Supporting Information

Antiaromaticity Gain Increases the Potential for *n*-Type Charge Transport in Hydrogen-Bonded π-Conjugated Cores

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Table S1: Computed orbital energies and HOMO-LUMO gap (in eV) for DPP monomer, hydrogen-bonded trimer, and tautomer at TD-ωB97X-D/6-311+G(d,p).

DPP	Monomer	Hydrogen-bonded trimer	Tautomer
HOMO	–7.38	–7.48	–7.54
LUMO	–4.52	–4.64	–4.81
HOMO-LUMO Gap	2.89	2.84	2.73

Table S2: Computed orbital energies and HOMO-LUMO gap (in eV) for NDP monomer, hydrogen-bonded trimer, and tautomer at TD-ωB97X-D/6-311+G(d,p).

NDP	Monomer	Hydrogen-bonded trimer	Tautomer
HOMO	–6.94	–7.01	–7.14
LUMO	–4.82	–5.01	–5.05
HOMO-LUMO Gap	2.12	2.00	2.09

Table S3: Computed orbital energies and HOMO-LUMO gap (in eV) for indigo monomer, hydrogen-bonded trimer, and tautomer at TD-ωB97X-D/6-311+G(d,p).

Indigo	Monomer	Hydrogen-bonded trimer	Tautomer
HOMO	–7.41	–7.38	–7.15
LUMO	–4.86	–5.07	–5.75
HOMO-LUMO Gap	2.55	2.31	1.40

Table S4: Computed orbital energies and HOMO-LUMO gap (in eV) for isoindigo monomer, hydrogen-bonded trimer, and tautomer at TD-ωB97X-D/6-311+G(d,p).

Isoindigo	Monomer	Hydrogen-bonded trimer	Tautomer
HOMO	–7.90	–7.93	–8.27
LUMO	–4.93	–5.16	–5.48
HOMO-LUMO Gap	2.97	2.77	2.79

Table S5: Computed orbital energies and HOMO-LUMO gap (in eV) for tyrian purple monomer, hydrogen-bonded trimer, and tautomer at TD-ωB97X-D/6-311+G(d,p).

Tyrian purple	Monomer	Hydrogen-bonded trimer	Tautomer
HOMO	–7.76	–7.74	–7.43
LUMO	-5.17	–5.40	–6.02
HOMO-LUMO Gap	2.59	2.34	1.41

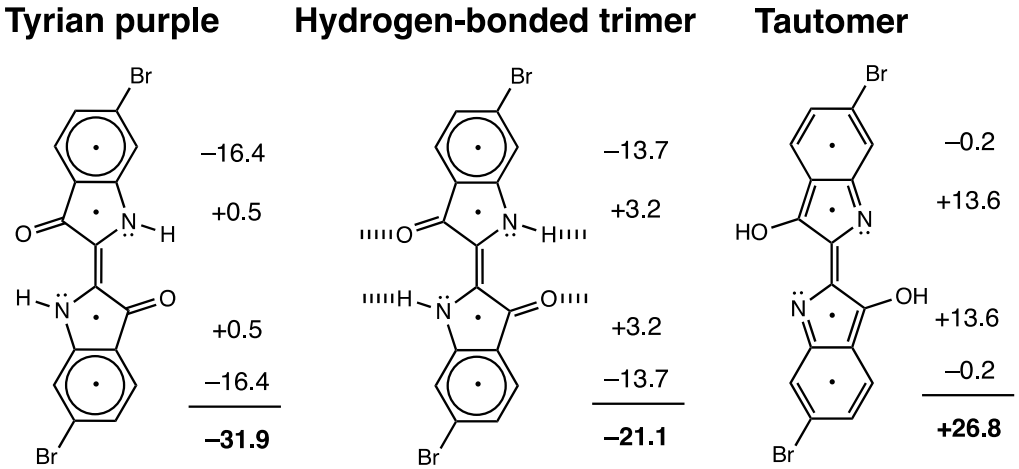

Figure S1: Computed NICS(1)$_{zz}$ (in ppm) for tyrian purple monomer, hydrogen-bonded trimer, and tautomer (NICS points were added at 1 Å above the center of each ring).

Optimized Cartesian coordinates at B3LYP-D3/6-311+G(d,p), in the gas-phase, for all monomers, hydrogen-boned trimers, and tautomers.

DPP System

Monomer

	X	Y	Z
C	3.31043	-1.22129	0.00000
N	4.08464	-0.03299	0.00000
C	3.31903	1.12634	0.00000
C	1.99691	0.71838	0.00000
C	0.63015	1.22460	0.00000
O	0.14377	2.34330	0.00000
N	-0.14406	0.03630	0.00000
H	-1.14995	0.08162	0.00000
C	0.62155	-1.12303	0.00000
C	1.94367	-0.71506	0.00000
H	5.09052	-0.07831	0.00000
O	3.79681	-2.33999	0.00000
C	3.91139	2.45463	0.00000
C	0.02919	-2.45132	0.00000
C	-1.36661	-2.63392	0.00000
C	-1.91576	-3.91022	0.00000
C	-1.08439	-5.03036	0.00000
C	0.85867	-3.58987	0.00000
C	0.30070	-4.86242	0.00000
H	-2.03924	-1.78421	0.00000
H	-2.99284	-4.03115	0.00000
H	-1.51381	-6.02568	0.00000
H	1.93559	-3.47157	0.00000
H	0.95279	-5.72821	0.00000
C	5.30719	2.63723	0.00000
C	5.85634	3.91353	0.00000
C	5.02497	5.03367	0.00000
C	3.08190	3.59318	0.00000
C	3.63987	4.86573	0.00000
H	5.97982	1.78752	0.00000
H	6.93342	4.03446	0.00000
H	5.45438	6.02899	0.00000
H	2.00498	3.47488	0.00000
H	2.98779	5.73152	0.00000

Total electronic energy with ZPE = –953.14101 a.u.

NIm = 0

Point Group (P.G.) = C_s

Hydrogen-bonded trimer

	X	Y	Z
C	-1.70327	0.57549	0.00000
N	-1.96009	-0.80279	0.00000
C	-0.80217	-1.56298	0.00000
C	0.25957	-0.66778	0.00000
C	1.70338	-0.57504	0.00000
O	2.59636	-1.43130	0.00000
N	1.96018	0.80323	0.00000
H	2.92438	1.15667	0.00000
C	0.80225	1.56340	0.00000
C	-0.25946	0.66817	0.00000
H	-2.92424	-1.15628	0.00000
O	-2.59623	1.43177	0.00000
C	-0.82770	-3.01680	0.00000
C	0.82783	3.01721	0.00000
C	2.04402	3.72807	0.00000
C	2.04295	5.11778	0.00000
C	0.83969	5.82379	0.00000
C	-0.38247	3.73837	0.00000
C	-0.36969	5.12740	0.00000
H	2.99234	3.20699	0.00000
H	2.98628	5.65201	0.00000
H	0.84461	6.90795	0.00000
H	-1.32463	3.20473	0.00000
H	-1.30822	5.67011	0.00000
C	-2.04384	-3.72773	0.00000
C	-2.04269	-5.11744	0.00000
C	-0.83940	-5.82338	0.00000
C	0.38264	-3.73788	0.00000
C	0.36994	-5.12692	0.00000
H	-2.99220	-3.20671	0.00000
H	-2.98600	-5.65172	0.00000
H	-0.84425	-6.90754	0.00000
H	1.32477	-3.20420	0.00000
H	1.30851	-5.66957	0.00000
C	5.57385	0.73030	0.00000
N	5.32133	-0.64269	0.00000
C	6.48452	-1.40351	0.00000
C	7.54317	-0.50867	0.00000

