

Supplementary Data

Solvatochromic, Spectral, and Geometrical Properties of Nifenazone: A DFT/TD-DFT and Experimental Study

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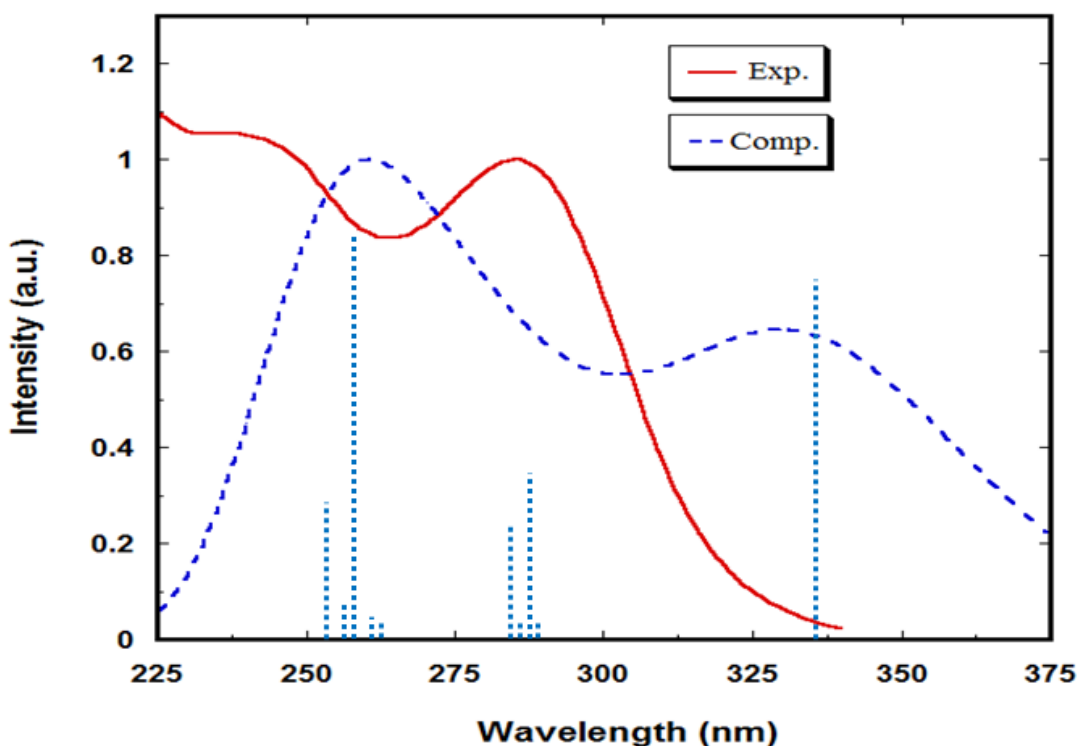


Figure S1: Experimental and simulated electronic absorption spectra of NIF in 1,4-dioxane obtained at the B3LYP/6-31G+(d) level of theory. The vertical lines in (A) represent the relative oscillator strength of each transition.

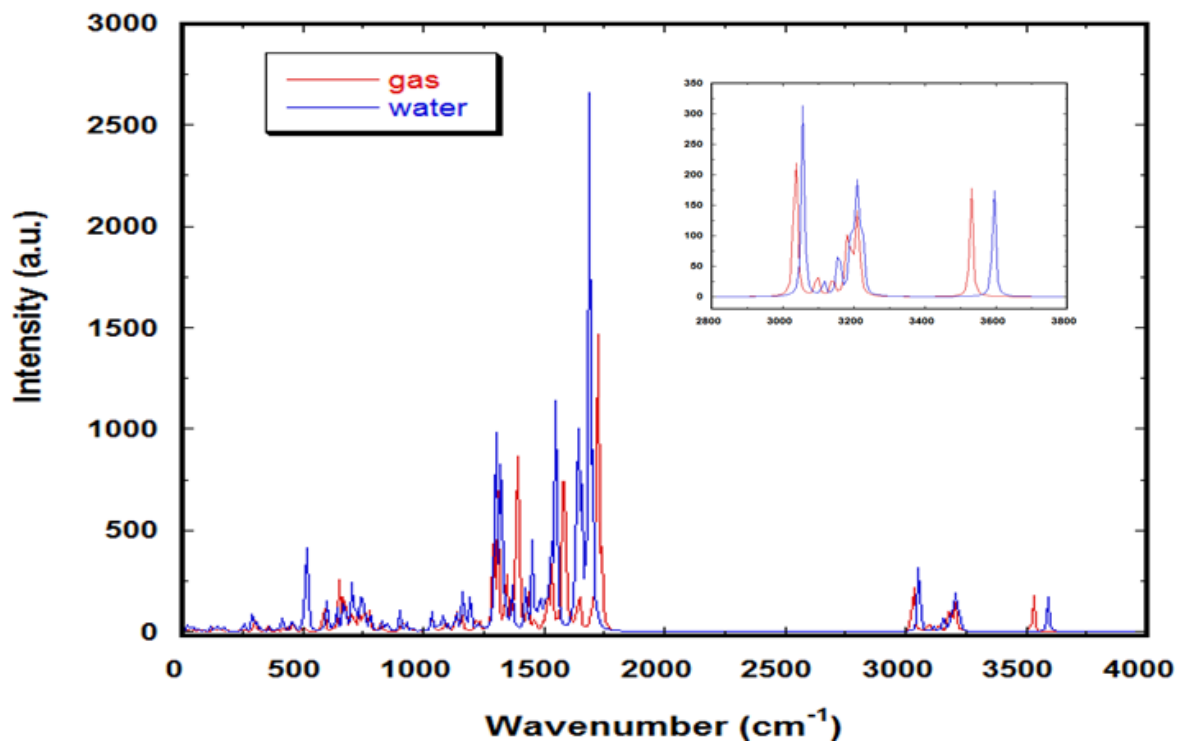


Figure S1: Simulated IR spectra of NIF in vacuo and in water obtained at the B3LYP/6-31G+(d) level of theory.

