

Electronic Supplementary Information

Out of cross-conjugation: The unexpected structure of tetrazinones

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Crystallographic results

Structure of **2** has already been published. It was determined and refined again to be included here for completeness of the present study.

Table S1 Crystallographic data and structure refinement results for structures 1-5

Compound	1	2	3	4	5
Formula	C ₁₀ H ₁₄ N ₆ O	C ₂₃ H ₂₄ N ₆ O	C ₂₁ H ₂₀ N ₆ O	C ₂₂ H ₂₄ N ₆ O	C ₂₂ H ₁₅ N ₇ O
Formula weight	234.27	400.48	372.43	388.47	393.41
Crystal system	Tetragonal	Monoclinic	Orthorhombic	Orthorhombic	Triclinic
Space group (No.)	P4 ₂ /n (86)	P2 ₁ /n (14)	C222 ₁ (20)	P2 ₁ 2 ₁ 2 ₁ (19)	P-1 (2)
<i>a</i> / Å	17.028(4)	11.7079(10)	6.159(1)	9.7674(10)	9.1009(10)
<i>b</i> / Å	17.028(4)	15.3735(10)	18.715(2)	13.8678(10)	9.7574(10)
<i>c</i> / Å	8.0005(10)	11.8425(10)	15.977(2)	14.871(1)	11.9033(10)
α / °	90.00	90.00	90.00	90.00	97.231(10)
β / °	90.00	90.763(10)	90.00	90.00	112.188(10)
γ / °	90.00	90.00	90.00	90.00	95.337(10)
<i>V</i> / Å ³	2319.8(8)	2131.4(3)	1841.6(4)	2014.3(3)	960.48(17)
<i>Z</i>	8	4	4	4	2
<i>D</i> _c / g cm ⁻³	1.342	1.248	1.343	1.281	1.36
<i>F</i> (000)	992	848	784	824	408
μ / mm ⁻¹	0.09	0.08	0.09	0.08	0.09
Reflections collected	4528	4730	1031	2317	3876
Unique reflections with <i>I</i> > 2 σ (<i>I</i>),	494	2258	817	1546	3207
Parameters refined	156	277	130	266	271
GOF on <i>F</i> ²	0.84	1.16	0.800	1.08	1.17
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)]	0.092	0.063	0.044	0.051	0.046
<i>R</i> _{int}	0.068	0.034	0.008	0.01	0.009
<i>wR</i> (<i>F</i> ²)	0.181	0.243	0.131	0.128	0.131
$\Delta\rho_{\max}, \Delta\rho_{\min}$ / e Å ⁻³	0.20, -0.18	0.22, -0.28	0.16, -0.15	0.18, -0.18	0.23, -0.24

Crystallographic Figures

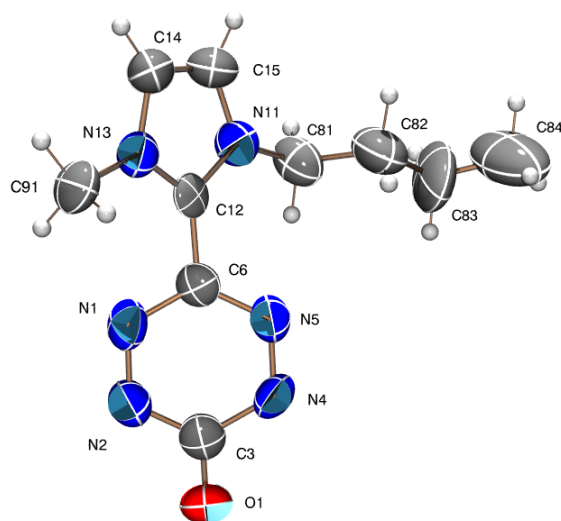


Figure S1. ORTEP view of molecule **1** at 50% probability level with numbering scheme.