C	8.99545	-0.42803	0.00000
O	9.89181	-1.25398	0.00000
N	9.23209	0.97682	0.00000
H	10.17285	1.33613	0.00000
C	8.07058	1.73133	0.00000
C	7.02063	0.82652	0.00000
H	4.35821	-0.99858	0.00000
O	4.68293	1.59040	0.00000
C	6.45890	-2.85680	0.00000
C	8.07897	3.18625	0.00000
C	9.28269	3.91564	0.00000
C	9.27112	5.30518	0.00000
C	8.05937	5.99617	0.00000
C	6.86172	3.89503	0.00000
C	6.85938	5.28423	0.00000
H	10.24034	3.40848	0.00000
H	10.20825	5.84961	0.00000
H	8.05190	7.08010	0.00000
H	5.92601	3.35010	0.00000
H	5.91432	5.81542	0.00000
C	5.24229	-3.56750	0.00000
C	5.24290	-4.95710	0.00000
C	6.44642	-5.66269	0.00000
C	7.66966	-3.57752	0.00000
C	7.65612	-4.96676	0.00000
H	4.29356	-3.04739	0.00000
H	4.29932	-5.49093	0.00000
H	6.44168	-6.74690	0.00000
H	8.61405	-3.04675	0.00000
H	8.59501	-5.50842	0.00000
C	-8.99551	0.42778	0.00000
N	-9.23211	-0.97708	0.00000
C	-8.07058	-1.73156	0.00000
C	-7.02067	-0.82671	0.00000
C	-5.57389	-0.73050	0.00000
O	-4.68297	-1.59060	0.00000
N	-5.32139	0.64252	0.00000
H	-4.35833	0.99846	0.00000
C	-6.48460	1.40332	0.00000
C	-7.54323	0.50846	0.00000
H	-10.17287	-1.33639	0.00000
O	-9.89189	1.25370	0.00000
C	-8.07893	-3.18648	0.00000

C	-6.45906	2.85662	0.00000
C	-5.24253	3.56742	0.00000
C	-5.24326	4.95703	0.00000
C	-6.44684	5.66250	0.00000
C	-7.66990	3.57723	0.00000
C	-7.65648	4.96646	0.00000
H	-4.29374	3.04743	0.00000
H	-4.29973	5.49094	0.00000
H	-6.44222	6.74672	0.00000
H	-8.61424	3.04637	0.00000
H	-8.59543	5.50803	0.00000
C	-9.28263	-3.91591	0.00000
C	-9.27103	-5.30544	0.00000
C	-8.05925	-5.99640	0.00000
C	-6.86167	-3.89522	0.00000
C	-6.85928	-5.28443	0.00000
H	-10.24030	-3.40877	0.00000
H	-10.20814	-5.84990	0.00000
H	-8.05176	-7.08033	0.00000
H	-5.92597	-3.35028	0.00000
H	-5.91421	-5.81559	0.00000

Total electronic energy with ZPE = –2859.48850 a.u.
NIm = 1 (7.03*i* cm^{-1})
P.G. = C_s

Tautomer

	X	Y	Z
C	3.34216	-1.05766	0.00000
N	4.14492	0.01222	0.00000
C	3.33141	1.12068	0.00000
C	1.97431	0.71418	0.00000
C	0.59842	1.06097	0.00000
O	0.08642	2.29364	0.00000
N	-0.20435	-0.00891	0.00000
C	0.60917	-1.11737	0.00000
C	1.96627	-0.71087	0.00000
O	3.85416	-2.29033	0.00000
C	3.90668	2.45553	0.00000
C	0.03389	-2.45222	0.00000
C	-1.36503	-2.61429	0.00000
C	-1.92647	-3.88407	0.00000
C	-1.10664	-5.01475	0.00000

C	0.85045	-3.59835	0.00000
C	0.28109	-4.86623	0.00000
H	-1.98938	-1.73048	0.00000
H	-3.00479	-3.99637	0.00000
H	-1.54705	-6.00557	0.00000
H	1.92716	-3.49538	0.00000
H	0.92045	-5.74169	0.00000
C	5.30561	2.61760	0.00000
C	5.86705	3.88738	0.00000
C	5.04721	5.01806	0.00000
C	3.09013	3.60166	0.00000
C	3.65949	4.86954	0.00000
H	5.92996	1.73379	0.00000
H	6.94537	3.99969	0.00000
H	5.48762	6.00888	0.00000
H	2.01342	3.49869	0.00000
H	3.02013	5.74500	0.00000
H	-0.87845	2.20403	0.00000
H	4.81903	-2.20072	0.00000

Total electronic energy = –953.09372 a.u.
NIm = 0
Point Group (P.G.) = C_s

NDP System
Monomer

	X	Y	Z
C	-1.57718	0.92334	0.00000
C	-2.58479	-0.12565	0.00000
C	-2.10247	-1.47907	0.00000
C	-0.76684	-1.73730	0.00000
C	-3.62042	1.94770	0.00000
C	-3.84898	0.46358	0.00000
H	-2.78705	-2.31111	0.00000
H	-0.43690	-2.76982	0.00000
C	1.57709	-0.92339	0.00000
C	2.58471	0.12561	0.00000
C	2.10239	1.47903	0.00000
C	0.76675	1.73725	0.00000
C	-0.21710	0.68937	0.00000
C	0.21702	-0.68941	0.00000
C	3.62034	-1.94774	0.00000
C	3.84890	-0.46362	0.00000

H	2.78696	2.31106	0.00000
H	0.43682	2.76978	0.00000
O	-4.39927	2.88244	0.00000
O	4.39918	-2.88249	0.00000
N	-2.23223	2.12523	0.00000
N	2.23215	-2.12527	0.00000
H	-1.82152	3.04447	0.00000
H	1.82144	-3.04452	0.00000
C	-5.18886	-0.12149	0.00000
C	-6.33739	0.70445	0.00000
C	-5.40789	-1.51719	0.00000
C	-7.61663	0.16077	0.00000
H	-6.21736	1.77674	0.00000
C	-6.68829	-2.05405	0.00000
H	-4.57798	-2.20362	0.00000
C	-7.80566	-1.21949	0.00000
H	-8.47279	0.82609	0.00000
H	-6.81333	-3.13110	0.00000
H	-8.80492	-1.63963	0.00000
C	5.18877	0.12145	0.00000
C	6.33730	-0.70450	0.00000
C	5.40781	1.51715	0.00000
C	7.61654	-0.16082	0.00000
H	6.21728	-1.77678	0.00000
C	6.68821	2.05400	0.00000
H	4.57789	2.20357	0.00000
C	7.80558	1.21944	0.00000
H	8.47270	-0.82613	0.00000
H	6.81325	3.13106	0.00000
H	8.80484	1.63959	0.00000