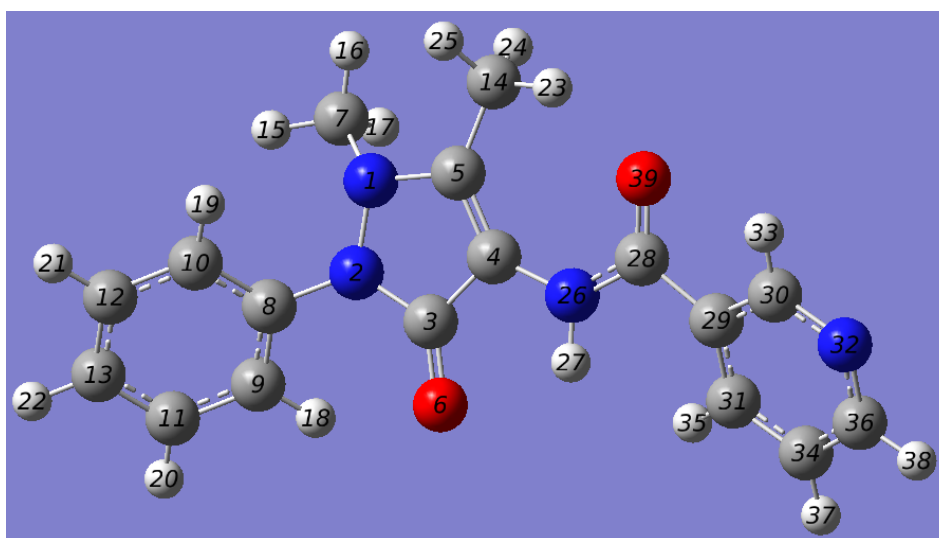


Figure S3. Numbering format for NIF generated by Gaussian G09. See Table S3 for simulated structural information

Table S1. Energy (eV) of selected frontier orbitals in different solvents obtained at the TD-DFT/CAM-B3LYP/6-31G+(d) theoretical level

Solvent	HOMO	LUMO	HOMO -1	HOMO -2	HOMO -3	HOMO -4	LUMO +1	LUMO +2	ΔE^*
Vacuu	-0.2731	-0.0210	-0.2913	-0.3195	-0.3267	-0.6321	0.0025	0.0070	0.2521
Water	-0.2808	-0.0195	-0.3010	-0.3211	-0.3311	-0.3396	0.0018	0.0053	0.2613
Methanol	-0.2802	-0.0194	-0.3002	-0.3208	-0.3308	-0.3394	0.0020	0.0054	0.2609
Ethanol	-0.2776	-0.0200	-0.2986	-0.3208	-0.3309	-0.3394	0.0019	0.0056	0.2576
1-Propanol	-0.2775	-0.0200	-0.2983	-0.3207	-0.3308	-0.3393	0.0019	0.0057	0.2574
2-Propanol	-0.2774	-0.0200	-0.2982	-0.3207	-0.3308	-0.3392	0.0019	0.0057	0.2574
Acetonitrile	-0.2779	-0.0201	-0.2990	-0.3210	-0.3310	-0.3397	0.0018	0.0056	0.2578
Ethylacetate	-0.2744	-0.0202	-0.2952	-0.3197	-0.3300	-0.3375	0.0024	0.0063	0.2542
Chloroform	-0.2743	-0.0202	-0.2942	-0.3194	-0.3297	-0.3371	0.0024	0.0060	0.2541
1,4-Dioxane	-0.2730	-0.0206	-0.2923	-0.3191	-0.3284	-0.3345	0.0028	0.0065	0.2524
n-Hexane	-0.2730	-0.0206	-0.2920	-0.3191	-0.3281	-0.3340	0.0028	0.0066	0.2524

$$*\Delta E = (E_{\text{LUMO}} - E_{\text{HOMO}})$$

Table S2. Energy (eV) of selected frontier orbitals in different solvents obtained at the TD-DFT/B3LYP/6-31G+(d) theoretical level

Solvent	HOMO	LUMO	HOMO -1	HOMO -2	HOMO -3	HOMO -4	LUMO +1	LUMO +2	ΔE^*
Vacuu	-0.2219	-0.0660	-0.2397	-0.2651	-0.2661	-0.2752	-0.0436	-0.0391	0.1559
water	-0.2275	-0.0651	-0.2477	-0.2672	-0.2732	-0.2786	-0.0452	-0.0398	0.1624
Methanol	-0.2271	-0.0650	-0.2469	-0.2668	-0.2728	-0.2784	-0.0450	-0.0397	0.1621
Isopropanol	-0.2246	-0.0655	-0.2452	-0.2668	-0.2726	-0.2789	-0.0450	-0.0394	0.1591
AcNT	-0.2251	-0.0656	-0.2459	-0.2672	-0.2730	-0.2792	-0.0452	-0.0394	0.1595
1,4-Dioxane	-0.2214	-0.0657	-0.2404	-0.2656	-0.2682	-0.2768	-0.0436	-0.0392	0.1557