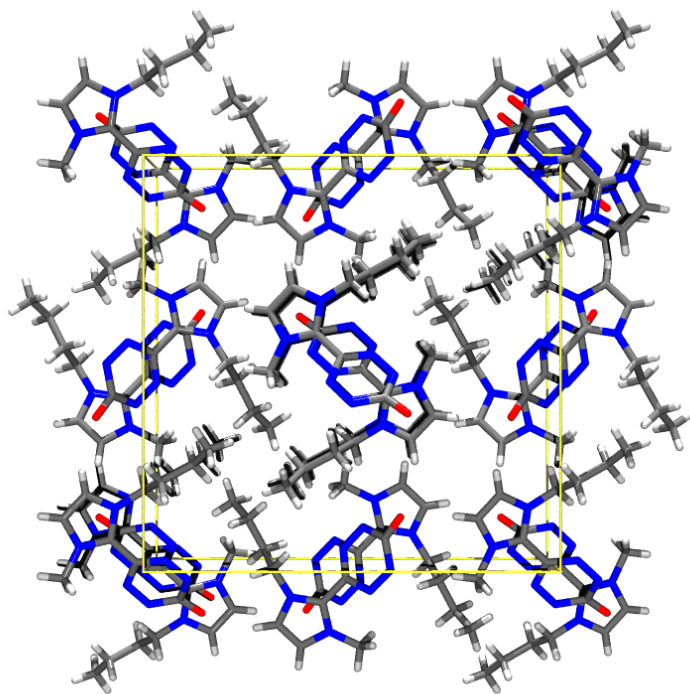


Figure S2. Packing diagram of **1** normal to (001).

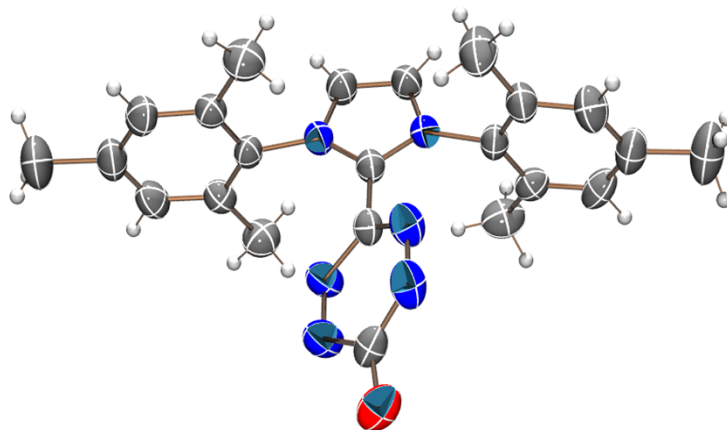


Figure S3. ORTEP view of molecule **2** at 50% probability level with numbering scheme.

