0.411431	-0.000152
17	1	0	0.428009	-0.661180	-0.000583
18	6	0	1.413878	1.270769	0.000082
19	8	0	1.217382	2.616708	0.000530
20	6	0	2.799012	0.879430	-0.000057
21	1	0	3.496345	1.712512	0.000155
22	6	0	3.248848	-0.421966	-0.000491
23	1	0	2.512277	-1.224972	-0.000718
24	6	0	4.626915	-0.870168	-0.000746
25	6	0	5.740163	0.023451	-0.000364
26	6	0	4.884882	-2.267488	-0.001426
27	1	0	5.570223	1.093991	0.000193
28	1	0	4.050810	-2.964886	-0.001695
29	6	0	7.047095	-0.463693	-0.000712
30	6	0	6.194197	-2.757685	-0.001805
31	1	0	6.393100	-3.824785	-0.002361
32	6	0	7.299644	-1.878100	-0.001487
33	8	0	8.193767	0.328057	-0.000366
34	6	0	8.042963	1.784541	0.000118
35	1	0	7.511354	2.122858	-0.898159
36	1	0	7.511676	2.122289	0.898800
37	1	0	9.059733	2.179814	0.000066
38	8	0	8.546801	-2.413046	-0.001983
39	1	0	9.408561	-1.825858	-0.001086
40	8	0	-8.405057	0.490399	0.000602
41	6	0	-8.461889	1.953220	-0.000419
42	1	0	-7.984284	2.364902	0.897663
43	1	0	-7.983729	2.363663	-0.898771
44	1	0	-9.524424	2.200666	-0.000904
45	8	0	-8.347081	-2.282528	0.001130
46	1	0	-9.283149	-1.830110	0.000766
47	5	0	-0.116810	3.265495	-0.000367
48	9	0	-0.233218	4.102756	-1.166479
49	9	0	-0.233222	4.105910	1.163361
50	7	0	-10.818576	-1.593674	0.000221
51	6	0	-12.001147	-1.423047	-0.000320
52	6	0	12.027131	-1.031942	0.000881
53	7	0	10.881568	-1.371009	-0.000031
54	16	0	13.646781	-0.552325	0.002162
55	16	0	-13.673360	-1.181496	-0.001072

Optimized geometric parameters for **1e- SCN**$^{-}$ in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.088677	-0.167251	-0.021195
2	6	0	-5.876448	0.506838	-0.033975
3	6	0	-7.105325	-1.577434	0.104346
4	1	0	-5.859128	1.584695	-0.129452
5	6	0	-4.648043	-0.184034	0.076601
6	6	0	-5.889457	-2.261941	0.214949
7	1	0	-5.920345	-3.340988	0.310596
8	6	0	-4.681230	-1.584848	0.201923
9	1	0	-3.762464	-2.150811	0.290230
10	6	0	-3.423773	0.587323	0.057579
11	1	0	-3.547832	1.662141	-0.039650
12	6	0	-2.151099	0.122389	0.147912
13	1	0	-1.939755	-0.935309	0.247347
14	6	0	-1.000964	0.986340	0.115975
15	8	0	-1.206477	2.281540	-0.029615
16	6	0	0.292695	0.474270	0.208329
17	1	0	0.425247	-0.589747	0.324735
18	6	0	1.397576	1.322813	0.080264
19	8	0	1.218920	2.623554	-0.048522
20	6	0	2.776237	0.910113	0.049786
21	1	0	3.478991	1.730820	-0.038692
22	6	0	3.207868	-0.376277	0.122081
23	1	0	2.466763	-1.166441	0.201735
24	6	0	4.573586	-0.847303	0.105272
25	6	0	5.689498	0.017781	0.008556
26	6	0	4.808195	-2.231095	0.188538
27	1	0	5.536205	1.085654	-0.055297
28	1	0	3.967506	-2.911385	0.262967
29	6	0	6.979134	-0.482839	-0.004265
30	6	0	6.099481	-2.738277	0.176990
31	1	0	6.280975	-3.804481	0.240912
32	6	0	7.200376	-1.885436	0.080810
33	8	0	8.112037	0.263362	-0.094120
34	6	0	7.992286	1.684345	-0.195144
35	1	0	7.437572	1.967620	-1.094169
36	1	0	7.501851	2.100562	0.689358
37	1	0	9.010189	2.062285	-0.259801
38	8	0	8.427268	-2.424213	0.073299
39	1	0	9.188225	-1.790334	-0.005234
40	8	0	-8.315285	0.415310	-0.121037
41	6	0	-8.389630	1.836158	-0.255735
42	1	0	-7.954723	2.336520	0.614200
43	1	0	-7.884421	2.171269	-1.166099
44	1	0	-9.449703	2.071649	-0.319311
45	8	0	-8.241141	-2.293248	0.123394
46	1	0	-9.084712	-1.779169	0.029033
47	5	0	-0.110256	3.261636	0.109472
48	9	0	-0.252680	4.240621	-0.876526
49	9	0	-0.177760	3.850271	1.385346
50	7	0	-10.873184	-1.584167	-0.093649
51	6	0	-12.027279	-1.384564	-0.174538