$$*\Delta E = (E_{\text{LUMO}} - E_{\text{HOMO}})$$

Table S3. Mulliken atomic charges of non-H atoms of NIF

Atom	Vacuo	water	MeOH	EthOH	2-PropOH	1-PropOH	AcNT	Ethy.Ac.	Chloroform	Dioxane	n-Hexane
N3	-0.1603	-0.1435	-0.0704	-0.0943	-0.1121	-0.0786	-0.0886	-0.0934	-0.1417	-0.0664	-0.0906
N4	0.1684	0.1942	0.2977	0.3129	0.2114	0.2762	0.0145	0.3058	0.1844	0.2804	0.2951
C9	0.3838	0.2922	0.8890	0.7891	0.4213	1.0924	0.4838	0.7842	0.2729	0.8787	0.7734
C7	0.4299	0.8307	-0.3772	0.0438	0.6152	-1.3443	-0.1458	0.0543	0.8535	-0.3613	0.0736
C8	0.4595	0.2058	0.5572	0.2757	0.3457	1.1897	0.3795	0.2689	0.1961	0.5449	0.2551
O2	-0.5600	-0.6210	-0.5978	-0.6008	-0.6331	-0.6165	-0.6122	-0.5790	-0.5969	-0.5332	-0.5340
C11	-0.4062	-0.3921	-0.4056	-0.4194	-0.3998	-0.3704	-0.2031	-0.4151	-0.3881	-0.3932	-0.4081
C12	-1.1135	-1.3969	-1.6444	-1.6271	-1.3487	-1.5306	-1.0752	-1.6300	-1.3995	-1.6639	-1.6460
C17	-0.5502	-0.3628	-0.0981	-0.1635	-0.2833	-0.0979	-0.1970	-0.1605	-0.3637	-0.0889	-0.1506
C13	0.7907	1.0351	0.9652	1.0082	0.9323	0.9516	0.6580	1.0037	1.0314	0.9560	0.9960
C16	-0.2510	-0.3744	-0.3086	-0.3089	-0.3940	-0.3408	-0.3148	-0.3040	-0.3645	-0.2928	-0.2910
C14	-0.0552	-0.2782	-0.4101	-0.3881	-0.3054	-0.4343	-0.0097	-0.3752	-0.2586	-0.3754	-0.3524
C15	-0.1659	-0.1116	-0.0694	-0.0804	-0.1095	-0.0723	-0.0685	-0.0729	-0.1008	-0.0491	-0.0586
C10	-1.2841	-1.2248	-1.0065	-0.9817	-1.2331	-1.1029	-0.5473	-0.9819	-1.2229	-1.0074	-0.9821
N2	-0.6115	-0.5973	-0.5638	-0.5668	-0.5689	-0.4792	-0.3912	-0.5728	-0.6098	-0.5746	-0.5813
C6	0.2556	-0.1179	-0.7956	-0.7812	-0.3177	-0.7724	0.1623	-0.7988	-0.1418	-0.8440	-0.8315
C2	0.5086	0.8099	1.3189	1.2605	0.9352	1.3594	0.4099	1.2759	0.8241	1.3656	1.3034
C1	-0.1899	-0.2950	-0.2537	-0.2455	-0.2366	-0.2738	-0.0957	-0.2499	-0.2960	-0.2663	-0.2555
C3	-0.1878	-0.0896	-0.1196	-0.1348	-0.1548	0.0512	0.1070	-0.1488	-0.1075	-0.1595	-0.1773
N1	-0.1678	-0.2398	-0.2320	-0.2317	-0.2402	-0.2306	-0.2606	-0.2155	-0.2153	-0.1869	-0.1822
C4	-0.0736	-0.0243	-0.0493	-0.0169	-0.0123	-0.1656	-0.1271	-0.0112	-0.0160	-0.0325	0.0026
C5	-0.3245	-0.3404	-0.3345	-0.3380	-0.3445	-0.3154	-0.2513	-0.3378	-0.3401	-0.3349	-0.3384
O1	-0.5699	-0.6149	-0.5451	-0.5533	-0.6254	-0.5267	-0.6090	-0.5365	-0.5936	-0.4974	-0.5038

Table S4. Structural parameters of NIF in different solvents obtained at the DFT/B3LYP/6-31G+(d) theoretical level. Items' numbers correspond to atoms as displayed in Fig. S3.