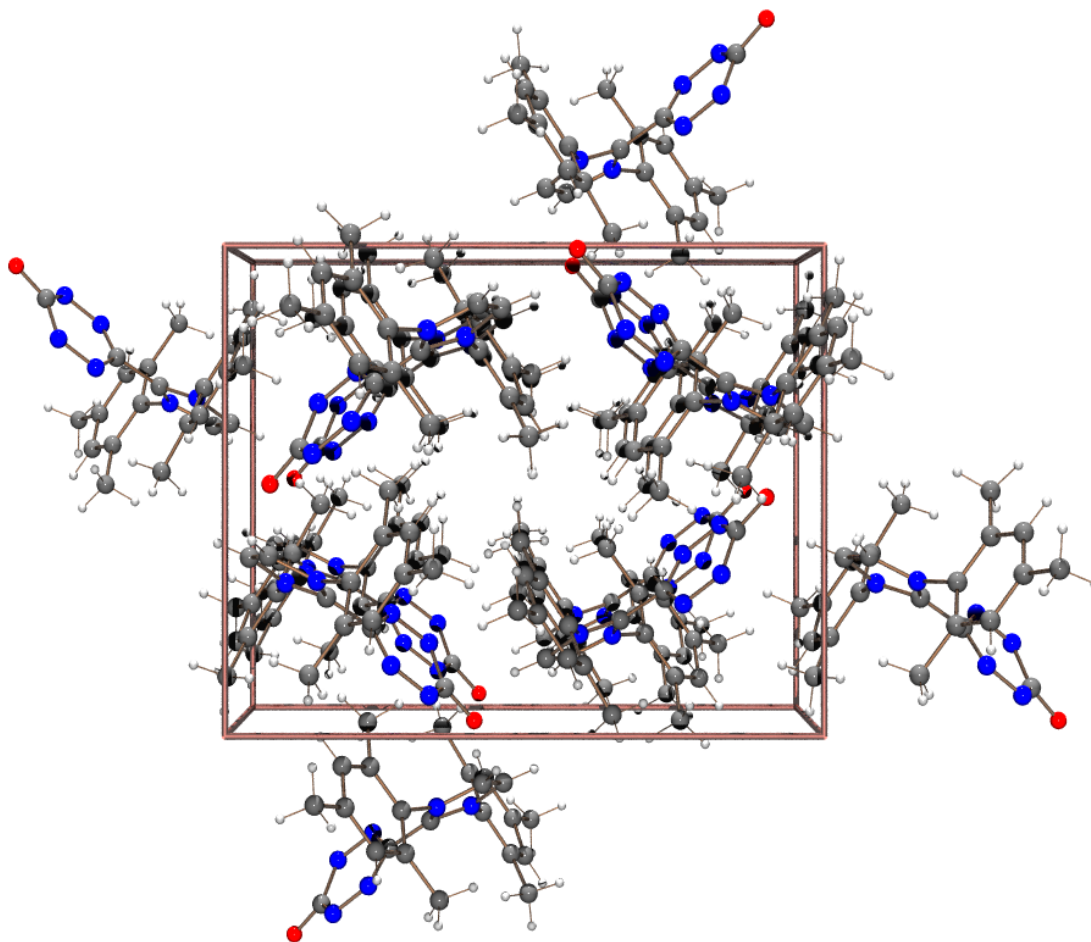


Figure S4. Packing diagram of **2** normal to (100).

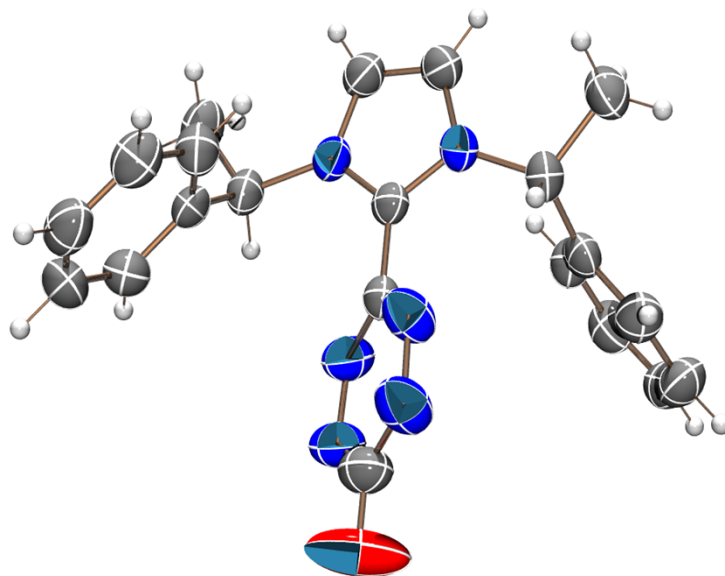


Figure S5. ORTEP view of molecule 3 at 50% probability level with numbering scheme.

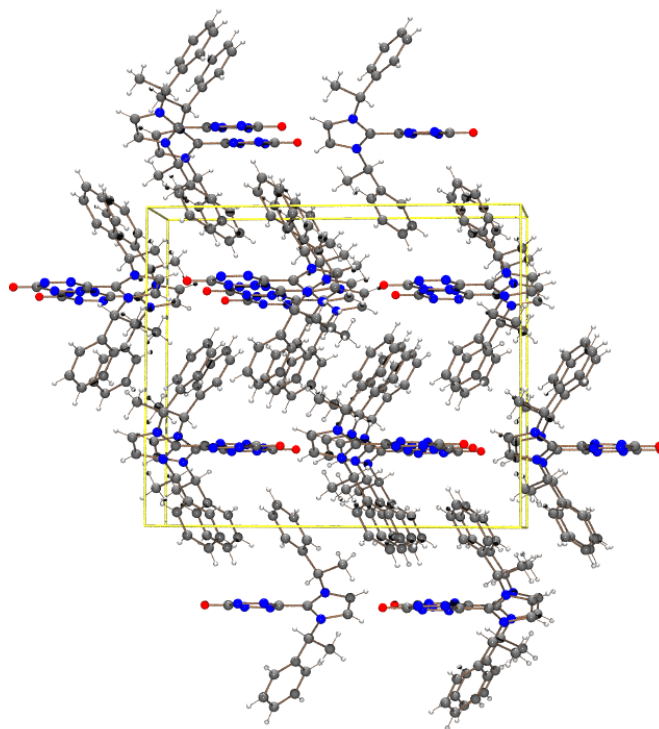


Figure S6. Packing diagram of 3 normal to (100).

