Supporting Information for:

Perylene Diimide Triple Helix Formation in the Solid-state

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Experimental Methods

^{1}H and ^{13}C NMR spectra were recorded using Bruker spectrometers. MALDI-TOF M/S spectra were recorded with a Bruker Ultraflex III mass spectrometer using trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]-malononitrile (DCTB) as the matrix. Elemental analysis was performed using an automated CE-440 Elemental Analyser.

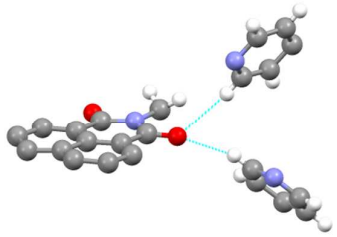

Figure S1. C-H…O hydrogen-bonding interactions adopted between C-H groups *ortho* to the pyridyl nitrogens and a carbonyl group of an adjacent PDI.

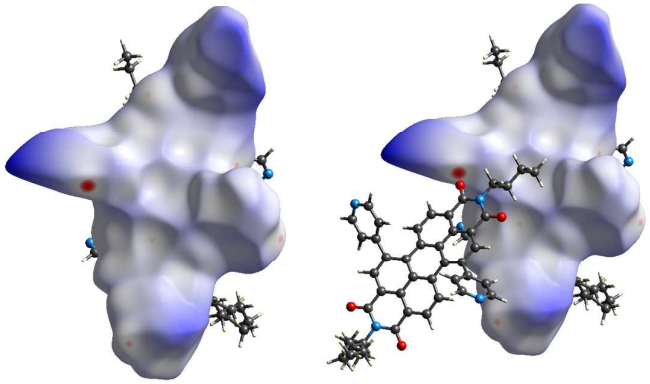

Figure S2. Views of the Hirshfeld surface calculated for **1** illustrating the intermolecular C-H…O interaction between one of the C-H *ortho* to the pyridyl nitrogen and carbonyl group on an adjacent PDI.

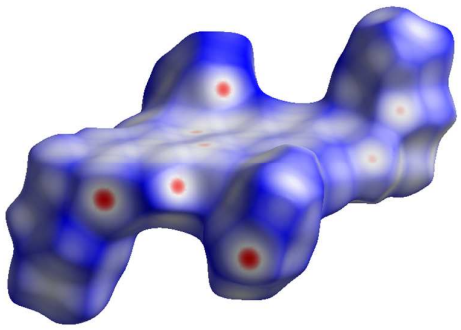

Figure S3. View of the Hirshfeld surface calculated for **2** indicating the intermolecular interactions that facilitate arrangement of the molecules into extended stacks.

Additional Experimental Description

Single Crystal X-ray Diffraction. Diffraction data for **1** were collected at Diamond Light Source, Beamline I19, on a CrystalLogic Kappa 4-circle diffractometer equipped with a Rigaku Saturn 724+ CCD detector using synchrotron radiation with a wavelength of 0.6889 Å.[S1] The raw data were reduced and corrected for Lorentz and polarisation effects using CrystalClear[S2] and corrected for the effects of adsorption using Scale implemented in CrystalClear. Diffraction data for **2** were collected on a Bruker P4 diffractometer equipped with a Bruker-Nonius FR591 rotating anode source, Mo Kα radiation (λ = 0.71073 Å). Both structures were solved by direct methods (SHELXS) and refined by full-matrix least-squares (SHELXL).[S3] Regions of diffuse solvent in the solvated structures were treated with the PLATON SQUEEZE routine.[S4]

For **1** disorder was observed in the pendant *n*-butyl group of molecule A. The terminal CH_3 of one of the pendant *n*-butyl group of molecule A is disordered over two positions. The occupancies of the two components were refined competitively, converging to a ratio of 0.54:0.46. The terminal $CH_2CH_2CH_3$ of one of the pendant *n*-butyl group of molecule B is disordered over two positions. The occupancies of the two components were refined competitively, converging to a ratio of 0.68:0.32. Enhanced rigid bond and similarity restraints were applied to the displacement parameters of these atoms. Chemically-equivalent bond lengths in the four *n*-butyl groups were restrained to be approximately equal.