Item	Vacuo	water	MeOH	EthOH	2-PropOH	1-PropOH	AcNT	Eth.Ac.	Chloroform	Dioxane	n-Hexane
<i>Bond Length (Å)</i>											
R(1,2)	1.4138	1.4106	1.4110	1.4111	1.4113	1.4112	1.4109	1.4121	1.4123	1.4128	1.4131
R(1,5)	1.4091	1.3764	1.3773	1.3800	1.3805	1.3804	1.3793	1.3880	1.3921	1.4016	1.4030
R(1,7)	1.4727	1.4676	1.4677	1.4679	1.4679	1.4680	1.4678	1.4688	1.4705	1.4722	1.4724
R(2,3)	1.3937	1.4048	1.4053	1.4037	1.4039	1.4037	1.4035	1.4017	1.3998	1.3951	1.3949
R(2,8)	1.4222	1.4275	1.4274	1.4272	1.4271	1.4272	1.4273	1.4261	1.4254	1.4237	1.4233
R(3,4)	1.4585	1.4463	1.4466	1.4464	1.4466	1.4466	1.4462	1.4487	1.4503	1.4542	1.4550
R(3,6)	1.2330	1.2407	1.2401	1.2405	1.2402	1.2403	1.2409	1.2383	1.2377	1.2360	1.2354
R(4,5)	1.3658	1.3717	1.3712	1.3707	1.3705	1.3705	1.3710	1.3685	1.3679	1.3672	1.3668
R(4,26)	1.3994	1.4097	1.4094	1.4077	1.4075	1.4076	1.4078	1.4056	1.4047	1.4019	1.4014
R(5,14)	1.4954	1.4923	1.4923	1.4924	1.4925	1.4924	1.4924	1.4932	1.4938	1.4948	1.4949
R(7,15)	1.0912	1.0903	1.0903	1.0904	1.0904	1.0904	1.0903	1.0905	1.0906	1.0909	1.0910
R(7,16)	1.0908	1.0904	1.0904	1.0904	1.0904	1.0904	1.0904	1.0906	1.0905	1.0905	1.0905
R(7,17)	1.0993	1.0970	1.0971	1.0973	1.0973	1.0973	1.0972	1.0979	1.0980	1.0985	1.0987
R(8,9)	1.4012	1.3993	1.3993	1.3993	1.3993	1.3993	1.3993	1.3997	1.4001	1.4007	1.4008
R(8,10)	1.4015	1.4011	1.4011	1.4010	1.4010	1.4010	1.4010	1.4010	1.4012	1.4013	1.4013
R(9,11)	1.3955	1.3971	1.3971	1.3971	1.3971	1.3971	1.3971	1.3967	1.3966	1.3961	1.3960
R(9,18)	1.0836	1.0849	1.0848	1.0848	1.0848	1.0848	1.0849	1.0845	1.0843	1.0839	1.0838
R(10,12)	1.3964	1.3970	1.3970	1.3970	1.3970	1.3970	1.3970	1.3969	1.3967	1.3966	1.3965
R(10,19)	1.0853	1.0858	1.0858	1.0857	1.0857	1.0857	1.0858	1.0856	1.0855	1.0854	1.0854
R(11,13)	1.3982	1.3989	1.3988	1.3988	1.3988	1.3988	1.3989	1.3986	1.3986	1.3984	1.3984
R(11,20)	1.0868	1.0866	1.0866	1.0866	1.0866	1.0866	1.0866	1.0866	1.0867	1.0867	1.0867
R(12,13)	1.3974	1.3990	1.3990	1.3990	1.3989	1.3989	1.3990	1.3986	1.3984	1.3980	1.3979
R(12,21)	1.0870	1.0866	1.0866	1.0866	1.0866	1.0866	1.0866	1.0867	1.0867	1.0868	1.0869
R(13,22)	1.0866	1.0865	1.0865	1.0865	1.0865	1.0865	1.0865	1.0866	1.0866	1.0866	1.0866
R(14,23)	1.0899	1.0916	1.0915	1.0907	1.0907	1.0907	1.0908	1.0895	1.0894	1.0899	1.0899
R(14,24)	1.0989	1.0965	1.0965	1.0964	1.0964	1.0964	1.0964	1.0973	1.0978	1.0985	1.0986
R(14,25)	1.0960	1.0955	1.0956	1.0958	1.0959	1.0958	1.0958	1.0958	1.0955	1.0955	1.0955
R(26,27)	1.0175	1.0133	1.0133	1.0133	1.0133	1.0133	1.0132	1.0142	1.0147	1.0164	1.0166
R(26,28)	1.3726	1.3708	1.3715	1.3720	1.3724	1.3723	1.3716	1.3743	1.3736	1.3726	1.3727
R(28,29)	1.5009	1.5000	1.4999	1.4996	1.4996	1.4996	1.4996	1.4992	1.4992	1.4998	1.4999
R(28,39)	1.2303	1.2347	1.2342	1.2343	1.2341	1.2341	1.2345	1.2328	1.2329	1.2321	1.2318
R(29,30)	1.4052	1.4037	1.4037	1.4039	1.4039	1.4039	1.4039	1.4042	1.4042	1.4047	1.4048
R(29,31)	1.4009	1.4010	1.4009	1.4011	1.4011	1.4011	1.4012	1.4010	1.4010	1.4009	1.4009
R(30,32)	1.3365	1.3380	1.3380	1.3380	1.3379	1.3380	1.3380	1.3376	1.3375	1.3371	1.3370
R(30,33)	1.0865	1.0867	1.0867	1.0867	1.0867	1.0867	1.0867	1.0866	1.0866	1.0865	1.0865
R(31,34)	1.3941	1.3944	1.3944	1.3944	1.3944	1.3944	1.3944	1.3943	1.3943	1.3941	1.3941
R(31,35)	1.0871	1.0864	1.0864	1.0865	1.0865	1.0865	1.0865	1.0866	1.0867	1.0868	1.0869
R(32,36)	1.3408	1.3440	1.3439	1.3438	1.3438	1.3438	1.3439	1.3432	1.3431	1.3422	1.3420
R(34,36)	1.3967	1.3960	1.3960	1.3960	1.3960	1.3960	1.3960	1.3962	1.3963	1.3964	1.3965