Total electronic energy with ZPE = –1260.39761 a.u.
NIm = 2 (82.91*i* cm^{-1}, 78.33*i* cm^{-1})
Point Group (P.G.) = C_s

Hydrogen-bonded trimer

	X	Y	Z
C	0.47713	-1.75921	0.00000
C	1.93115	-1.71603	0.00000
C	2.53908	-0.41422	0.00000
C	1.76943	0.70794	0.00000
C	1.19199	-3.90060	0.00000
C	2.40722	-3.02834	0.00000

H	3.61082	-0.30052	0.00000
H	2.24916	1.67944	0.00000
C	-0.47721	1.75909	0.00000
C	-1.93124	1.71593	0.00000
C	-2.53916	0.41410	0.00000
C	-1.76951	-0.70806	0.00000
C	-0.33074	-0.64169	0.00000
C	0.33066	0.64157	0.00000
C	-1.19202	3.90049	0.00000
C	-2.40726	3.02828	0.00000
H	-3.61089	0.30038	0.00000
H	-2.24924	-1.67955	0.00000
O	1.09582	-5.13204	0.00000
O	-1.09587	5.13193	0.00000
N	0.08912	-3.07189	0.00000
N	-0.08917	3.07176	0.00000
H	-0.87571	-3.42712	0.00000
H	0.87567	3.42698	0.00000
C	3.76934	-3.56141	0.00000
C	4.00428	-4.95603	0.00000
C	4.90751	-2.72518	0.00000
C	5.29514	-5.47132	0.00000
H	3.16345	-5.63129	0.00000
C	6.19488	-3.24569	0.00000
H	4.79965	-1.65358	0.00000
C	6.40156	-4.62470	0.00000
H	5.43554	-6.54667	0.00000
H	7.04183	-2.56865	0.00000
H	7.40695	-5.02986	0.00000
C	-3.76929	3.56159	0.00000
C	-4.00380	4.95628	0.00000
C	-4.90772	2.72571	0.00000
C	-5.29450	5.47197	0.00000
H	-3.16275	5.63128	0.00000
C	-6.19493	3.24662	0.00000
H	-4.80020	1.65409	0.00000
C	-6.40118	4.62569	0.00000
H	-5.43457	6.54737	0.00000
H	-7.04209	2.56984	0.00000
H	-7.40645	5.03116	0.00000
C	1.90702	7.52299	0.00000
C	3.35926	7.56219	0.00000
C	3.96762	8.86277	0.00000

C	3.19571	9.98433	0.00000
C	2.61970	5.37940	0.00000
C	3.83422	6.24812	0.00000
H	5.03949	8.97601	0.00000
H	3.68459	10.95187	0.00000
C	0.95121	11.04587	0.00000
C	-0.50404	10.99958	0.00000
C	-1.10780	9.69493	0.00000
C	-0.33803	8.57416	0.00000
C	1.10009	8.64135	0.00000
C	1.75904	9.92676	0.00000
C	0.20946	13.20618	0.00000
C	-0.99402	12.30458	0.00000
H	-2.17909	9.58047	0.00000
H	-0.81713	7.60239	0.00000
O	2.52021	4.14725	0.00000
O	0.30621	14.41827	0.00000
N	1.51807	6.21049	0.00000
N	1.32532	12.36228	0.00000
H	0.55360	5.85621	0.00000
H	2.26238	12.73053	0.00000
C	5.19579	5.71340	0.00000
C	5.42802	4.31837	0.00000
C	6.33578	6.54700	0.00000
C	6.71790	3.80048	0.00000
H	4.58552	3.64509	0.00000
C	7.62228	6.02402	0.00000
H	6.23095	7.61905	0.00000
C	7.82620	4.64463	0.00000
H	6.85592	2.72481	0.00000
H	8.47059	6.69939	0.00000
H	8.83076	4.23742	0.00000
C	-2.36011	12.82489	0.00000
C	-2.60258	14.21871	0.00000
C	-3.49300	11.98059	0.00000
C	-3.89683	14.72535	0.00000
H	-1.76685	14.90107	0.00000
C	-4.78314	12.49308	0.00000
H	-3.37949	10.90973	0.00000
C	-4.99739	13.87121	0.00000
H	-4.04316	15.79969	0.00000
H	-5.62614	11.81118	0.00000
H	-6.00530	14.27017	0.00000

C	-0.95122	-11.04597	0.00000
C	0.50403	-10.99967	0.00000
C	1.10778	-9.69501	0.00000
C	0.33799	-8.57425	0.00000
C	-0.20946	-13.20627	0.00000
C	0.99401	-12.30468	0.00000
H	2.17906	-9.58052	0.00000
H	0.81707	-7.60247	0.00000
C	-1.90707	-7.52310	0.00000
C	-3.35931	-7.56231	0.00000
C	-3.96765	-8.86291	0.00000
C	-3.19573	-9.98446	0.00000
C	-1.75906	-9.92687	0.00000
C	-1.10013	-8.64146	0.00000
C	-2.61976	-5.37952	0.00000
C	-3.83427	-6.24823	0.00000
H	-5.03952	-8.97616	0.00000
H	-3.68460	-10.95200	0.00000
O	-0.30618	-14.41836	0.00000
O	-2.52027	-4.14737	0.00000
N	-1.32532	-12.36238	0.00000
N	-1.51813	-6.21060	0.00000
H	-2.26238	-12.73063	0.00000
H	-0.55366	-5.85631	0.00000
C	2.36006	-12.82507	0.00000
C	2.60238	-14.21891	0.00000
C	3.49305	-11.98090	0.00000
C	3.89656	-14.72571	0.00000
H	1.76656	-14.90117	0.00000
C	4.78313	-12.49354	0.00000
H	3.37967	-10.91002	0.00000
C	4.99722	-13.87169	0.00000
H	4.04277	-15.80007	0.00000
H	5.62621	-11.81174	0.00000
H	6.00509	-14.27077	0.00000
C	-5.19582	-5.71346	0.00000
C	-5.42796	-4.31841	0.00000
C	-6.33588	-6.54698	0.00000
C	-6.71779	-3.80043	0.00000
H	-4.58540	-3.64520	0.00000
C	-7.62234	-6.02389	0.00000
H	-6.23114	-7.61903	0.00000
C	-7.82616	-4.64449	0.00000

H	-6.85573	-2.72475	0.00000
H	-8.47070	-6.69920	0.00000
H	-8.83069	-4.23721	0.00000

Total electronic energy with ZPE = –3781.25845 a.u.
NIm = 6(81.63*i* cm^{-1}, 80.99*i* cm^{-1}, 79.15*i* cm^{-1}, 76.81*i* cm^{-1}, 76.68*i* cm^{-1}, 76.05*i* cm^{-1})
P.G. = C_s