52	6	0	12.044596	-1.008432	-0.192153
53	7	0	10.922747	-1.346470	-0.118281
54	16	0	13.626448	-0.531931	-0.296244
55	16	0	-13.654720	-1.102979	-0.288210

Optimized geometric parameters for **1e- NO_3^-** in B3LYP/SDD (gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.148864	-0.257718	-0.413767
2	6	0	-5.929028	0.417733	-0.349144
3	6	0	-7.184165	-1.692087	-0.431638
4	1	0	-5.916611	1.505105	-0.324351
5	6	0	-4.685380	-0.281780	-0.330942
6	6	0	-5.942509	-2.384350	-0.431646
7	1	0	-5.984830	-3.469544	-0.449889
8	6	0	-4.726429	-1.703989	-0.382725
9	1	0	-3.801119	-2.274329	-0.373494
10	6	0	-3.455098	0.481353	-0.281543
11	1	0	-3.553658	1.566756	-0.246602
12	6	0	-2.165406	0.000869	-0.281603
13	1	0	-1.958128	-1.065527	-0.313828
14	6	0	-1.011447	0.864351	-0.247126
15	8	0	-1.223920	2.194280	-0.213102
16	6	0	0.303798	0.355434	-0.254623
17	1	0	0.448583	-0.715957	-0.282113
18	6	0	1.413724	1.227991	-0.233085
19	8	0	1.212956	2.560422	-0.200295
20	6	0	2.805449	0.836577	-0.248714
21	1	0	3.495353	1.675989	-0.235219
22	6	0	3.266462	-0.459145	-0.281285
23	1	0	2.527582	-1.262270	-0.288161
24	6	0	4.641769	-0.912435	-0.313493
25	6	0	5.761752	-0.026369	-0.334845
26	6	0	4.901845	-2.309937	-0.343906
27	1	0	5.596746	1.046665	-0.328315
28	1	0	4.063143	-3.004570	-0.331941
29	6	0	7.065573	-0.516018	-0.381866
30	6	0	6.207182	-2.806372	-0.374157
31	1	0	6.409682	-3.873121	-0.375481
32	6	0	7.324353	-1.933931	-0.377123
33	8	0	8.206568	0.272143	-0.469867
34	6	0	8.164701	1.635769	0.035699
35	1	0	7.578312	2.289269	-0.627935
36	1	0	7.751134	1.658386	1.052111
37	1	0	9.205074	1.964217	0.058742
38	8	0	8.560065	-2.457114	-0.378985
39	1	0	9.418451	-1.853986	-0.184243
40	8	0	-8.392107	0.363378	-0.511431
41	6	0	-8.585227	1.649502	0.144184
42	1	0	-8.243725	1.605538	1.185688
43	1	0	-8.066045	2.455813	-0.396194
44	1	0	-9.662606	1.822921	0.124254
45	8	0	-8.320924	-2.408956	-0.453240
46	1	0	-9.256613	-1.953959	-0.244781
47	5	0	-0.135492	3.227627	-0.185091
48	9	0	-0.251840	4.057256	-1.337146
49	9	0	-0.255795	3.999852	1.004731
50	7	0	10.959415	-0.489283	0.996780
51	8	0	10.755336	-1.336809	-0.018257
52	8	0	12.058933	0.189893	1.022764
53	8	0	10.052096	-0.375977	1.919984
54	7	0	-11.003137	-0.906235	1.004407
55	8	0	-10.674315	-1.666778	-0.044395
56	8	0	-12.217155	-0.471129	1.098265
57	8	0	-10.097136	-0.627548	1.894900

Optimized geometric parameters for **1e- NO_3^-** in B3LYP/SDD (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.151720	-0.102758	-0.273418
2	6	0	-5.929967	0.573408	-0.210792
3	6	0	-7.176130	-1.523660	-0.421884
4	1	0	-5.909541	1.653086	-0.097038
5	6	0	-4.693054	-0.130146	-0.295152
6	6	0	-5.949445	-2.220154	-0.509092
7	1	0	-5.985713	-3.299343	-0.623282
8	6	0	-4.728727	-1.543166	-0.447775
9	1	0	-3.807483	-2.112899	-0.517563
10	6	0	-3.459719	0.633160	-0.221055
11	1	0	-3.566906	1.711866	-0.110157
12	6	0	-2.176304	0.143209	-0.273597
13	1	0	-1.976363	-0.918491	-0.380414
14	6	0	-1.015952	0.990177	-0.187384
15	8	0	-1.219402	2.327375	-0.059971
16	6	0	0.293331	0.478444	-0.232136
17	1	0	0.428753	-0.588870	-0.335152
18	6	0	1.410186	1.336319	-0.148991
19	8	0	1.211390	2.674472	-0.018319
20	6	0	2.796733	0.948546	-0.188467
21	1	0	3.493180	1.779210	-0.116332
22	6	0	3.246299	-0.347172	-0.299423
23	1	0	2.510054	-1.147826	-0.363089
24	6	0	4.625650	-0.794032	-0.338685
25	6	0	5.737853	0.098479	-0.281615