R(34,37)	1.0861	1.0854	1.0855	1.0855	1.0855	1.0855	1.0854	1.0856	1.0857	1.0859	1.0859
R(36,38)	1.0884	1.0876	1.0877	1.0877	1.0877	1.0877	1.0877	1.0878	1.0878	1.0880	1.0881
Bond Angle (°)											
A(2,1,5)	106.98	107.23	107.21	107.17	107.16	107.16	107.18	107.07	107.05	107.01	107.00
A(2,1,7)	112.69	116.24	116.10	115.96	115.89	115.90	116.04	115.11	114.49	113.44	113.28
A(5,1,7)	117.52	121.77	121.62	121.40	121.32	121.32	121.50	120.29	119.56	118.44	118.24
A(1,2,3)	109.60	109.33	109.32	109.33	109.33	109.33	109.33	109.38	109.45	109.56	109.57
A(1,2,8)	119.73	119.46	119.39	119.43	119.39	119.40	119.46	119.45	119.41	119.67	119.68
A(3,2,8)	124.95	123.79	123.72	123.85	123.83	123.85	123.87	124.03	124.32	124.79	124.82
A(2,3,4)	105.38	104.56	104.56	104.65	104.65	104.65	104.64	104.82	104.93	105.22	105.24
A(2,3,6)	127.17	124.93	124.98	125.22	125.25	125.24	125.18	125.78	126.05	126.73	126.82
A(4,3,6)	127.42	130.49	130.44	130.12	130.09	130.09	130.16	129.39	129.00	128.04	127.92
A(3,4,5)	108.80	108.82	108.84	108.87	108.88	108.88	108.86	108.92	108.90	108.84	108.84
A(3,4,26)	114.76	123.37	123.24	122.45	122.36	122.38	122.55	120.44	119.36	116.53	116.23
A(5,4,26)	136.43	127.73	127.83	128.62	128.70	128.68	128.53	130.62	131.73	134.62	134.93
A(1,5,4)	108.91	109.37	109.38	109.27	109.28	109.27	109.27	109.15	109.10	108.94	108.94
A(1,5,14)	118.54	121.62	121.58	121.35	121.31	121.31	121.39	120.54	120.09	119.21	119.10
A(4,5,14)	132.51	129.00	129.03	129.36	129.39	129.40	129.33	130.26	130.75	131.79	131.90
A(1,7,15)	108.96	109.15	109.13	109.09	109.09	109.09	109.10	109.06	109.04	108.99	108.99
A(1,7,16)	108.52	108.19	108.21	108.20	108.21	108.20	108.19	108.24	108.36	108.49	108.50
A(1,7,17)	111.55	111.30	111.32	111.42	111.44	111.43	111.41	111.53	111.46	111.46	111.47
A(15,7,16)	108.55	108.46	108.45	108.41	108.41	108.41	108.41	108.42	108.45	108.50	108.51
A(15,7,17)	109.37	109.67	109.65	109.65	109.63	109.64	109.66	109.55	109.54	109.48	109.45
A(16,7,17)	109.83	110.01	110.01	110.00	110.00	110.00	110.00	109.98	109.93	109.87	109.86
A(2,8,9)	118.96	118.63	118.63	118.67	118.67	118.67	118.66	118.71	118.82	118.89	118.91
A(2,8,10)	120.71	120.85	120.86	120.82	120.83	120.82	120.82	120.83	120.74	120.70	120.70
A(9,8,10)	120.33	120.51	120.50	120.50	120.50	120.50	120.51	120.46	120.44	120.40	120.39
A(8,9,11)	119.42	119.55	119.54	119.53	119.52	119.52	119.53	119.51	119.49	119.45	119.44
A(8,9,18)	119.67	119.62	119.63	119.64	119.64	119.64	119.64	119.64	119.67	119.70	119.70
A(11,9,18)	120.91	120.83	120.83	120.84	120.83	120.83	120.84	120.85	120.84	120.85	120.86
A(8,10,12)	119.58	119.48	119.49	119.50	119.50	119.50	119.49	119.51	119.53	119.54	119.55
A(8,10,19)	119.66	119.86	119.85	119.82	119.82	119.82	119.83	119.78	119.76	119.72	119.71
A(12,10,19)	120.75	120.66	120.66	120.68	120.68	120.68	120.68	120.71	120.71	120.74	120.74
A(9,11,13)	120.67	120.33	120.34	120.36	120.37	120.37	120.35	120.43	120.47	120.56	120.58
A(9,11,20)	119.22	119.49	119.47	119.46	119.46	119.46	119.47	119.41	119.37	119.30	119.28
A(13,11,20)	120.11	120.18	120.18	120.17	120.17	120.17	120.18	120.16	120.15	120.14	120.13
A(10,12,13)	120.47	120.36	120.36	120.35	120.35	120.35	120.35	120.38	120.40	120.44	120.44
A(10,12,21)	119.34	119.46	119.45	119.45	119.45	119.45	119.46	119.42	119.40	119.37	119.37
A(13,12,21)	120.18	120.18	120.19	120.19	120.20	120.20	120.19	120.19	120.19	120.19	120.19
A(11,13,12)	119.52	119.77	119.76	119.75	119.74	119.74	119.76	119.69	119.66	119.60	119.58
A(11,13,22)	120.25	120.13	120.13	120.13	120.13	120.13	120.13	120.16	120.17	120.20	120.21
A(12,13,22)	120.23	120.10	120.11	120.12	120.12	120.12	120.12	120.15	120.17	120.20	120.21
A(5,14,23)	109.49	109.64	109.65	109.79	109.80	109.80	109.78	110.01	109.91	109.60	109.57
A(5,14,24)	111.15	111.24	111.24	111.20	111.20	111.19	111.20	110.94	110.93	110.99	111.02