One solvent position with the structure could be identified as a mixture of one molecule of $CHCl_3$ and half a molecule of *n*-hexane (the solvents used for crystallisation). The

occupancies of these two molecules were refined competitively, then fixed to a ratio of 0.7:0.3, respectively. The *n*-hexane molecule, which is on a centre of symmetry, was refined with isotropic displacement parameters. No other solvent molecules could be sensibly refined, so the structure was treated with PLATON SQUEEZE[S4]. Examination of the results from PLATON SQUEEZE, and the shape of the voids present after this procedure, revealed two types of void, both of which are continuous in the *c*-direction. The narrower voids had an electron density count of 28 electrons, and were assigned as a half an *n*-hexane molecule (half an *n*-hexane per void, 3 per cell). The larger voids, with an electron count of 138 electrons, have broad nodes part way along the channel, were assigned as containing $CHCl_3$ molecules (2 per void, 6 per cell). These solvent molecules were included in the formula and calculation of derived parameters.

Powder X-ray Diffraction.

Powder X-ray diffraction (PXRD) data were collected over the 2θ range 4-50^{o} on a Philips X'pert diffractometer using Cu-*Kα* radiation (λ = 1.5418 Å) at 40 kV and 40mA. Patterns were calculated for the single crystal structures of **1** and **2** using Mercury.[S5]

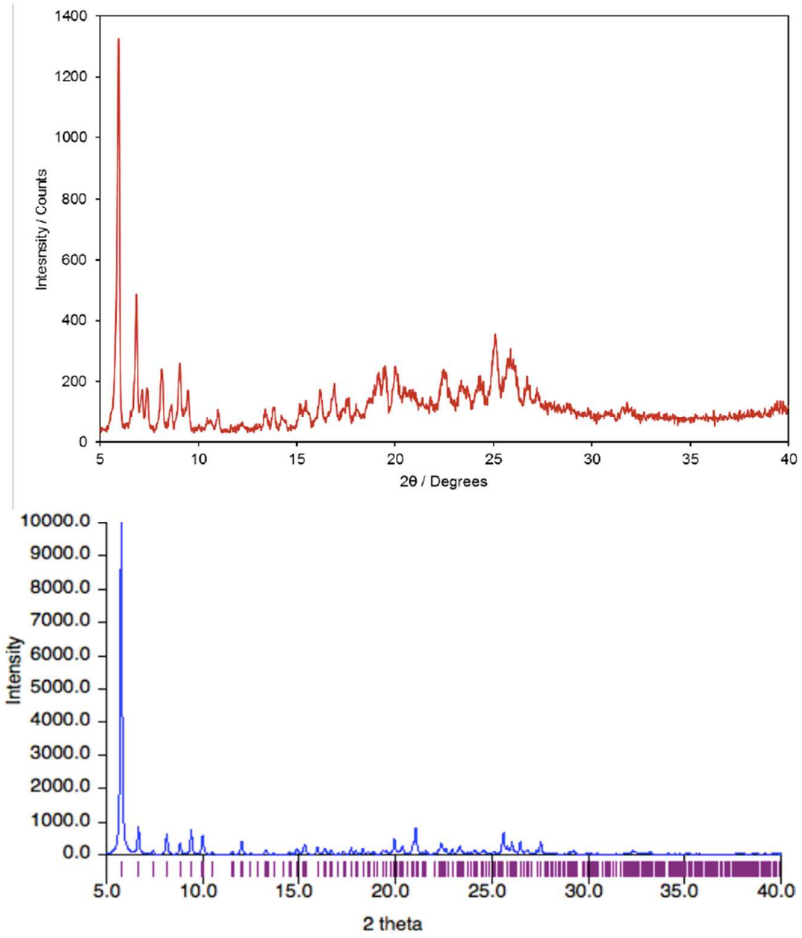

Fig. S4. PXRD patterns for **1**. Experimental above and calculated below.