26	6	0	4.881537	-2.187743	-0.438338
27	1	0	5.568572	1.166876	-0.212175
28	1	0	4.046760	-2.882553	-0.484267
29	6	0	7.043931	-0.389758	-0.319403
30	6	0	6.190959	-2.679044	-0.473516
31	1	0	6.389244	-3.743735	-0.545773
32	6	0	7.291331	-1.799548	-0.411754
33	8	0	8.195416	0.392882	-0.279106
34	6	0	8.057042	1.846078	-0.161912
35	1	0	7.520247	2.257891	-1.025534
36	1	0	7.536635	2.114521	0.765847
37	1	0	9.076996	2.232228	-0.140617
38	8	0	8.546626	-2.329044	-0.449078
39	1	0	9.362061	-1.720737	-0.334909
40	8	0	-8.408237	0.497969	-0.206180
41	6	0	-8.485715	1.949896	-0.034529
42	1	0	-8.006934	2.258622	0.903130
43	1	0	-8.019705	2.469061	-0.881340
44	1	0	-9.551527	2.179980	0.000035
45	8	0	-8.332460	-2.246614	-0.488642
46	1	0	-9.232028	-1.776767	-0.369090
47	5	0	-0.124363	3.315609	0.070017
48	9	0	-0.243218	4.299661	-0.972429
49	9	0	-0.240280	3.991469	1.336554
50	7	0	11.420312	-0.980916	0.851740
51	8	0	10.877807	-1.245767	-0.331343
52	8	0	12.626917	-0.506417	0.896292
53	8	0	10.734005	-1.203719	1.934032
54	7	0	-11.411309	-1.435214	0.798408
55	8	0	-10.812990	-1.538226	-0.382747
56	8	0	-12.681785	-1.174497	0.838457
57	8	0	-10.714129	-1.598492	1.884479

Optimized geometric parameters for **1e- NO_3^-** in B3LYP/6-311++G** (solvent phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.081872	-0.141650	-0.212097
2	6	0	-5.870680	0.533187	-0.172656
3	6	0	-7.094304	-1.556010	-0.269397
4	1	0	-5.855845	1.614499	-0.130518
5	6	0	-4.639947	-0.162262	-0.185433
6	6	0	-5.876891	-2.245329	-0.283311
7	1	0	-5.904956	-3.327745	-0.327967
8	6	0	-4.669566	-1.567451	-0.242007
9	1	0	-3.748694	-2.136660	-0.256545
10	6	0	-3.416004	0.609204	-0.141970
11	1	0	-3.541297	1.688061	-0.121696
12	6	0	-2.142408	0.138956	-0.122380
13	1	0	-1.930204	-0.923137	-0.133597
14	6	0	-0.992001	1.002913	-0.086782
15	8	0	-1.199573	2.305233	-0.101305
16	6	0	0.301974	0.484393	-0.060475
17	1	0	0.434648	-0.585861	-0.048681
18	6	0	1.406283	1.341652	-0.105905
19	8	0	1.227996	2.648386	-0.113908
20	6	0	2.785743	0.933903	-0.165073
21	1	0	3.487723	1.759846	-0.182734
22	6	0	3.218889	-0.353555	-0.192659
23	1	0	2.479029	-1.148773	-0.179195
24	6	0	4.586138	-0.819228	-0.237568
25	6	0	5.699810	0.053776	-0.257149
26	6	0	4.824154	-2.204604	-0.262199
27	1	0	5.543663	1.122988	-0.241416
28	1	0	3.984951	-2.890633	-0.248381
29	6	0	6.990900	-0.441360	-0.296724
30	6	0	6.117299	-2.706524	-0.300891
31	1	0	6.301341	-3.774062	-0.317124
32	6	0	7.215362	-1.845649	-0.315923
33	8	0	8.122663	0.311767	-0.323053
34	6	0	8.000384	1.735890	-0.290449
35	1	0	7.447747	2.101700	-1.160416
36	1	0	7.506313	2.065243	0.627932
37	1	0	9.017606	2.120191	-0.316192
38	8	0	8.446579	-2.375863	-0.352789
39	1	0	9.194532	-1.725343	-0.309919
40	8	0	-8.311628	0.443110	-0.203682
41	6	0	-8.392907	1.868386	-0.132677
42	1	0	-7.934280	2.242339	0.787142
43	1	0	-7.915041	2.333100	-0.999805
44	1	0	-9.454948	2.103640	-0.132409
45	8	0	-8.231494	-2.270556	-0.313121
46	1	0	-9.068064	-1.740383	-0.293313
47	5	0	-0.101577	3.278011	0.071608
48	9	0	-0.247140	4.294946	-0.876431
49	9	0	-0.165859	3.818190	1.367957
50	7	0	11.446074	-0.852093	0.651634
51	8	0	10.867123	-1.223918	-0.414824
52	8	0	12.574422	-0.318173	0.581720
53	8	0	10.883742	-1.025594	1.756051
54	7	0	-11.514072	-1.296661	0.540748
55	8	0	-10.803534	-1.495686	-0.491425
56	8	0	-12.713093	-0.968194	0.405738
57	8	0	-11.008888	-1.432744	1.677942