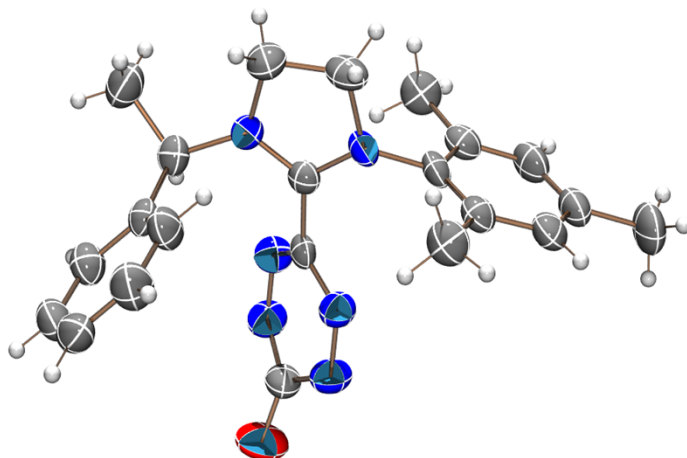


Figure S7. ORTEP view of structure **4** at 50% probability level.

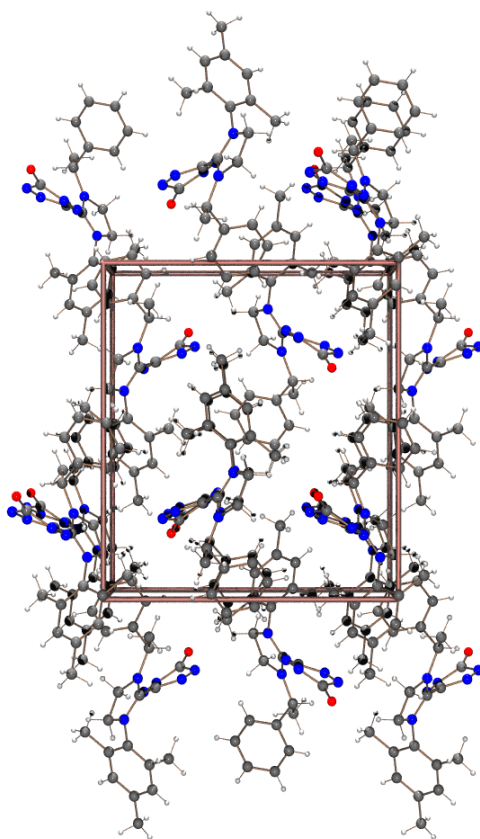


Figure S8. Packing diagram of **4** normal to (100).

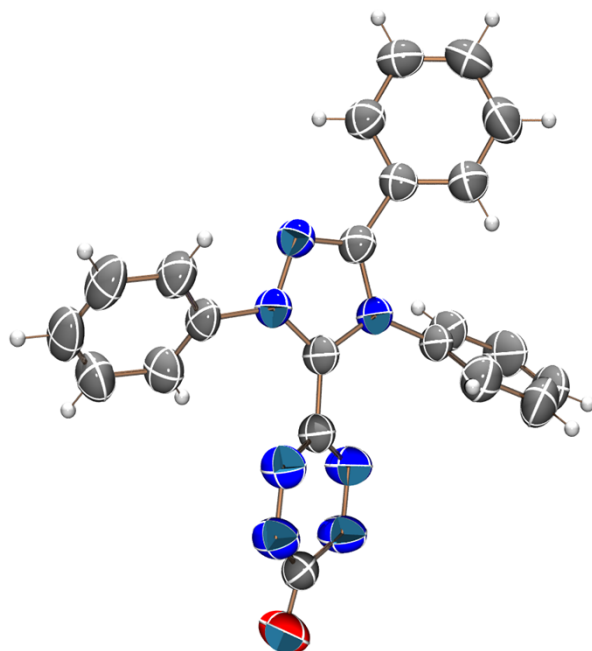


Figure S9. ORTEP view of structure **5** at 50% probability level.