A(5,14,25)	110.79	111.32	111.32	111.27	111.27	111.27	111.27	111.24	111.16	110.99	110.96
A(23,14,24)	108.56	108.11	108.13	108.25	108.26	108.26	108.23	108.57	108.77	108.77	108.75
A(23,14,25)	108.89	108.49	108.46	108.26	108.24	108.25	108.29	108.02	108.04	108.47	108.53
A(24,14,25)	107.91	107.93	107.94	107.97	107.97	107.97	107.96	107.96	107.94	107.94	107.94
A(4,26,27)	110.58	116.72	116.58	115.78	115.69	115.71	115.88	113.99	113.31	111.51	111.33
A(4,26,28)	129.29	123.78	123.77	124.35	124.34	124.34	124.35	125.12	126.00	127.99	128.18
A(27,26,28)	117.86	117.88	117.79	117.65	117.61	117.62	117.70	117.16	117.07	117.26	117.34
A(26,28,29)	115.25	115.78	115.72	115.69	115.67	115.68	115.70	115.46	115.34	115.27	115.25
A(26,28,39)	123.34	122.82	122.83	122.83	122.83	122.83	122.83	122.87	122.98	123.19	123.22
A(29,28,39)	121.41	121.40	121.45	121.48	121.49	121.49	121.46	121.66	121.67	121.54	121.53
A(28,29,30)	117.76	118.14	118.13	118.09	118.09	118.08	118.09	118.07	118.13	117.96	117.93
A(28,29,31)	124.55	124.01	124.02	124.09	124.09	124.10	124.09	124.13	124.05	124.29	124.32
A(30,29,31)	117.68	117.83	117.84	117.81	117.81	117.81	117.81	117.80	117.80	117.74	117.73
A(29,30,32)	123.92	123.82	123.82	123.84	123.84	123.84	123.84	123.83	123.82	123.87	123.87
A(29,30,33)	119.18	119.48	119.47	119.43	119.43	119.43	119.44	119.40	119.41	119.31	119.29
A(32,30,33)	116.90	116.69	116.70	116.73	116.73	116.73	116.72	116.77	116.77	116.82	116.83
A(29,31,34)	118.91	118.85	118.85	118.85	118.85	118.85	118.85	118.87	118.87	118.90	118.90
A(29,31,35)	121.26	121.25	121.23	121.30	121.28	121.29	121.31	121.20	121.16	121.21	121.21
A(34,31,35)	119.81	119.88	119.90	119.83	119.84	119.83	119.82	119.90	119.95	119.87	119.87
A(30,32,36)	117.45	117.47	117.47	117.47	117.48	117.48	117.47	117.48	117.48	117.47	117.47
A(31,34,36)	118.55	118.65	118.64	118.65	118.65	118.65	118.66	118.62	118.61	118.58	118.58
A(31,34,37)	121.00	121.00	121.00	120.99	120.99	120.99	120.98	121.01	121.02	121.00	121.01
A(36,34,37)	120.45	120.35	120.35	120.36	120.36	120.36	120.36	120.37	120.37	120.41	120.42
A(32,36,34)	123.50	123.37	123.38	123.37	123.37	123.37	123.37	123.40	123.41	123.44	123.45
A(32,36,38)	116.00	116.19	116.18	116.18	116.17	116.18	116.18	116.14	116.12	116.07	116.06
A(34,36,38)	120.51	120.44	120.44	120.45	120.45	120.45	120.45	120.46	120.47	120.49	120.49

Dihedral angle (°)

D(5,1,2,3)	5.74	8.66	8.66	8.81	8.78	8.78	8.85	8.37	7.70	6.61	6.44
D(5,1,2,8)	160.36	159.71	159.43	159.94	159.80	159.86	160.08	160.01	160.01	160.67	160.63
D(7,1,2,3)	136.38	148.78	148.38	148.01	147.76	147.78	148.29	144.97	142.66	139.10	138.53
D(7,1,2,8)	-68.99	-60.16	-60.85	-60.86	-61.22	-61.14	-60.48	-63.39	-65.03	-66.84	-67.28
D(2,1,5,4)	-5.44	-6.91	-6.96	-7.38	-7.38	-7.37	-7.36	-7.48	-6.97	-6.24	-6.10
D(2,1,5,14)	172.51	171.99	171.91	171.25	171.21	171.22	171.29	170.25	170.64	171.30	171.50
D(7,1,5,4)	-133.32	-144.34	-143.97	-143.88	-143.66	-143.67	-144.12	-141.38	-139.22	-135.94	-135.40
D(7,1,5,14)	44.64	34.56	34.90	34.75	34.94	34.92	34.54	36.35	38.40	41.60	42.20
D(2,1,7,15)	57.34	54.60	54.64	54.45	54.43	54.45	54.46	55.18	55.95	57.12	57.25
D(2,1,7,16)	175.37	172.43	172.46	172.20	172.18	172.20	172.22	172.94	173.81	175.08	175.23
D(2,1,7,17)	-63.51	-66.60	-66.53	-66.75	-66.76	-66.74	-66.75	-65.94	-65.10	-63.83	-63.67
D(5,1,7,15)	-177.57	-171.48	-171.85	-172.56	-172.80	-172.76	-172.30	-174.34	-175.10	-176.20	-176.42
D(5,1,7,16)	-59.55	-53.65	-54.03	-54.81	-55.05	-55.01	-54.55	-56.58	-57.24	-58.23	-58.44
D(5,1,7,17)	61.58	67.32	66.98	66.24	66.02	66.05	66.49	64.54	63.85	62.86	62.66
D(1,2,3,4)	-3.78	-6.84	-6.80	-6.65	-6.60	-6.60	-6.71	-5.90	-5.34	-4.37	-4.23
D(1,2,3,6)	174.50	171.73	171.82	172.08	172.15	172.13	171.99	172.97	173.44	174.18	174.28
D(8,2,3,4)	-156.78	-156.38	-156.04	-156.22	-156.05	-156.13	-156.40	-155.95	-156.00	-156.80	-156.80