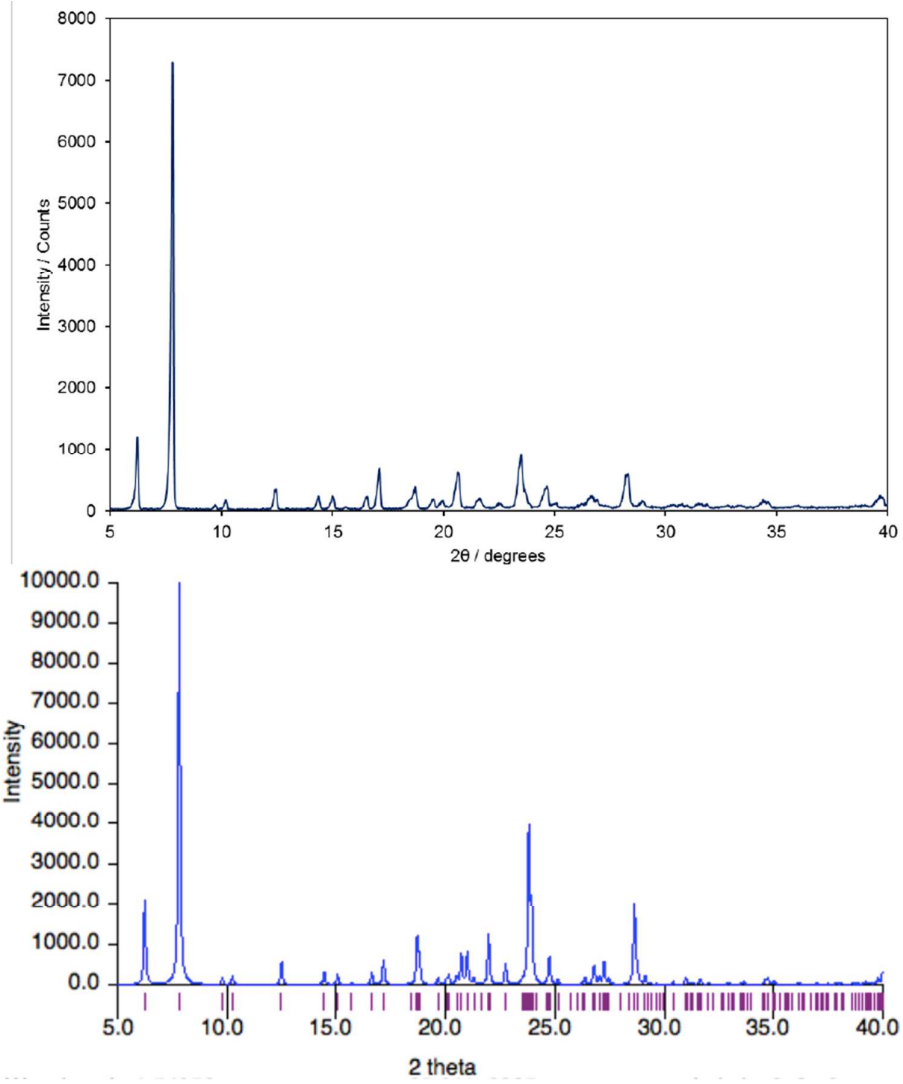

Fig. S5. PXRD patterns for **2**. Experimental above and calculated below.

UV-visible Spectra

UV-visible spectra were recorded for 10^{-5} M solutions of **1** and **2** in CH_2Cl_2 at 298 K. Thin films of each compound were studied by depositing a CH_2Cl_2 solution of the compound on the inside surface of a cuvette and evaporated under a stream of N_2.

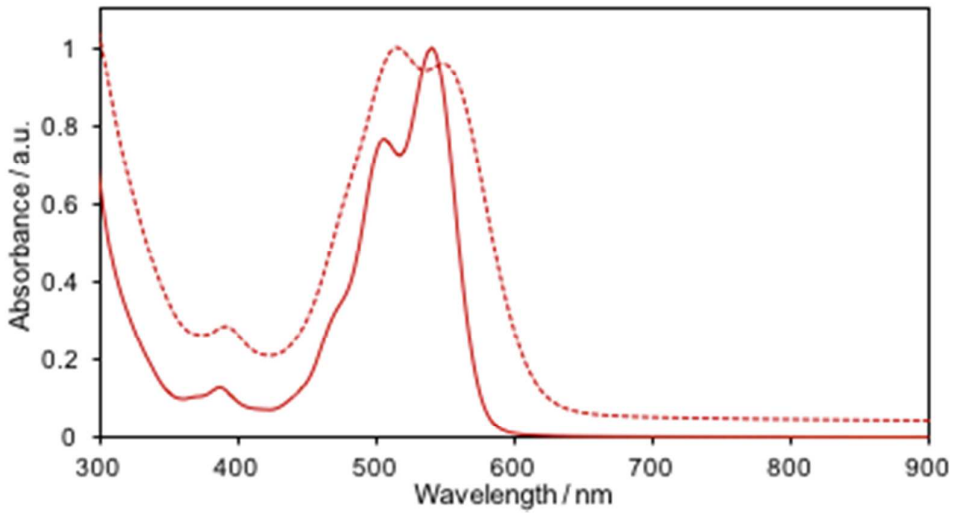

Fig. S6. UV-visible spectra for **1**. Solution spectra (CH_2Cl_2 solution) shown with continuous line; thin film, deposited from CH_2Cl_2 solution, shown with dotted line.