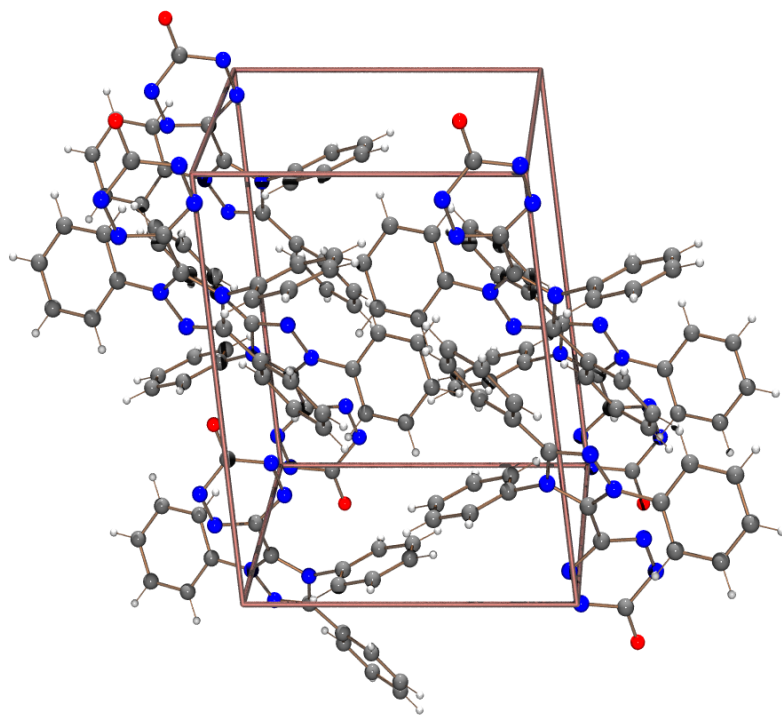


Figure S10. Packing diagram of **5** normal to (100).

Basis set effects in periodic calculations with BLYP+D3 functional.

Comparison of the results obtained by using DZVP (valence double-zeta plus a polarization function) and with TZV2P (valence triple-zeta plus two polarization functions) for molecule **3** in solid state.

	τ_1	τ_2	d(C-C)
DZVP	52.9	52.8	1.466
TZV2P	54.7	53.8	1.464

The results show that the agreement is very good between the two methods and the effect of the basis set increase is small.

Basis set and functional effects in gas-phase calculations

Basis set effects, calculated by employing different basis sets and ω B97xD functional for molecule **4**. Angles (τ) are in degree, distances (d) between the five membered and tetrazine rings are in Å.

	τ_1	τ_2	d(C-C)
ω B97xD/6-31G*	36.3	25.9	1.440
ω B97xD/6-31+G*	38.4	28.0	1.444
ω B97xD/6-311+G*	37.8	27.2	1.442
ω B97xD/6-311++G(3df,3pd)	34.4	25.2	1.437

The calculated parameters are nicely converged with respect to the size of the basis.

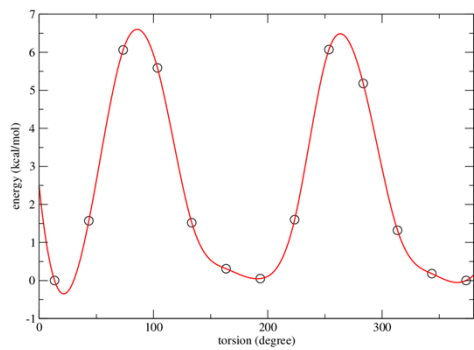
Functional effects, calculated for molecule **4** employing 6-31G* basis set (DZVP in periodic (PBC) calculations).