D(8,2,3,6)	21.50	22.19	22.58	22.50	22.69	22.61	22.30	22.92	22.79	21.75	21.72
D(1,2,8,9)	156.53	144.50	145.37	145.31	145.76	145.65	144.81	148.47	150.37	153.14	153.84
D(1,2,8,10)	-23.76	-36.48	-35.61	-35.51	-35.05	-35.16	-36.03	-32.18	-30.10	-27.20	-26.50
D(3,2,8,9)	-52.97	-68.83	-68.28	-67.96	-67.63	-67.67	-68.35	-64.27	-61.66	-56.98	-56.13
D(3,2,8,10)	126.74	110.20	110.75	111.21	111.55	111.51	110.80	115.09	117.87	122.68	123.53
D(2,3,4,5)	0.37	2.61	2.54	2.12	2.06	2.08	2.19	1.28	1.03	0.48	0.43
D(2,3,4,26)	179.62	179.60	179.44	179.61	179.52	179.54	179.70	179.72	-179.72	-179.71	-179.81
D(6,3,4,5)	-177.90	-175.85	-175.97	-176.52	-176.60	-176.57	-176.42	-177.53	-177.71	-178.04	-178.06
D(6,3,4,26)	1.35	1.14	0.93	0.97	0.86	0.89	1.10	0.91	1.54	1.77	1.69
D(3,4,5,1)	3.17	2.68	2.76	3.29	3.33	3.31	3.23	3.88	3.73	3.60	3.55
D(3,4,5,14)	-174.40	-176.11	-176.00	-175.19	-175.12	-175.14	-175.28	-173.55	-173.55	-173.52	-173.64
D(26,4,5,1)	-175.84	-174.14	-173.97	-174.00	-173.92	-173.95	-174.09	-174.34	-175.40	-176.16	-176.15
D(26,4,5,14)	6.59	7.07	7.28	7.52	7.63	7.61	7.40	8.22	7.32	6.72	6.67
D(3,4,26,27)	6.00	57.13	55.00	44.14	43.18	43.42	45.31	29.10	24.39	12.53	11.33
D(3,4,26,28)	-156.21	-108.01	-109.08	-118.47	-118.91	-118.78	-117.89	-128.41	-133.36	-146.32	-147.77
D(5,4,26,27)	-175.04	-126.48	-128.71	-138.90	-139.91	-139.65	-137.70	-152.85	-156.56	-167.72	-168.99
D(5,4,26,28)	22.75	68.38	67.21	58.49	58.01	58.14	59.10	49.64	45.69	33.43	31.91
D(1,5,14,23)	160.92	175.73	175.98	178.34	178.34	178.17	178.30	173.19	165.93	160.32	160.09
D(1,5,14,24)	-79.16	-64.74	-64.46	-61.89	-61.87	-62.05	-61.95	-66.66	-73.74	-79.52	-79.78
D(1,5,14,25)	40.80	55.68	55.97	58.51	58.54	58.35	58.44	53.54	46.37	40.52	40.26
D(4,5,14,23)	-21.70	-5.60	-5.39	-3.34	-3.37	-3.55	-3.34	-9.62	-17.04	-22.80	-22.96
D(4,5,14,24)	98.22	113.93	114.17	116.43	116.42	116.23	116.41	110.53	103.28	97.36	97.17
D(4,5,14,25)	-141.82	-125.66	-125.41	-123.17	-123.18	-123.37	-123.20	-129.28	-136.61	-142.60	-142.79
D(2,8,9,11)	179.46	178.41	178.42	178.59	178.62	178.62	178.56	178.88	179.05	179.22	179.26
D(2,8,9,18)	0.42	-1.60	-1.56	-1.39	-1.34	-1.35	-1.44	-0.90	-0.62	-0.17	-0.07
D(10,8,9,11)	-0.25	-0.62	-0.62	-0.58	-0.57	-0.57	-0.60	-0.48	-0.49	-0.43	-0.40
D(10,8,9,18)	-179.29	179.37	179.41	179.44	179.47	179.46	179.40	179.74	179.84	-179.83	-179.73
D(2,8,10,12)	179.61	-179.49	-179.49	-179.67	-179.69	-179.69	-179.63	-179.92	179.92	179.78	179.75
D(2,8,10,19)	-1.32	0.46	0.39	0.21	0.16	0.17	0.28	-0.24	-0.50	-0.89	-0.98
D(9,8,10,12)	-0.68	-0.48	-0.49	-0.51	-0.52	-0.52	-0.49	-0.57	-0.55	-0.57	-0.59
D(9,8,10,19)	178.38	179.46	179.40	179.37	179.33	179.34	179.42	179.11	179.03	178.76	178.68
D(8,9,11,13)	0.95	1.13	1.13	1.12	1.11	1.11	1.12	1.07	1.08	1.04	1.02
D(8,9,11,20)	-179.52	-179.67	-179.64	-179.67	-179.66	-179.67	-179.68	-179.59	-179.56	-179.53	-179.52
D(18,9,11,13)	179.97	-178.86	-178.89	-178.90	-178.92	-178.92	-178.87	-179.15	-179.26	-179.57	-179.66
D(18,9,11,20)	-0.49	0.35	0.33	0.31	0.30	0.30	0.32	0.19	0.11	-0.14	-0.20
D(8,10,12,13)	0.93	1.08	1.08	1.07	1.07	1.07	1.07	1.05	1.01	0.98	0.97
D(8,10,12,21)	-179.94	-179.60	-179.63	-179.64	-179.65	-179.64	-179.62	-179.75	-179.80	-179.89	-179.90
D(19,10,12,13)	-178.12	-178.86	-178.80	-178.81	-178.77	-178.78	-178.84	-178.63	-178.57	-178.34	-178.29
D(19,10,12,21)	1.01	0.46	0.49	0.49	0.51	0.50	0.47	0.57	0.62	0.79	0.84
D(9,11,13,12)	-0.70	-0.54	-0.54	-0.56	-0.57	-0.57	-0.55	-0.60	-0.63	-0.63	-0.65
D(9,11,13,22)	179.47	179.33	179.34	179.33	179.34	179.34	179.32	179.41	179.42	179.47	179.47
D(20,11,13,12)	179.77	-179.74	-179.76	-179.77	-179.79	-179.78	-179.74	-179.94	-179.98	179.94	179.90
D(20,11,13,22)	-0.06	0.13	0.12	0.13	0.12	0.12	0.13	0.07	0.06	0.04	0.02
D(10,12,13,11)	-0.25	-0.58	-0.57	-0.54	-0.53	-0.53	-0.55	-0.46	-0.43	-0.38	-0.36