Tautomer

	X	Y	Z
C	-1.58165	0.91288	0.00000
C	-2.56371	-0.16944	0.00000
C	-2.07783	-1.52268	0.00000
C	-0.74040	-1.76322	0.00000
C	-3.47156	1.88687	0.00000
C	-3.81848	0.43989	0.00000
H	-2.75468	-2.36296	0.00000
H	-0.35729	-2.77544	0.00000
C	1.58157	-0.91292	0.00000
C	2.56362	0.16939	0.00000
C	2.07774	1.52264	0.00000
C	0.74032	1.76318	0.00000
C	-0.22331	0.68873	0.00000
C	0.22323	-0.68877	0.00000
C	3.47147	-1.88691	0.00000
C	3.81840	-0.43994	0.00000
H	2.75459	2.36291	0.00000
H	0.35721	2.77539	0.00000
O	-4.38049	2.86948	0.00000
O	4.38040	-2.86952	0.00000
N	-2.19906	2.15626	0.00000
N	2.19898	-2.15630	0.00000
C	-5.16976	-0.11893	0.00000
C	-6.31501	0.70967	0.00000
C	-5.39640	-1.51338	0.00000
C	-7.59771	0.17292	0.00000
H	-6.20297	1.78183	0.00000
C	-6.67877	-2.04475	0.00000
H	-4.56609	-2.19958	0.00000
C	-7.79328	-1.20611	0.00000
H	-8.45070	0.84237	0.00000
H	-6.80791	-3.12134	0.00000
H	-8.79443	-1.62151	0.00000

C	5.16968	0.11889	0.00000
C	6.31492	-0.70972	0.00000
C	5.39632	1.51334	0.00000
C	7.59763	-0.17296	0.00000
H	6.20288	-1.78188	0.00000
C	6.67869	2.04471	0.00000
H	4.56601	2.19953	0.00000
C	7.79320	1.20606	0.00000
H	8.45062	-0.84241	0.00000
H	6.80783	3.12129	0.00000
H	8.79434	1.62146	0.00000
H	-3.88801	3.70412	0.00000
H	3.88793	-3.70417	0.00000

Total electronic energy = –1260.35022 a.u.
NIm = 2 (79.22*i* cm^{-1}, 75.00*i* cm^{-1})
Point Group (P.G.) = C_s

Indigo System
Monomer

	X	Y	Z
O	-0.50393	2.32026	0.00000
O	1.95301	-2.33351	0.00000
N	-0.72378	-1.17717	0.00000
N	2.17296	1.16391	0.00000
C	0.04617	-0.03230	0.00000
C	-2.21370	0.56406	0.00000
C	-2.07044	-0.84057	0.00000
C	1.40300	0.01907	0.00000
C	-0.86819	1.14799	0.00000
C	3.66287	-0.57734	0.00000
C	2.31734	-1.16125	0.00000
C	3.51962	0.82729	0.00000
C	-3.47693	1.15210	0.00000
C	-3.18557	-1.67520	0.00000
C	4.92610	-1.16537	0.00000
C	4.63474	1.66192	0.00000
C	-4.59621	0.32588	0.00000
C	-4.44154	-1.06997	0.00000
C	6.04538	-0.33915	0.00000
C	5.89072	1.05670	0.00000
H	-0.32064	-2.10381	0.00000
H	-3.56790	2.23207	0.00000

H	-3.08293	-2.75387	0.00000
H	5.01709	-2.24534	0.00000
H	4.53210	2.74059	0.00000
H	-5.59087	0.75453	0.00000
H	-5.32473	-1.69914	0.00000
H	7.04004	-0.76780	0.00000
H	6.77391	1.68587	0.00000
H	1.76983	2.09055	0.00000

Total electronic energy with ZPE = –875.72845 a.u.
NIm = 0
Point Group (P.G.) = C_s

Hydrogen-bonded trimer

	X	Y	Z
O	2.18438	-1.49105	0.00000
O	-2.18462	1.49117	0.00000
N	-1.32087	-1.31579	0.00000
N	1.32062	1.31586	0.00000
C	-0.10190	-0.67407	0.00000
C	0.24808	-2.98858	0.00000
C	-1.13017	-2.68736	0.00000
C	0.10164	0.67417	0.00000
C	0.97214	-1.71746	0.00000
C	-0.24829	2.98868	0.00000
C	-0.97237	1.71757	0.00000
C	1.12995	2.68743	0.00000
C	0.67566	-4.31925	0.00000
C	-2.09282	-3.69433	0.00000
C	-0.67581	4.31939	0.00000
C	2.09265	3.69435	0.00000
C	-0.27570	-5.33060	0.00000
C	-1.64515	-5.01075	0.00000
C	0.27560	5.33069	0.00000
C	1.64504	5.01080	0.00000
H	-2.22337	-0.85697	0.00000
H	1.73090	-4.55653	0.00000
H	-3.13896	-3.42772	0.00000
H	-1.73103	4.55677	0.00000
H	3.13877	3.42766	0.00000
H	0.03361	-6.36867	0.00000
H	-2.37378	-5.81453	0.00000
H	-0.03368	6.36877	0.00000

H	2.37370	5.81455	0.00000
H	2.22312	0.85702	0.00000
O	8.75068	-1.52527	0.00000
O	4.39641	1.44457	0.00000
N	5.24887	-1.43786	0.00000
N	7.89596	1.18251	0.00000
C	6.44681	-0.76966	0.00000
C	6.85963	-3.07651	0.00000
C	5.47621	-2.81011	0.00000
C	6.65168	0.57563	0.00000
C	7.55212	-1.78863	0.00000
C	6.37660	2.89274	0.00000
C	5.61477	1.63905	0.00000
C	7.74982	2.55566	0.00000
C	7.33355	-4.38799	0.00000
C	4.54403	-3.84142	0.00000
C	5.98305	4.23255	0.00000
C	8.73654	3.54141	0.00000
C	6.40919	-5.42724	0.00000
C	5.03211	-5.14632	0.00000
C	6.95950	5.22081	0.00000
C	8.32041	4.86932	0.00000
H	4.33281	-1.00565	0.00000
H	8.40074	-4.57668	0.00000
H	3.49010	-3.60728	0.00000
H	4.93291	4.49450	0.00000
H	9.78859	3.28223	0.00000
H	6.74651	-6.45655	0.00000
H	4.32672	-5.97052	0.00000
H	6.67633	6.26623	0.00000
H	9.06892	5.65385	0.00000
H	8.75601	0.65115	0.00000
O	-4.39667	-1.44451	0.00000
O	-8.75084	1.52549	0.00000
N	-7.89622	-1.18236	0.00000
N	-5.24903	1.43791	0.00000
C	-6.65192	-0.57551	0.00000
C	-6.37690	-2.89262	0.00000
C	-7.75011	-2.55551	0.00000
C	-6.44701	0.76978	0.00000
C	-5.61504	-1.63895	0.00000
C	-6.85970	3.07665	0.00000
C	-7.55226	1.78881	0.00000