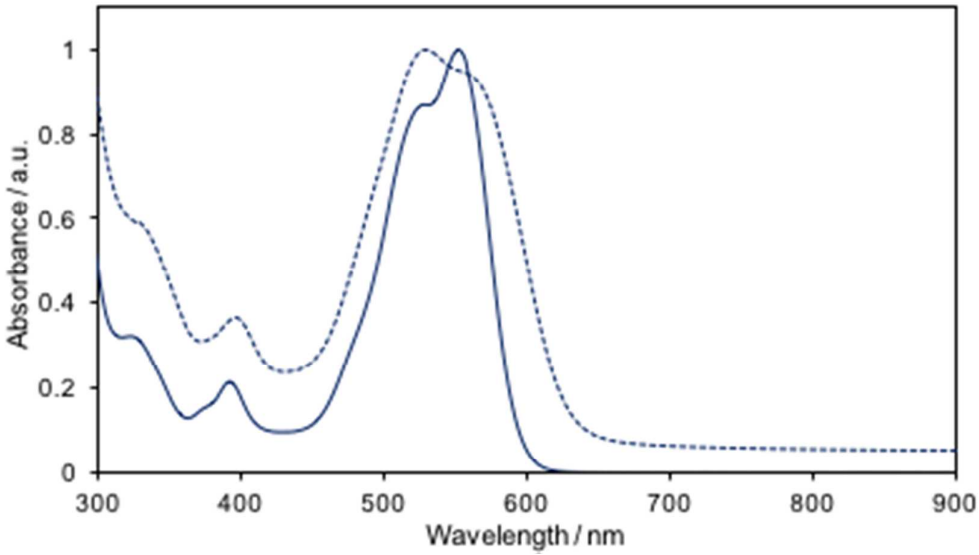

Fig. S7. UV-visible spectra for **2**. Solution spectra (CH_2Cl_2 solution) shown with continuous line; thin film, deposited from CH_2Cl_2 solution, shown with dotted line.

DFT Calculations

Density Functional Theory (DFT) calculations were performed using Gaussian 09 software with the B3LYP exchange-correlation function and a 6-311g(d,p) basis set for all atoms.[S6-S8] Geometry optimizations on models of **1** and **2** were performed in the gas phase. The calculated geometries were recognized as local minima by frequency calculations. Single

point calculations were accomplished in the gas phase for each molecule of **1** and **2** using the coordinates determined from X-ray crystallography.

Geometry Optimization of **1**

C	1.53892	2.40790	0.07303
C	2.94349	2.32173	-0.00862
H	3.54913	3.19397	0.20340
C	3.58434	1.15187	-0.35048
C	3.48777	-1.23383	-0.86272
C	2.74469	-2.38197	-1.05260
H	3.25428	-3.29375	-1.33745
C	1.36142	-2.36864	-0.85276
H	0.81875	-3.29069	-0.99133
C	-1.53607	-2.33073	0.11233
C	-2.94279	-2.24501	0.08672
H	-3.53921	-3.11980	0.31374
C	-3.59710	-1.07254	-0.21869
C	-3.52253	1.31919	-0.70539
C	-2.78828	2.47047	-0.90968
H	-3.30932	3.38540	-1.16185
C	-1.39798	2.45610	-0.76597
H	-0.86244	3.38070	-0.91454
C	-0.69998	1.29420	-0.43864
C	0.75646	1.27453	-0.22588
C	1.41291	0.01627	-0.41176
C	2.83100	-0.02595	-0.54055
C	0.67889	-1.21072	-0.48166
C	-0.76714	-1.19381	-0.20782
C	-1.43057	0.06598	-0.35316
C	-2.85267	0.10829	-0.42448
C	5.06424	1.14155	-0.47409
O	5.73851	2.13720	-0.28366

