Electronic Supplementary Information

An efficient implementation of spin-orbit coupling within the framework of semiempirical orthogonalization-corrected method for ultrafast intersystem crossing dynamics

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Molecular Geometry Structures

Cartesian coordinates in Angstrom

Formaldehyde

C	-0.132229	-0.000002	0.000010
O	1.064400	0.000002	-0.000012
H	-0.717794	0.939142	0.000000
H	-0.717798	-0.939142	0.000039

Acetone

C	-0.166195	0.001194	-0.173304
O	0.995476	0.002610	-0.496361
C	-0.968665	1.278406	-0.070441
H	-0.314973	2.141560	-0.175067
H	-1.722697	1.297114	-0.861767
H	-1.501870	1.323562	0.881793
C	-0.902277	-1.278207	0.154427
H	-1.095277	-1.316243	1.230069
H	-1.871297	-1.310577	-0.347823
H	-0.301731	-2.139413	-0.130635

Acrolein

C	-0.531880	-2.174920	0.633970
H	-0.020600	-3.134960	0.633970
H	-1.616080	-2.211970	0.633970
C	0.141290	-1.022970	0.633970

H	-0.346570	-0.046800	0.633970
C	1.622460	-1.006920	0.633970
H	2.155600	-2.011370	0.633970
O	2.214650	0.062810	0.633970

Formamide

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.225060
N	1.119392	0.000000	-0.775069
H	-0.927427	0.000000	-0.600301
H	1.070498	0.000000	-1.782390
H	2.024514	0.000000	-0.325050

Acetamide

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.229432
N	1.158961	0.000000	-0.727714
C	-1.267035	0.000000	-0.831605
H	1.173203	0.000000	-1.735754
H	2.035830	0.000000	-0.226200
H	-2.121178	0.000000	-0.156088
H	-1.310640	0.885499	-1.472734
H	-1.310640	-0.885499	-1.472734

Propanamide

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.230366
N	1.159094	0.000000	-0.726405
C	-1.272720	0.000000	-0.833211
C	-2.523363	0.000000	0.033790
H	1.171881	0.000000	-1.734644
H	2.036497	0.000000	-0.225525
H	-1.256730	0.877192	-1.492360
H	-1.256730	-0.877192	-1.492360
H	-3.420921	0.000000	-0.590418
H	-2.544300	-0.880205	0.678537
H	-2.544300	0.880205	0.678537

Thymine

C	-2.909875	-0.629050	-0.750426
C	-0.969207	0.789501	-0.288958
C	-1.853272	1.844318	0.067623
C	-3.262872	1.547385	0.254145
H	-3.983226	2.239771	0.660440
O	-3.385348	-1.615949	-1.278475

O	0.248383	0.881498	-0.508213
C	-1.400473	3.243296	0.147397
H	-1.641309	3.662743	1.134181
H	-0.331135	3.324808	-0.036402
H	-1.941543	3.870633	-0.574804
N	-1.583501	-0.490619	-0.420219
H	-0.982147	-1.215500	-0.786819
N	-3.713370	0.446397	-0.387742
H	-4.702890	0.311532	-0.560634

2-Thiothymine

N	-1.812458	-0.393339	0.564053
C	-3.193236	-0.497647	0.446440
N	-3.844849	0.727222	0.400820
C	-3.182787	1.890877	0.147251
C	-1.838212	1.960323	0.056073
C	-1.069971	0.745890	0.326133
S	-3.900754	-1.711592	-0.613819
O	0.152551	0.704996	0.383914
C	-1.102378	3.229382	-0.235122
H	-3.812160	2.766764	0.047198
H	-0.389778	3.462163	0.559503
H	-0.533579	3.151194	-1.165183
H	-1.799275	4.062677	-0.331434
H	-4.844612	0.746269	0.519835
H	-1.281199	-1.231706	0.748732

4-Thiothymine

N	-1.849545	-0.436139	0.362328
C	-3.213053	-0.450129	0.523403
N	-3.827070	0.740518	0.284492
C	-3.150749	1.901485	-0.101755
C	-1.808952	1.903194	-0.257845
C	-1.110224	0.694914	-0.019118
O	-3.814395	-1.461620	0.856259
S	0.589846	0.528584	-0.157243
C	-1.058533	3.135119	-0.669847
H	-3.767423	2.772650	-0.261638
H	-0.316476	3.413561	0.083639
H	-0.530266	2.975915	-1.614157
H	-1.739102	3.976314	-0.801042
H	-4.827252	0.751073	0.393826
H	-1.391740	-1.316080	0.538097