C	-5.47630	2.81017	0.00000
C	-5.98337	-4.23243	0.00000
C	-8.73684	-3.54125	0.00000
C	-7.33353	4.38816	0.00000
C	-4.54404	3.84141	0.00000
C	-6.95982	-5.22068	0.00000
C	-8.32072	-4.86916	0.00000
C	-6.40909	5.42734	0.00000
C	-5.03203	5.14634	0.00000
H	-8.75626	-0.65098	0.00000
H	-4.93322	-4.49435	0.00000
H	-9.78889	-3.28207	0.00000
H	-8.40070	4.57693	0.00000
H	-3.49014	3.60714	0.00000
H	-6.67666	-6.26610	0.00000
H	-9.06924	-5.65369	0.00000
H	-6.74635	6.45667	0.00000
H	-4.32659	5.97049	0.00000
H	-4.33300	1.00564	0.00000

Total electronic energy with ZPE = –2627.22315 a.u.
NIm = 5 (26.83*i* cm^{-1}, 26.03*i* cm^{-1}, 22.24*i* cm^{-1}, 15.28*i* cm^{-1}, 1.22*i* cm^{-1})
P.G. = C_s

Tautomer

	X	Y	Z
O	-0.40230	2.33962	0.00000
O	1.85111	-2.35261	0.00000
N	-0.64998	-1.23007	0.00000
N	2.09916	1.21703	0.00000
C	0.03587	-0.06684	0.00000
C	-2.14594	0.59093	0.00000
C	-1.96908	-0.84986	0.00000
C	1.41321	0.05390	0.00000
C	-0.84553	1.10424	0.00000
C	3.59497	-0.60413	0.00000
C	2.29450	-1.11732	0.00000
C	3.41825	0.83667	0.00000
C	-3.43343	1.17369	0.00000
C	-3.10608	-1.67209	0.00000
C	4.88239	-1.18701	0.00000
C	4.55531	1.65878	0.00000
C	-4.52784	0.33886	0.00000

C	-4.35446	-1.07177	0.00000
C	5.97689	-0.35229	0.00000
C	5.80364	1.05835	0.00000
H	-3.54380	2.25187	0.00000
H	-2.99787	-2.74990	0.00000
H	4.99266	-2.26521	0.00000
H	4.44720	2.73660	0.00000
H	-5.52998	0.74958	0.00000
H	-5.23821	-1.70099	0.00000
H	6.97899	-0.76311	0.00000
H	6.68745	1.68748	0.00000
H	0.59901	2.30298	0.00000
H	0.84975	-2.31579	0.00000

Total electronic energy = –875.66972 a.u.
NIm = 0
Point Group (P.G.) = C_s

Isoindigo System
Monomer

	X	Y	Z
C	-0.32929	-0.60293	0.00000
C	-1.85442	-0.71746	0.00000
C	0.32846	0.60526	0.00000
C	1.85359	0.71981	0.00000
C	0.99555	2.84496	0.00000
O	-2.71385	0.14243	0.00000
O	2.71304	-0.14008	0.00000
C	0.32995	-4.81976	0.00000
C	1.47782	-4.02990	0.00000
C	1.39846	-2.63595	0.00000
C	0.14655	-2.00305	0.00000
C	-0.99640	-2.84264	0.00000
C	-0.93341	-4.22511	0.00000
H	0.41233	-5.90071	0.00000
H	2.45438	-4.49919	0.00000
H	2.29640	-2.04524	0.00000
H	-1.83810	-4.82193	0.00000
C	0.93254	4.22743	0.00000
C	-0.33083	4.82207	0.00000
H	1.83723	4.82426	0.00000
C	-1.39931	2.63824	0.00000
C	-1.47868	4.03220	0.00000

H	-0.41322	5.90302	0.00000
H	-2.29724	2.04752	0.00000
H	-2.45525	4.50148	0.00000
C	-0.14739	2.00536	0.00000
N	-2.14230	-2.06108	0.00000
N	2.14146	2.06344	0.00000
H	-3.09298	-2.39557	0.00000

Total electronic energy with ZPE = –875.73987 a.u.
NIm = 1 (29.05*i* cm^{-1})
Point Group (P.G.) = C_s

Hydrogen-bonded trimer

	X	Y	Z
C	0.48793	-0.47863	0.81648
C	1.96249	-0.17056	0.60267
C	-0.48690	0.48495	0.81346
C	-1.96177	0.17524	0.60413
C	-1.75219	2.43170	0.78581
O	2.50201	0.91851	0.41272
O	-2.50155	-0.91525	0.42336
C	1.05857	-4.66639	1.19694
C	-0.25280	-4.21988	1.36767
C	-0.57568	-2.86821	1.24236
C	0.42915	-1.94190	0.93679
C	1.75319	-2.42554	0.80207
C	2.08749	-3.76392	0.91706
H	1.28667	-5.72205	1.29128
H	-1.03656	-4.93162	1.59847
H	-1.59372	-2.54019	1.36364
H	3.11477	-4.08961	0.80648
C	-2.08633	3.77093	0.89093
C	-1.05702	4.67553	1.16237
H	-3.11377	4.09576	0.77930
C	0.57730	2.87774	1.21934
C	0.25460	4.23034	1.33467
H	-1.28498	5.73188	1.24888
H	1.59552	2.55066	1.34170
H	1.03868	4.94383	1.55885
C	-0.42795	1.94910	0.92237
N	2.62106	-1.36084	0.58332
N	-2.62037	1.36535	0.57653
H	3.63214	-1.42697	0.41367

H	-3.63168	1.43017	0.40781
C	8.40031	-0.89600	-0.36486
C	9.88120	-0.58389	-0.17706
C	7.42873	0.07162	-0.35317
C	5.95218	-0.23405	-0.14495
C	6.16668	2.02141	-0.32796
O	10.44766	0.48192	-0.03964
O	5.40913	-1.32274	0.04183
C	8.92219	-5.09964	-0.70236
C	7.61843	-4.63601	-0.88178
C	7.31587	-3.27881	-0.77083
C	8.33071	-2.36062	-0.47265
C	9.64811	-2.86250	-0.33212
C	9.96178	-4.20780	-0.43042
H	9.13635	-6.15928	-0.78284
H	6.82489	-5.33826	-1.10791
H	6.30313	-2.93794	-0.89884
H	10.98226	-4.55241	-0.31069
C	5.83406	3.36083	-0.42683
C	6.86774	4.26748	-0.67588
H	4.80547	3.68510	-0.32429
C	8.50257	2.46882	-0.72351
C	8.18118	3.82300	-0.82990
H	6.64158	5.32477	-0.75576
H	9.52372	2.14442	-0.82688
H	8.97055	4.53779	-1.02956
C	7.49155	1.53717	-0.45458
N	10.52277	-1.80312	-0.12612
N	5.29488	0.95554	-0.12847
H	11.52152	-1.86978	-0.00893
H	4.28418	1.02291	0.04049
C	-7.42930	-0.07426	-0.34235
C	-5.95247	0.23301	-0.13848
C	-8.40092	0.89325	-0.36015
C	-9.88154	0.58257	-0.16796
C	-9.64872	2.85992	-0.34084
O	-5.40918	1.32309	0.03921
O	-10.44779	-0.48217	-0.02160
C	-6.86872	-4.27247	-0.63361
C	-8.18237	-3.82918	-0.78923
C	-8.50362	-2.47422	-0.69280
C	-7.49225	-1.54054	-0.43242
C	-6.16720	-2.02379	-0.30389