N	5.65728	-0.07629	-0.82881
C	4.96236	-1.27906	-1.02254
O	5.55289	-2.30388	-1.30918
C	-5.08051	-1.06355	-0.28847
O	-5.74540	-2.06380	-0.08933
N	-5.68815	0.15809	-0.60321
C	-5.00236	1.36431	-0.80707
O	-5.60458	2.39180	-1.05765
C	1.00124	3.71201	0.55777
C	0.21966	3.78814	1.71615
H	-0.05600	2.89074	2.25689
C	-0.19260	5.03475	2.17383
H	-0.79501	5.11170	3.07465
N	0.11047	6.18875	1.56946
C	0.86319	6.11367	0.46949
H	1.10527	7.05789	-0.01045
C	1.33492	4.91753	-0.06756
H	1.94154	4.92723	-0.96577
C	-0.97788	-3.63799	0.56401
C	-0.13613	-3.72134	1.67906
H	0.17112	-2.82710	2.20784
C	0.29625	-4.97089	2.10909
H	0.94570	-5.05310	2.97611
N	-0.04250	-6.12170	1.51755
C	-0.85289	-6.03997	0.45996
H	-1.12363	-6.98153	-0.00978
C	-1.34817	-4.84024	-0.04706
H	-2.00136	-4.84479	-0.91202
C	7.12645	-0.10402	-0.97795
H	7.42477	0.87806	-1.34217
H	7.35128	-0.85724	-1.73162
C	7.84763	-0.42861	0.33342

H	7.50012	-1.39998	0.70053
H	7.57787	0.32189	1.08375
C	9.37001	-0.45921	0.15909
H	9.71085	0.51078	-0.22202
H	9.63201	-1.19961	-0.60605
C	10.11143	-0.78563	1.45854
H	9.89614	-0.04348	2.23329
H	11.19370	-0.80192	1.30540
H	9.81534	-1.76515	1.84606
C	-7.16207	0.18498	-0.70001
H	-7.46638	-0.79518	-1.06048
H	-7.41504	0.94318	-1.44022
C	-7.82982	0.50955	0.64113
H	-7.43188	1.46184	1.00429
H	-7.55564	-0.26046	1.37022
C	-9.35978	0.60815	0.54340
H	-9.73948	0.97268	1.50368
H	-9.62531	1.37395	-0.19546
C	-10.06244	-0.70979	0.19645
H	-9.79130	-1.07137	-0.79901
H	-11.14884	-0.58863	0.21315
H	-9.80313	-1.49450	0.91368

Energy: -2140.29784343 A.U.

Single Point on Molecule A in **1**

C	-1.40585	-2.33859	0.35866
C	-2.82215	-2.28737	0.39802
H	-3.30877	-3.08748	0.55675
C	-3.51752	-1.10157	0.21189
C	-3.51926	1.33234	-0.11965

C	-2.82535	2.51887	-0.32583
H	-3.30262	3.32771	-0.46741
C	-1.42185	2.52626	-0.32603
H	-0.96684	3.34756	-0.47047
C	1.61784	2.52544	0.10584
C	3.01287	2.46132	-0.16550
H	3.53828	3.24608	-0.06103
C	3.62891	1.29242	-0.57678
C	3.51472	-1.10799	-1.07642
C	2.78302	-2.28877	-1.14644
H	3.19674	-3.08357	-1.46181
C	1.43229	-2.31091	-0.75213
H	0.95960	-3.13464	-0.77552
C	0.76058	-1.15120	-0.32474
C	-0.67231	-1.16365	0.05043
C	-1.37080	0.10212	-0.01225
C	-2.80356	0.11606	0.03049
C	-0.66748	1.35686	-0.11913
C	0.81735	1.36330	-0.08521
C	1.47445	0.10508	-0.34944
C	2.87593	0.09027	-0.65965
C	-5.00452	-1.12089	0.28517
O	-5.65087	-2.15628	0.39928
N	-5.64819	0.13303	0.24579
C	-5.00555	1.34663	-0.05345
O	-5.66523	2.37605	-0.23358
C	5.09975	1.29346	-0.85534
O	5.78231	2.31107	-0.74504
N	5.67686	0.07840	-1.26447
C	4.95635	-1.11020	-1.46477
O	5.49429	-2.10465	-1.94254
C	-0.82043	-3.66302	0.76198