	τ_1	τ_2	d(C-C)
HF	31.5	30.5	1.437
BLYP	36.6	23.4	1.447
M062X	32.9	23.8	1.438
ω B97xD	36.3	25.9	1.440

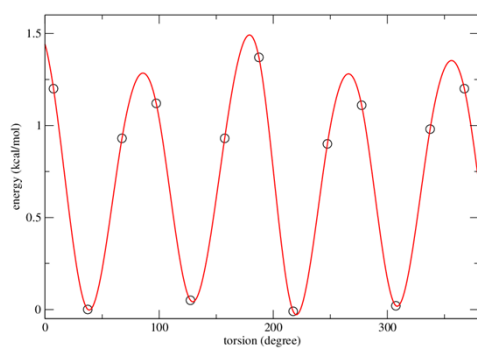
The calculated gas-phase Hartree-Fock (HF) and the DFT structural values are convincingly similar and show unequivocally the non-planar structure. Note that torsion is somewhat sensitive to correlation whereas the bond length is not.

Rotational curves of molecules 1-5

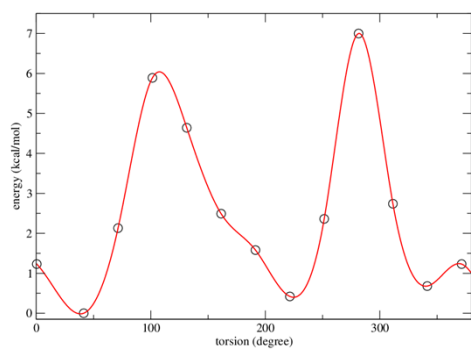
Molecule 1



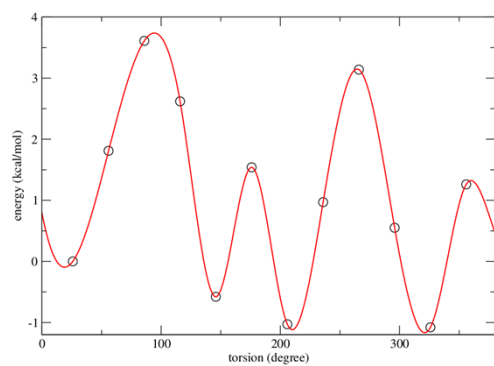
Molecule 2



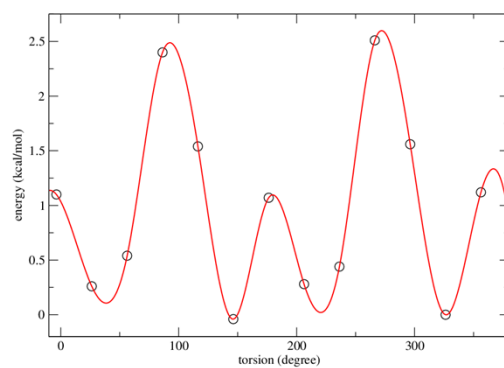
Molecule 3



Molecule 4



Molecule 5



N-N distances in the terazine rings of molecules 1-7 (Å)

	1	2	3	4	5	6	7
Experiment	1.315	1.307	1.321	1.304	1.305		
Theory, PBC ^a	1.326	1.324	1.325	1.325	1.322		
Theory, gas-phase ^b	1.285	1.287	1.289	1.285	1.286	1.284	1.282

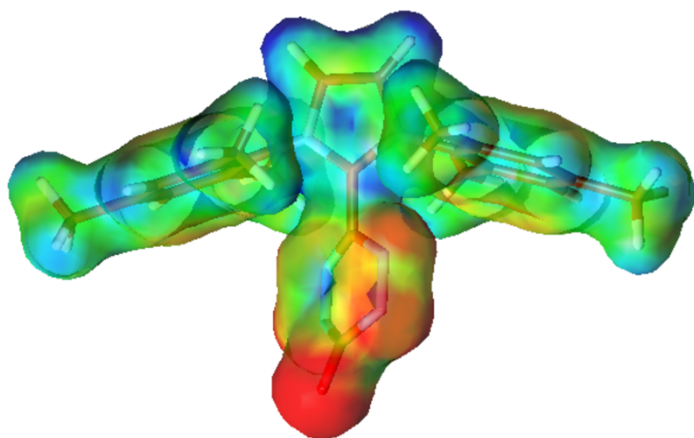
^aperiodic calculation employing BLYP functional and DZVP basis set^bgas-phase calculation employing ω B97X-D functional and 6-31G* basis set**Calculated dipole moments (gas-phase, ω B97X-D/6-31G* methodology, in Debye)**