C	-5.83471	-3.36393	-0.39294
H	-6.64266	-5.33034	-0.70568
H	-8.97201	-4.54548	-0.98232
H	-9.52493	-2.15063	-0.79726
H	-4.80598	-3.68741	-0.28931
C	-9.96256	4.20441	-0.44905
C	-8.92336	5.09416	-0.72923
H	-10.98288	4.54992	-0.33059
C	-7.31709	3.27288	-0.78588
C	-7.61983	4.62919	-0.90685
H	-9.13766	6.15314	-0.81757
H	-6.30451	2.93105	-0.91264
H	-6.82661	5.32968	-1.13944
C	-8.33150	2.35699	-0.47929
N	-5.29514	-0.95643	-0.11378
N	-10.52307	1.80214	-0.12553
H	-4.28421	-1.02250	0.05434
H	-11.52166	1.86968	-0.00750

Total electronic energy with ZPE = –2627.27277 a.u.
NIm = 0
P.G. = C_1

Tautomer

	X	Y	Z
C	-0.31669	-0.60829	0.00000
C	-1.80465	-0.83644	0.00000
C	0.31552	0.61062	0.00000
C	1.80349	0.83860	0.00000
C	0.98904	2.82929	0.00000
O	-2.71355	0.14662	0.00000
O	2.71226	-0.14460	0.00000
C	0.31096	-4.82794	0.00000
C	1.47006	-4.05768	0.00000
C	1.41449	-2.65869	0.00000
C	0.17426	-2.01568	0.00000
C	-0.98993	-2.82704	0.00000
C	-0.94335	-4.20869	0.00000
H	0.37815	-5.91003	0.00000
H	2.43940	-4.54244	0.00000
H	2.33097	-2.10042	0.00000
H	-1.86354	-4.77979	0.00000
C	0.94265	4.21094	0.00000

C	-0.31158	4.83038	0.00000
H	1.86292	4.78192	0.00000
C	-1.41541	2.66128	0.00000
C	-1.47078	4.06028	0.00000
H	-0.37861	5.91247	0.00000
H	-2.33197	2.10316	0.00000
H	-2.44005	4.54518	0.00000
C	-0.17527	2.01808	0.00000
N	-2.17209	-2.06604	0.00000
N	2.17110	2.06814	0.00000
H	3.57912	0.28854	0.00000
H	-3.58036	-0.28666	0.00000

Total electronic energy = –875.68650 a.u.
NIm = 1 (53.44*i* cm^{-1})
Point Group (P.G.) = C_s

Tyrian purple System
Monomer

	X	Y	Z
O	-0.50143	2.32181	0.00000
O	1.95049	-2.33503	0.00000
N	-0.72493	-1.17632	0.00000
N	2.17413	1.16306	0.00000
C	0.04652	-0.03104	0.00000
C	-2.21102	0.56709	0.00000
C	-2.06884	-0.83764	0.00000
C	1.40265	0.01783	0.00000
C	-0.86635	1.15049	0.00000
C	3.66019	-0.58038	0.00000
C	2.31549	-1.16374	0.00000
C	3.51804	0.82436	0.00000
C	-3.47540	1.15016	0.00000
C	-3.17863	-1.67813	0.00000
C	4.92456	-1.16346	0.00000
C	4.62783	1.66483	0.00000
C	-4.59870	0.33138	0.00000
C	-4.42766	-1.06136	0.00000
C	6.04788	-0.34469	0.00000
C	5.87687	1.04805	0.00000
H	-0.32309	-2.10385	0.00000
H	-3.57384	2.22931	0.00000
H	-3.08285	-2.75570	0.00000

H	5.02301	-2.24261	0.00000
H	4.53206	2.74240	0.00000
H	-5.59458	0.75247	0.00000
Br	-5.98619	-2.17257	0.00000
H	7.04375	-0.76580	0.00000
Br	7.43540	2.15924	0.00000
H	1.77231	2.09061	0.00000

Total electronic energy with ZPE = –6022.83770 a.u.
NIm = 0
Point Group (P.G.) = C_s

Hydrogen-bonded trimer

	X	Y	Z
O	-1.91567	-1.82715	0.00000
O	1.91587	1.82740	0.00000
N	1.51781	-1.08532	0.00000
N	-1.51755	1.08530	0.00000
C	0.20890	-0.64847	0.00000
C	0.23704	-2.98593	0.00000
C	1.54986	-2.46852	0.00000
C	-0.20861	0.64854	0.00000
C	-0.68266	-1.85166	0.00000
C	-0.23695	2.98601	0.00000
C	0.68286	1.85181	0.00000
C	-1.54972	2.46849	0.00000
C	0.02849	-4.36538	0.00000
C	2.66442	-3.30471	0.00000
C	-0.02854	4.36549	0.00000
C	-2.66438	3.30456	0.00000
C	1.12070	-5.21954	0.00000
C	2.41305	-4.67189	0.00000
C	-1.12085	5.21952	0.00000
C	-2.41314	4.67177	0.00000
H	2.33392	-0.48551	0.00000
H	-0.96781	-4.78194	0.00000
H	3.65716	-2.88168	0.00000
H	0.96771	4.78213	0.00000
H	-3.65704	2.88133	0.00000
H	0.98277	-6.29189	0.00000
Br	3.89850	-5.88568	0.00000
H	-0.98302	6.29189	0.00000
Br	-3.89871	5.88541	0.00000

H	-2.33360	0.48541	0.00000
O	4.59658	-0.69499	0.00000
O	8.39012	2.97323	0.00000
N	7.99827	0.17726	0.00000
N	4.94702	2.31358	0.00000
C	6.66728	0.55859	0.00000
C	6.79953	-1.76950	0.00000
C	8.09283	-1.19902	0.00000
C	6.24132	1.84974	0.00000
C	5.82979	-0.67191	0.00000
C	6.27137	4.18987	0.00000
C	7.16475	3.03386	0.00000
C	4.94951	3.70149	0.00000
C	6.64894	-3.15570	0.00000
C	9.23981	-1.99032	0.00000
C	6.52292	5.55980	0.00000
C	3.85826	4.56341	0.00000
C	7.77666	-3.96506	0.00000
C	9.04724	-3.36828	0.00000
C	5.44895	6.44177	0.00000
C	4.14385	5.92524	0.00000
H	8.75255	0.85137	0.00000
H	5.66796	-3.60916	0.00000
H	10.23182	-1.55894	0.00000
H	7.54336	5.92433	0.00000
H	2.85609	4.16500	0.00000
H	7.68324	-5.04225	0.00000
Br	10.58924	-4.50178	0.00000
H	5.60700	7.51140	0.00000
Br	2.68220	7.16817	0.00000
H	4.11356	1.73756	0.00000
O	-8.39011	-2.97338	0.00000
O	-4.59670	0.69500	0.00000
N	-4.94704	-2.31352	0.00000
N	-7.99836	-0.17730	0.00000
C	-6.24137	-1.84974	0.00000
C	-6.27130	-4.18988	0.00000
C	-4.94946	-3.70144	0.00000
C	-6.66737	-0.55860	0.00000
C	-7.16474	-3.03392	0.00000
C	-6.79966	1.76951	0.00000
C	-5.82991	0.67192	0.00000
C	-8.09295	1.19898	0.00000