C	0.10821	-3.75825	1.80760
H	0.45066	-2.97474	2.22189
C	0.52237	-5.02403	2.23099
H	1.15400	-5.07185	2.93910
N	0.08233	-6.18426	1.69735
C	-0.80250	-6.07406	0.69934
H	-1.12415	-6.87589	0.30386
C	-1.28747	-4.85969	0.19696
H	-1.92001	-4.84622	-0.51174
C	1.12871	3.83225	0.66685
C	0.29847	3.88470	1.80314
H	-0.00710	3.08233	2.20977
C	-0.07150	5.12219	2.32722
H	-0.63745	5.13386	3.09033
N	0.32717	6.30607	1.81355
C	1.12037	6.25053	0.72504
H	1.40478	7.07132	0.34043
C	1.55299	5.06237	0.12477
H	2.12226	5.08460	-0.63526
C	-7.12814	0.14771	0.38911
H	-7.40823	0.99785	0.81233
H	-7.40784	-0.59493	0.98064
C	-7.82302	0.00383	-0.97130
H	-7.54390	0.75168	-1.55706
H	-7.52851	-0.83992	-1.39658
C	-9.34764	0.00072	-0.85954
H	-9.63501	-0.77021	-0.30872
H	-9.64592	0.82880	-0.40694
C	-10.00162	-0.08889	-2.23836
H	-9.75911	0.70039	-2.76667
H	-10.97556	-0.12645	-2.13604
H	-9.68959	-0.89693	-2.69636

C	7.13233	0.07555	-1.60340
H	7.36692	0.93031	-2.04411
H	7.31748	-0.65787	-2.24241
C	8.01183	-0.10842	-0.34851
H	8.95626	0.04089	-0.60461
H	7.76848	0.59185	0.30802
C	7.91127	-1.46192	0.33801
H	8.11931	-2.16744	-0.32462
H	6.97593	-1.59683	0.63342
C	8.83736	-1.64248	1.55143
H	9.76847	-1.67985	1.24796
H	8.61049	-2.47603	2.01379
H	8.72311	-0.88681	2.16422

Energy: -2139.92641261 A.U.

Single Point on Molecule B in **1**

C	1.66373	2.47799	0.04785
C	3.07523	2.32359	-0.06540
H	3.63603	3.07290	0.09952
C	3.65317	1.11244	-0.40958
C	3.42043	-1.25915	-0.99899
C	2.62378	-2.38552	-1.14344
H	3.00515	-3.19755	-1.45662
C	1.25218	-2.33092	-0.82778
H	0.73420	-3.12627	-0.87325
C	-1.62776	-2.17623	0.14714
C	-3.04107	-2.05268	0.07503
H	-3.58172	-2.81431	0.24924
C	-3.65079	-0.85054	-0.24256
C	-3.51640	1.56760	-0.64034

C	-2.74577	2.72236	-0.74669
H	-3.16617	3.55411	-0.93092
C	-1.34468	2.66631	-0.58310
H	-0.84287	3.47144	-0.63677
C	-0.66819	1.45659	-0.34311
C	0.81024	1.37548	-0.20595
C	1.41161	0.07963	-0.42624
C	2.83097	-0.02586	-0.61863
C	0.62925	-1.12656	-0.44616
C	-0.81783	-1.05587	-0.16175
C	-1.44379	0.24031	-0.30131
C	-2.86823	0.32418	-0.39610
C	5.14286	0.98299	-0.44357
O	5.88546	1.88417	-0.05701
N	5.66146	-0.22501	-0.94249
C	4.88594	-1.34615	-1.27184
O	5.40506	-2.35638	-1.74024
C	-5.13321	-0.81306	-0.36665
O	-5.83342	-1.81843	-0.25390
N	-5.71933	0.43575	-0.64874
C	-5.00191	1.63584	-0.79740
O	-5.57989	2.68836	-1.05847
C	1.23945	3.81748	0.57306
C	0.53537	3.92412	1.78816
H	0.21391	3.14524	2.22760
C	0.31598	5.18607	2.33879
H	-0.14741	5.24100	3.16618
N	0.72718	6.33737	1.75826
C	1.37301	6.23091	0.58749
H	1.64983	7.03132	0.15719
C	1.66481	5.01003	-0.04202
H	2.13891	4.98923	-0.86497

C	-1.14470	-3.51137	0.63590
C	-0.26447	-3.63307	1.71869
H	0.14402	-2.86232	2.09554
C	0.00567	-4.90694	2.23885
H	0.59535	-4.96776	2.98098
N	-0.51928	-6.05226	1.75169
C	-1.33646	-5.91847	0.70108
H	-1.70321	-6.70983	0.32454
C	-1.69164	-4.69361	0.11503
H	-2.29148	-4.66591	-0.62107
C	7.14074	-0.34625	-1.05360
H	7.53436	0.55488	-1.16710
H	7.36479	-0.88015	-1.85660
C	7.75042	-1.00945	0.17694
H	7.45226	-1.95297	0.21460
H	7.41272	-0.55385	0.98834
C	9.27630	-0.97170	0.18662
H	9.57776	-0.02876	0.19317
H	9.61683	-1.39333	-0.64232
C	9.87378	-1.70431	1.40956
H	9.48557	-1.33712	2.23187
H	10.84548	-1.57874	1.42372
H	9.66827	-2.66057	1.35075
C	-7.20036	0.43822	-0.81919
H	-7.46686	-0.34521	-1.36271
H	-7.47010	1.25476	-1.30941
C	-7.93210	0.39153	0.52280
H	-7.86315	1.27709	0.96071
H	-7.49167	-0.27249	1.10983
C	-9.42214	0.01978	0.36597
H	-9.89415	0.29498	1.19149
H	-9.79442	0.55667	-0.37773