	1	2	3	4	5	6	7
Dipole moment	13.4	13.2	12.9	12.8	13.4	14.0	13.7

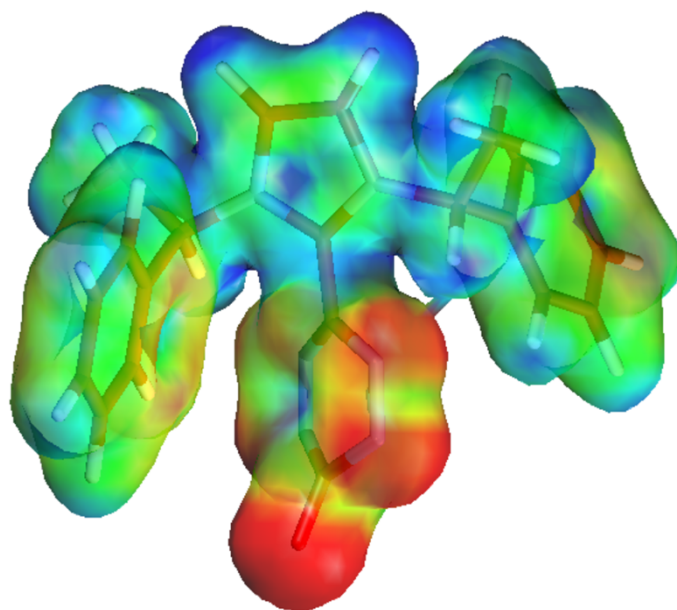
Molecular electrostatic potentials projected onto the total density for molecules 2-7.

The densities are generated with a contour value of 0.02 au for molecule 1. Blue and red colors indicate positive (0.1 au.) and negative (-0.1 au.) regions, respectively. The other colors indicate transient regions.