C	-6.52279	-5.55982	0.00000
C	-3.85817	-4.56331	0.00000
C	-6.64913	3.15571	0.00000
C	-9.23996	1.99023	0.00000
C	-5.44878	-6.44174	0.00000
C	-4.14371	-5.92516	0.00000
C	-7.77688	3.96502	0.00000
C	-9.04744	3.36820	0.00000
H	-4.11361	-1.73747	0.00000
H	-7.54322	-5.92439	0.00000
H	-2.85601	-4.16485	0.00000
H	-5.66819	3.60928	0.00000
H	-10.23196	1.55883	0.00000
H	-5.60678	-7.51138	0.00000
Br	-2.68201	-7.16803	0.00000
H	-7.68352	5.04222	0.00000
Br	-10.58948	4.50164	0.00000
H	-8.75262	-0.85143	0.00000

Total electronic energy with ZPE = –18068.56005 a.u.
NIm = 6(17.56*i* cm^{-1}, 14.98*i* cm^{-1}, 11.59*i* cm^{-1}, 9.17*i* cm^{-1}, 3.50*i* cm^{-1}, 2.97*i* cm^{-1})
P.G. = C_s

Tautomer

	X	Y	Z
O	-0.40472	2.34470	0.00000
O	1.85351	-2.35765	0.00000
N	-0.65205	-1.22818	0.00000
N	2.10126	1.21515	0.00000
C	0.03574	-0.06410	0.00000
C	-2.14294	0.59460	0.00000
C	-1.96750	-0.84647	0.00000
C	1.41335	0.05119	0.00000
C	-0.84379	1.10723	0.00000
C	3.59198	-0.60781	0.00000
C	2.29276	-1.12030	0.00000
C	3.41668	0.83327	0.00000
C	-3.43121	1.17236	0.00000
C	-3.09829	-1.67576	0.00000
C	4.88017	-1.18571	0.00000
C	4.54756	1.66243	0.00000
C	-4.52926	0.34496	0.00000
C	-4.33933	-1.06387	0.00000

C	5.97832	-0.35844	0.00000
C	5.78854	1.05040	0.00000
H	-3.54897	2.24957	0.00000
H	-2.99475	-2.75228	0.00000
H	4.99781	-2.26294	0.00000
H	4.44413	2.73897	0.00000
H	-5.53265	0.74743	0.00000
Br	-5.90116	-2.16541	0.00000
H	6.98166	-0.76102	0.00000
Br	7.35048	2.15179	0.00000
H	0.59480	2.31365	0.00000
H	0.85392	-2.32640	0.00000

Total electronic energy = –6022.78142 a.u.
NIm = 0
Point Group (P.G.) = C_s

Model A System
Monomer

	X	Y	Z
C	2.18359	-3.66468	0.00000
C	0.77183	-3.64081	0.00000
C	0.08825	-2.44569	0.00000
C	0.78022	-1.21070	0.00000
C	0.08285	0.03466	0.00000
C	0.80928	1.19114	0.00000
C	2.23487	1.17239	0.00000
C	2.71183	2.56501	0.00000
C	1.40655	3.43703	0.00000
N	0.36743	2.51983	0.00000
C	2.92837	-0.00750	0.00000
C	2.21743	-1.23597	0.00000
C	2.88832	-2.48433	0.00000
H	-0.99640	-2.43818	0.00000
H	0.22186	-4.57516	0.00000
H	2.70644	-4.61371	0.00000
H	3.97306	-2.49136	0.00000
H	-1.00127	0.04269	0.00000
H	4.01315	0.00178	0.00000
O	3.83274	3.00455	0.00000
O	1.31763	4.63643	0.00000

H	-0.60017	2.80514	0.00000

Total electronic energy with ZPE = –666.73013 a.u.
NIm = 0
Point Group (P.G.) = C_s

Hydrogen-bonded trimer

	X	Y	Z
C	0.54862	-5.71700	0.00000
C	-0.86239	-5.63354	0.00000
C	-1.50123	-4.41174	0.00000
C	-0.75635	-3.20803	0.00000
C	-1.40669	-1.93611	0.00000
C	-0.62848	-0.81605	0.00000
C	0.79739	-0.89049	0.00000
C	1.31146	0.47299	0.00000
C	0.04256	1.39528	0.00000
N	-1.02470	0.53068	0.00000
C	1.44731	-2.10287	0.00000
C	0.67898	-3.29380	0.00000
C	1.30455	-4.56764	0.00000
H	-2.58421	-4.35293	0.00000
H	-1.44952	-6.54552	0.00000
H	1.03100	-6.68743	0.00000
H	2.38851	-4.61099	0.00000
H	-2.48802	-1.88225	0.00000
H	2.53073	-2.16701	0.00000
O	2.45268	0.89453	0.00000
O	0.02333	2.60332	0.00000
H	-1.99368	0.82339	0.00000
C	9.86379	3.95724	0.00000
C	8.65156	4.68294	0.00000
C	7.43959	4.02850	0.00000
C	7.37463	2.61338	0.00000
C	6.12396	1.92646	0.00000
C	6.13444	0.56069	0.00000
C	7.35233	-0.17879	0.00000
C	7.00617	-1.60949	0.00000
C	5.43461	-1.63582	0.00000
N	5.04576	-0.32170	0.00000

C	8.56635	0.45605	0.00000
C	8.60912	1.87543	0.00000
C	9.83851	2.58195	0.00000
H	6.51369	4.59339	0.00000
H	8.67765	5.76694	0.00000
H	10.80931	4.48674	0.00000
H	10.76379	2.01532	0.00000
H	5.19380	2.48288	0.00000
H	9.48477	-0.12153	0.00000
O	7.71189	-2.58702	0.00000
O	4.72295	-2.61753	0.00000
H	4.07187	-0.00787	0.00000
C	-9.62214	4.44445	0.00000
C	-10.67039	3.49805	0.00000
C	-10.40124	2.14644	0.00000
C	-9.06874	1.67141	0.00000
C	-8.77641	0.27255	0.00000
C	-7.47033	-0.11922	0.00000
C	-6.40627	0.83080	0.00000
C	-5.14326	0.09484	0.00000
C	-5.55234	-1.41959	0.00000
N	-6.92965	-1.41655	0.00000
C	-6.65908	2.17958	0.00000
C	-8.00149	2.63528	0.00000
C	-8.31469	4.01855	0.00000
H	-11.21463	1.42908	0.00000
H	-11.69882	3.84091	0.00000
H	-9.85209	5.50311	0.00000
H	-7.50183	4.73664	0.00000
H	-9.58843	-0.44563	0.00000
H	-5.83737	2.88773	0.00000
O	-4.00015	0.48900	0.00000
O	-4.81642	-2.37602	0.00000
H	-7.47251	-2.26765	0.00000

Total electronic energy with ZPE = –2000.26287 a.u.