2,4-Thiothymine

N	-1.849597	-0.439399	0.257464
C	-3.197739	-0.498714	0.178537
N	-3.814670	0.659732	-0.097117
C	-3.143553	1.873525	-0.293316
C	-1.797095	1.931963	-0.217287
C	-1.095406	0.734827	0.066154
S	-4.031552	-1.942734	0.416010
S	0.607536	0.618256	0.175149
C	-1.043647	3.210682	-0.420485
H	-3.770420	2.725984	-0.502749
H	-0.469950	3.468154	0.474247
H	-0.338645	3.119587	-1.251494
H	-1.724296	4.032763	-0.639190
H	-4.819327	0.632279	-0.157057
H	-1.386158	-1.308939	0.468901

psoralen00

O	-4.022976	0.983961	0.000000
C	-3.003331	0.354454	0.000000
O	-1.811019	1.055041	0.000000
C	-2.893000	-1.094271	0.000000
C	-1.697697	-1.707320	0.000000
C	-0.477245	-0.953034	0.000000
C	-0.595087	0.454056	0.000000
C	0.511143	1.287736	0.000000
C	0.785333	-1.547040	0.000000
C	1.909768	-0.737538	0.000000
C	1.737466	0.658321	0.000000
O	2.940243	1.278519	0.000000
C	3.333491	-0.942117	0.000000
C	3.882011	0.287390	0.000000
H	-3.829527	-1.635518	0.000000
H	-1.635709	-2.791427	0.000000
H	0.867762	-2.628465	0.000000
H	0.399029	2.363736	0.000000
H	3.867102	-1.879343	0.000000
H	4.904183	0.629340	0.000000

psoralen0S

O	-4.477112	0.621239	0.000000
C	-3.334935	0.233828	0.000000
C	-2.931630	-1.158396	0.000000
C	-1.664873	-1.610948	0.000000
C	-0.463569	-0.820333	0.000000
C	-0.513687	0.595613	0.000000

C	0.650336	1.358530	0.000000
C	0.775055	-1.471417	0.000000
C	1.942257	-0.727952	0.000000
C	1.843685	0.672996	0.000000
O	3.078216	1.230536	0.000000
C	3.352340	-1.008775	0.000000
C	3.964994	0.190491	0.000000
H	-3.762942	-1.855206	0.000000
H	-1.517347	-2.687597	0.000000
H	0.802631	-2.555813	0.000000
H	0.619675	2.441384	0.000000
H	3.835735	-1.972817	0.000000
H	5.004204	0.476804	0.000000
S	-2.031091	1.484315	0.000000

psoralenSO

O	-4.107347	0.881651	0.000000
C	-3.062861	0.294171	0.000000
O	-1.900266	1.040072	0.000000
C	-2.899047	-1.151174	0.000000
C	-1.682977	-1.720953	0.000000
C	-0.493379	-0.918241	0.000000
C	-0.662591	0.481833	0.000000
C	0.415133	1.345669	0.000000
C	0.791493	-1.450680	0.000000
C	1.898093	-0.609589	0.000000
C	1.686170	0.789992	0.000000
C	3.294341	-0.939253	0.000000
C	4.087971	0.150926	0.000000
H	-3.815972	-1.725048	0.000000
H	-1.579979	-2.801848	0.000000
H	0.920954	-2.528125	0.000000
H	0.243810	2.414823	0.000000
H	3.671532	-1.953684	0.000000
H	5.167591	0.183633	0.000000
S	3.199271	1.652304	0.000000

m-rNDI

C	1.99223	-2.35362	0.18070
C	0.84368	-1.40019	0.14158
C	1.10732	0.00192	0.07508
C	2.43559	0.49085	0.04622

C	3.58149	-0.45324	0.08473
C	-0.42997	-1.89918	0.16961
C	0.01200	0.89150	0.04042
C	-1.31818	0.39012	0.06947
C	-1.56140	-1.00198	0.13357
C	-2.43966	1.33558	0.02742
C	-0.87137	3.24236	-0.06694
C	0.26889	2.28845	-0.02570
C	1.55721	2.78779	-0.05485
C	2.62721	1.86668	-0.01713
H	1.74994	3.85641	-0.10541
H	-0.58711	-2.97677	0.22737
N	-2.16544	2.71139	-0.04062
N	3.28717	-1.82969	0.14977
O	-3.63085	0.96834	0.04592
O	-0.69630	4.46679	-0.12379
O	4.75814	-0.08284	0.06308
O	1.80942	-3.57654	0.23835
Br	3.87404	2.36564	-0.04506
N	-2.82703	-1.48847	0.18174
H	-3.59191	-0.80458	0.13731
C	-3.18356	-2.89607	0.13127
H	-2.48064	-3.50934	0.78998
C	-4.61069	-3.05032	0.65880
H	-4.89573	-4.11069	0.64522
H	-4.67116	-2.67564	1.68976
H	-5.31338	-2.48420	0.03100
C	-3.09330	-3.39270	-1.31668
H	-3.36896	-4.45447	-1.36559
H	-3.77693	-2.81424	-1.95257
H	-2.07017	-3.27144	-1.69960
C	-3.29060	3.62706	-0.08362
H	-3.92071	3.41773	-0.97433
H	-3.92184	3.50079	0.82168
H	-2.92863	4.66903	-0.13166
C	4.40845	-2.75188	0.18372
H	5.01064	-2.65669	-0.74500
H	5.06747	-2.52090	1.04681
H	4.04307	-3.78991	0.27287