C	-9.72851	-1.33358	0.12048
H	-9.35016	-1.60320	-0.74201
H	-10.70159	-1.44984	0.10137
H	-9.34756	-1.88906	0.83254

Energy: -2139.91363401 A.U.

Geometry Optimization on **2**

C	0.41512	5.58616	-1.21991
C	0.12357	6.50952	-0.21635
C	8.60673	0.99702	-2.39623
C	-0.06317	4.28299	-1.13402
C	-0.66067	6.12341	0.86748
C	7.74514	1.02766	-1.13043
C	-0.84032	3.88016	-0.03973
C	-1.14672	4.81991	0.95164
C	-2.82804	2.48248	-0.13715
C	-1.42762	2.50414	-0.00117
C	7.90836	-0.23608	-0.27874
C	-4.99824	1.37766	-0.51455
C	-7.11458	0.24164	-1.03315
C	-3.52546	1.31588	-0.34255
C	-0.71041	1.28700	0.05866
C	1.44943	2.26914	0.88379
C	2.82459	2.21796	1.10917
C	-4.99423	-1.03737	-1.06849
C	0.72702	1.18830	0.37320
C	-2.82091	0.10052	-0.46331
C	-1.41082	0.06651	-0.22898
C	3.52512	1.05686	0.86142
C	-3.52518	-1.05690	-0.86128

C	4.99416	1.03734	1.06865
C	-7.90839	0.23623	0.27883
C	1.41078	-0.06656	0.22903
C	7.11454	-0.24163	1.03323
C	2.82087	-0.10055	0.46336
C	-2.82468	-2.21802	-1.10897
C	-0.72706	-1.18835	-0.37313
C	-1.44951	-2.26921	-0.88363
C	0.71039	-1.28705	-0.05866
C	3.52545	-1.31588	0.34253
C	4.99823	-1.37765	0.51454
C	2.82805	-2.48249	0.13705
C	1.42763	-2.50417	0.00109
C	1.14672	-4.81986	-0.95194
C	-7.74520	-1.02743	1.13063
C	0.84038	-3.88022	0.03956
C	0.66073	-6.12338	-0.86786
C	-8.60677	-0.99665	2.39644
C	0.06336	-4.28319	1.13390
C	-0.12338	-6.50963	0.21601
C	-0.41488	-5.58639	1.21970
H	1.01218	5.88334	-2.07464
H	8.46814	1.90204	-2.99377
H	0.49885	7.52410	-0.28384
H	9.67058	0.92211	-2.14977
H	8.35373	0.13931	-3.02744
H	0.16367	3.56962	-1.91819
H	7.99642	1.90856	-0.53039
H	-0.89939	6.83663	1.64828
H	6.69351	1.14565	-1.41400
H	-7.32452	1.15858	-1.58354
H	-3.37846	3.41475	-0.13206

H	8.96480	-0.35638	-0.00871
H	7.63804	-1.12179	-0.86169
H	-7.37570	-0.61812	-1.64715
H	-1.75724	4.52436	1.79784
H	0.94408	3.19066	1.11247
H	3.35760	3.08579	1.47608
H	-8.96483	0.35653	0.00879
H	7.37564	0.61809	1.64730
H	-7.63804	1.12199	0.86170
H	-3.35771	-3.08587	-1.47581
H	-0.94419	-3.19076	-1.11228
H	1.75714	-4.52419	-1.79816
H	7.32450	-1.15860	1.58354
H	3.37849	-3.41474	0.13189
H	-7.99651	-1.90838	0.53066
H	0.89940	-6.83651	-1.64875
H	-6.69357	-1.14542	1.41420
H	-9.67062	-0.92174	2.14997
H	-8.35374	-0.13890	3.02756
H	-0.16343	-3.56991	1.91815
H	-8.46820	-1.90163	2.99406
H	-0.49862	-7.52423	0.28344
H	-1.01184	-5.88368	2.07446
N	-5.64905	0.18252	-0.84131
N	5.64901	-0.18252	0.84138
O	-5.62521	2.41371	-0.38273
O	5.60998	2.02989	1.41237
O	-5.61007	-2.02994	-1.41212
O	5.62522	-2.41368	0.38263

Energy: -2108.21620830 A.U.