D(10,12,13,22)	179.58	179.56	179.54	179.57	179.56	179.56	179.57	179.52	179.52	179.52	179.52
D(21,12,13,11)	-179.37	-179.89	-179.86	-179.83	-179.81	-179.81	-179.86	-179.66	-179.61	-179.51	-179.48
D(21,12,13,22)	0.46	0.24	0.26	0.28	0.28	0.28	0.27	0.33	0.34	0.39	0.40
D(4,26,28,29)	177.13	177.24	176.73	176.63	176.39	176.44	176.89	174.28	175.13	175.85	175.99
D(4,26,28,39)	-2.89	-3.51	-4.07	-4.28	-4.56	-4.50	-3.97	-6.65	-5.79	-4.56	-4.37
D(27,26,28,29)	16.01	12.26	12.83	14.32	14.62	14.54	13.97	17.41	18.11	18.04	17.95
D(27,26,28,39)	-164.01	-168.49	-167.97	-166.59	-166.33	-166.39	-166.90	-163.52	-162.81	-162.38	-162.40
D(26,28,29,30)	-157.57	-152.11	-152.00	-152.85	-152.94	-152.97	-152.72	-153.79	-153.30	-155.48	-155.64
D(26,28,29,31)	23.76	29.15	29.22	28.50	28.43	28.38	28.60	27.39	28.08	25.82	25.68
D(39,28,29,30)	22.45	28.63	28.78	28.05	28.00	27.95	28.13	27.12	27.61	24.93	24.72
D(39,28,29,31)	-156.21	-150.11	-150.00	-150.60	-150.64	-150.69	-150.55	-151.70	-151.01	-153.77	-153.97
D(28,29,30,32)	-179.68	-179.57	-179.64	-179.52	-179.50	-179.51	-179.55	-179.80	-179.61	-179.65	-179.65
D(28,29,30,33)	0.39	0.86	0.82	0.86	0.86	0.86	0.84	0.56	0.74	0.59	0.57
D(31,29,30,32)	-0.92	-0.76	-0.78	-0.78	-0.78	-0.78	-0.78	-0.90	-0.91	-0.86	-0.88
D(31,29,30,33)	179.15	179.68	179.67	179.60	179.58	179.59	179.60	179.46	179.44	179.38	179.34
D(28,29,31,34)	179.25	179.05	179.12	179.02	179.00	179.01	179.05	179.32	179.12	179.20	179.21
D(28,29,31,35)	0.92	0.79	0.87	0.78	0.76	0.78	0.82	1.03	0.85	0.90	0.90
D(30,29,31,34)	0.58	0.31	0.33	0.36	0.36	0.36	0.36	0.49	0.50	0.50	0.52
D(30,29,31,35)	-177.74	-177.95	-177.91	-177.88	-177.88	-177.87	-177.87	-177.79	-177.77	-177.80	-177.79
D(29,30,32,36)	0.60	0.67	0.67	0.65	0.65	0.65	0.65	0.66	0.68	0.61	0.61
D(33,30,32,36)	-179.47	-179.76	-179.78	-179.71	-179.70	-179.71	-179.73	-179.69	-179.67	-179.63	-179.60
D(29,31,34,36)	0.00	0.17	0.17	0.12	0.12	0.12	0.12	0.08	0.07	0.03	0.03
D(29,31,34,37)	-179.49	-179.31	-179.33	-179.34	-179.34	-179.34	-179.34	-179.38	-179.38	-179.43	-179.44
D(35,31,34,36)	178.35	178.45	178.44	178.38	178.38	178.38	178.38	178.39	178.35	178.36	178.36
D(35,31,34,37)	-1.15	-1.04	-1.05	-1.08	-1.07	-1.08	-1.08	-1.08	-1.10	-1.11	-1.11
D(30,32,36,34)	0.05	-0.13	-0.11	-0.12	-0.12	-0.11	-0.11	-0.02	-0.05	0.00	0.00
D(30,32,36,38)	179.73	179.56	179.57	179.58	179.58	179.58	179.58	179.62	179.61	179.66	179.67
D(31,34,36,32)	-0.34	-0.28	-0.30	-0.26	-0.26	-0.26	-0.27	-0.34	-0.32	-0.31	-0.32
D(31,34,36,38)	-180.00	-179.96	-179.97	-179.94	-179.94	-179.94	-179.95	-179.97	-179.96	-179.95	-179.97
D(37,34,36,32)	179.15	179.21	179.20	179.20	179.20	179.20	179.20	179.13	179.13	179.16	179.16
D(37,34,36,38)	-0.50	-0.47	-0.47	-0.48	-0.48	-0.48	-0.48	-0.50	-0.50	-0.49	-0.49