NIm = 0

P.G. = C_s

Tautomer

	X	Y	Z
C	2.17395	-3.63934	0.00000
C	0.75297	-3.56173	0.00000
C	0.10217	-2.35469	0.00000
C	0.82244	-1.12693	0.00000
C	0.15186	0.11466	0.00000
C	0.87121	1.29842	0.00000
C	2.33993	1.19382	0.00000
C	2.73612	2.51791	0.00000
C	1.44455	3.37955	0.00000
N	0.37673	2.57697	0.00000
C	3.01618	-0.02849	0.00000
C	2.27606	-1.20926	0.00000
C	2.91069	-2.48910	0.00000
H	-0.98130	-2.31856	0.00000
H	0.17538	-4.47964	0.00000
H	2.65951	-4.60743	0.00000
H	3.99500	-2.52633	0.00000
H	-0.93070	0.14689	0.00000
H	4.10091	-0.05882	0.00000
O	3.87626	3.12003	0.00000
O	1.61755	4.59846	0.00000
H	3.63215	4.08295	0.00000

Total electronic energy = –666.67166 a.u.
NIm = 0
Point Group (P.G.) = C_s

Model B System
Monomer

	X	Y	Z
C	2.19552	-3.64820	0.00000
C	0.78275	-3.65346	0.00000
C	0.08360	-2.46959	0.00000
C	0.76060	-1.22459	0.00000
C	0.04935	0.00904	0.00000
C	0.76418	1.17190	0.00000
C	2.17818	1.17723	0.00000
C	2.64300	2.59421	0.00000

N	1.46314	3.35330	0.00000
C	0.28885	2.58571	0.00000
C	2.90155	0.01961	0.00000
C	2.19953	-1.21922	0.00000
C	2.88581	-2.45914	0.00000
H	-1.00096	-2.47279	0.00000
H	0.25072	-4.59775	0.00000
H	2.73458	-4.58850	0.00000
H	3.97037	-2.45425	0.00000
H	-1.03482	0.02054	0.00000
H	3.98562	0.03912	0.00000
O	3.76670	3.03287	0.00000
H	1.45953	4.36266	0.00000
O	-0.83804	3.01610	0.00000

Total electronic energy with ZPE = –666.76001 a.u.
NIm = 0
Point Group (P.G.) = C_s

Hydrogen-bonded trimer

	X	Y	Z
C	-9.53039	-0.60778	0.00000
C	-9.11542	-1.95768	0.00000
C	-7.77673	-2.27314	0.00000
C	-6.79002	-1.25672	0.00000
C	-5.39986	-1.57007	0.00000
C	-4.50332	-0.54204	0.00000
C	-4.91885	0.81214	0.00000
C	-3.69347	1.66128	0.00000
C	-6.23848	1.15856	0.00000
C	-7.21272	0.11854	0.00000
C	-8.60006	0.40517	0.00000
H	-7.45698	-3.30946	0.00000
H	-9.85856	-2.74664	0.00000
H	-10.58840	-0.37251	0.00000
H	-8.91806	1.44208	0.00000
H	-5.06602	-2.60166	0.00000
H	-6.54378	2.19892	0.00000
O	-3.60175	2.87479	0.00000
O	-2.26043	-1.51314	0.00000

C	-3.01232	-0.56079	0.00000
N	-2.62772	0.77380	0.00000
H	-1.64622	1.09289	0.00000
C	6.25496	4.21955	0.00000
C	6.07653	5.62083	0.00000
C	4.81174	6.16092	0.00000
C	3.66457	5.32911	0.00000
C	2.34904	5.87827	0.00000
C	1.28899	5.01877	0.00000
C	1.47572	3.61814	0.00000
C	0.13958	2.98191	0.00000
C	2.71250	3.03943	0.00000
C	3.84674	3.90091	0.00000
C	5.16502	3.38117	0.00000
H	4.67518	7.23694	0.00000
H	6.94367	6.27125	0.00000
H	7.25750	3.80740	0.00000
H	5.29658	2.30473	0.00000
H	2.20048	6.95230	0.00000
H	2.82061	1.95936	0.00000
O	-0.10961	1.79022	0.00000
O	-0.76364	6.34450	0.00000
C	-0.18043	5.29048	0.00000
N	-0.78369	4.01575	0.00000
H	-1.79214	3.85496	0.00000
C	6.32807	-6.39470	0.00000
C	7.04389	-5.17655	0.00000
C	6.37232	-3.97693	0.00000
C	4.95554	-3.93428	0.00000
C	4.24660	-2.69930	0.00000
C	2.88208	-2.73213	0.00000
C	2.16755	-3.94911	0.00000
C	0.70859	-3.62956	0.00000
C	2.80264	-5.15713	0.00000
C	4.22658	-5.17490	0.00000
C	4.95325	-6.39188	0.00000
H	6.92127	-3.04133	0.00000
H	8.12774	-5.19204	0.00000
H	6.86901	-7.33402	0.00000
H	4.40273	-7.32644	0.00000

H	4.78297	-1.75690	0.00000
H	2.23893	-6.08342	0.00000
O	-0.22725	-4.39044	0.00000
O	2.11946	-0.42188	0.00000
C	1.89438	-1.61063	0.00000
N	0.64134	-2.22779	0.00000
H	-0.25357	-1.73899	0.00000

Total electronic energy with ZPE = –2000.31652 a.u.
NIm = 2 (17.37*i* cm^{-1}, 6.86*i* cm^{-1})
P.G. = C_s

Tautomer

	X	Y	Z
C	2.19364	-3.65634	0.00000
C	0.78268	-3.66602	0.00000
C	0.08053	-2.48235	0.00000
C	0.75355	-1.23684	0.00000
C	0.03549	-0.00295	0.00000
C	0.75322	1.15730	0.00000
C	2.16805	1.17026	0.00000
C	2.57718	2.62100	0.00000
N	1.38128	3.41198	0.00000
C	0.38885	2.58578	0.00000
C	2.89226	0.01784	0.00000
C	2.19130	-1.22676	0.00000
C	2.88002	-2.46321	0.00000
H	-1.00420	-2.48933	0.00000
H	0.25249	-4.61137	0.00000
H	2.73655	-4.59445	0.00000
H	3.96461	-2.45513	0.00000
H	-1.04853	-0.00443	0.00000
H	3.97657	0.03795	0.00000
O	3.69674	3.06014	0.00000
O	-0.88664	2.95489	0.00000
H	-0.90686	3.92425	0.00000

Total electronic energy = –666.72574 a.u.
NIm = 0
Point Group (P.G.) = C_s