Single Point on Molecule **2**

C	0.51427	5.50857	-1.17890
C	0.20177	6.46678	-0.23277
C	8.26670	0.88738	-2.52067
C	0.03548	4.23043	-1.08178
C	-0.67642	6.13808	0.80264
C	7.55386	0.99658	-1.17857
C	-0.83336	3.87579	-0.02299
C	-1.20660	4.85352	0.89146
C	-2.83682	2.46738	-0.09943
C	-1.44214	2.49614	0.03829
C	7.80118	-0.23156	-0.30587
C	-4.98740	1.35658	-0.57048
C	-7.10573	0.19978	-1.03625
C	-3.52205	1.30190	-0.33632
C	-0.71859	1.28181	0.07715
C	1.45135	2.27414	0.86820
C	2.82457	2.22350	1.07932
C	-4.96886	-1.05372	-1.08145
C	0.72696	1.19321	0.36077
C	-2.82087	0.09224	-0.44674
C	-1.40544	0.05661	-0.21005
C	3.51105	1.07372	0.84262
C	-3.51105	-1.07372	-0.84262
C	4.96885	1.05372	1.08145
C	-7.80118	0.23156	0.30587
C	1.40544	-0.05661	0.21005
C	7.10573	-0.19978	1.03624
C	2.82087	-0.09224	0.44674
C	-2.82458	-2.22350	-1.07932
C	-0.72696	-1.19321	-0.36077

C	-1.45135	-2.27414	-0.86820
C	0.71859	-1.28181	-0.07715
C	3.52205	-1.30190	0.33632
C	4.98740	-1.35658	0.57048
C	2.83682	-2.46738	0.09943
C	1.44214	-2.49614	-0.03829
C	1.20660	-4.85352	-0.89146
C	-7.55386	-0.99659	1.17857
C	0.83336	-3.87579	0.02299
C	0.67642	-6.13808	-0.80264
C	-8.26670	-0.88739	2.52067
C	-0.03548	-4.23043	1.08178
C	-0.20176	-6.46678	0.23277
C	-0.51426	-5.50857	1.17890
H	1.07362	5.74187	-1.91119
H	8.08670	1.69010	-3.05263
H	0.57815	7.33745	-0.28627
H	9.23171	0.80348	-2.37160
H	7.94037	0.09730	-2.99997
H	0.28704	3.57937	-1.72650
H	7.87337	1.80492	-0.70376
H	-0.91198	6.79346	1.44815
H	6.58127	1.09828	-1.33254
H	-7.35732	1.00421	-1.55578
H	-3.32392	3.28002	-0.02502
H	8.77508	-0.32080	-0.15468
H	7.49961	-1.03504	-0.79891
H	-7.40481	-0.59674	-1.54287
H	-1.82651	4.64457	1.58013
H	0.98668	3.07637	1.07789
H	3.28477	2.99479	1.38961
H	-8.77508	0.32081	0.15468

H	7.40480	0.59674	1.54287
H	-7.49961	1.03504	0.79891
H	-3.28476	-2.99478	-1.38960
H	-0.98668	-3.07637	-1.07789
H	1.82651	-4.64457	-1.58013
H	7.35732	-1.00420	1.55578
H	3.32392	-3.28002	0.02502
H	-7.87337	-1.80492	0.70376
H	0.91198	-6.79346	-1.44815
H	-6.58127	-1.09828	1.33254
H	-9.23171	-0.80348	2.37160
H	-7.94038	-0.09730	2.99997
H	-0.28704	-3.57937	1.72650
H	-8.08669	-1.69010	3.05263
H	-0.57814	-7.33745	0.28627
H	-1.07362	-5.74187	1.91119
N	-5.62916	0.15693	-0.87952
N	5.62915	-0.15694	0.87953
O	-5.61335	2.39382	-0.49368
O	5.58102	2.05220	1.43208
O	-5.58101	-2.05220	-1.43208
O	5.61335	-2.39382	0.49368

Energy: -2107.81874951 A.U.

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