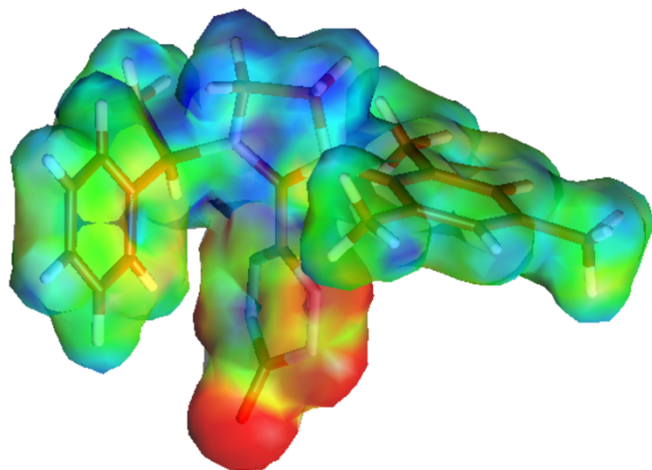
Molecule 2



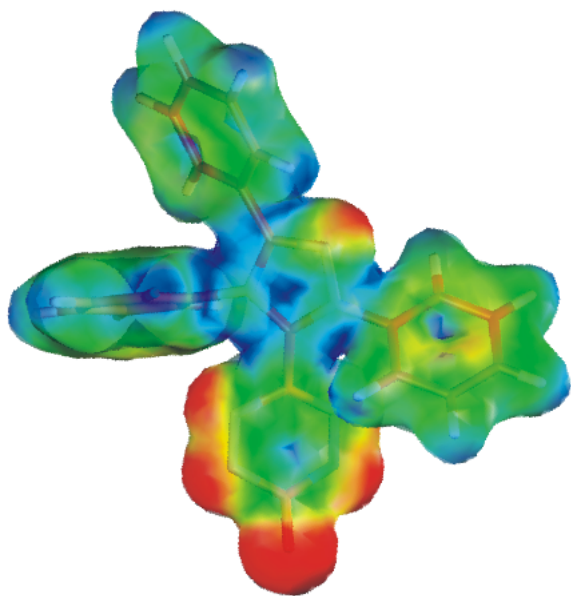
Molecule 3



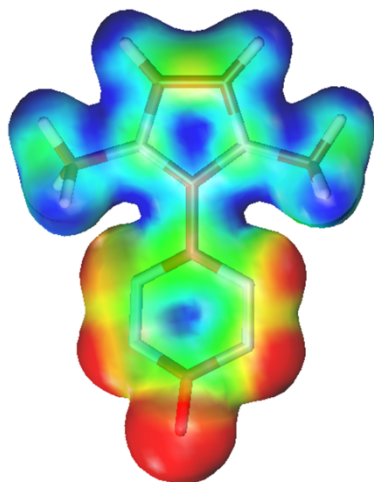
Molecule 4



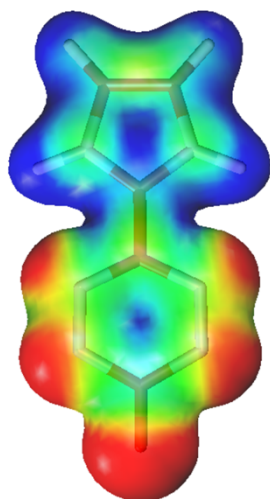
Molecule 5



Molecule 6



Molecule 7



Optimized XYZ coordinates and total energies of the molecules considered in this study

Molecule 1

Periodic calculation

BLYP

248
E = -1123.3723749298

C	18.3829466616	-1.3601707840	5.1278719314
C	16.5312225208	0.2483051992	6.1156540510
C	15.5297319431	1.2192980952	6.5516663670
C	13.6238758628	2.1691463139	7.2423083925
H	12.5811959014	2.1976620728	7.5325334001
C	14.5504371715	3.1582106567	7.0970577443
H	14.5090974375	4.2299342143	7.2378694330
C	16.9506931027	3.3122628692	6.3203051724
H	16.6195119429	4.2069467819	5.7884228684
H	17.5299737788	2.6930301598	5.6352172168
C	17.7658149995	3.7330943262	7.5508431551
H	17.9816017241	2.8546231156	8.1715980542
H	17.1602759022	4.4276190072	8.1445045929
C	19.0769542441	4.4146913499	7.1201360051
H	19.7193801727	3.6709963714	6.6334944667
H	18.8431524170	5.1712105759	6.3596502426
C	19.8269707870	5.0864702718	8.2746490338
H	20.7929227497	5.4757853480	7.9389833251
H	20.0240827219	4.3786347940	9.0880040390
H	19.2498953850	5.9234205334	8.6721064346
C	13.6111194602	-0.3541839574	7.0868551777
H	12.5378452110	-0.2096241058	7.2168988670
H	14.0408851656	-0.8189656468	7.9771046975
H	13.8019087492	-0.9712542430	6.2146572523
N	16.1227801996	-0.7699719875	5.3280615034
N	17.0283390768	-1.6171817327	4.8554699119
N	18.7283774237	-0.4440883986	6.1305599231
N	17.7926260205	0.3710280240	6.5981243490
N	15.7276884447	2.5578190304	6.6733132616
N	14.2365670800	0.9717548334	6.9008613381
O	19.2714238180	-1.9945736639	4.5153357924
C	7.1590533060	9.8741711804	5.1278717263
C	9.0107771057	8.2656946951	6.1156542797
C	10.0122678061	7.2947017863	6.5516655580
C	11.9181239582	6.3448539115	7.2423081385
H	12.9608036266	6.3163377550	7.5325332359
C	10.9915634865	5.3557894211	7.0970581810
H	11.0329026201	4.2840652495	7.2378697211
C	8.5912901545	5.2017532315	6.3203219032
H	8.9224888735	4.3070514057	5.7884222879
H	8.0120271867	5.8209686758	5.6352166533
C	7.7761887664	4.7809064239	7.5508414724
H	7.5603989675	5.6593766115	8.1715976059
H	8.3817243126	4.0863803265	8.1445047860
C	6.4650464120	4.0993091513	7.1201250968
H	5.8226179417	4.8430060240	6.6334932780
H	6.6988469603	3.3427921484	6.3596529104
C	5.7150289288	3.4275292869	8.2746500572
H	4.7490770028	3.0382148296	7.9389829129
H	5.5179174687	4.1353648611	9.0880034828
H	6.2921047011	2.5905791706	8.6721063590
C	11.9308803820	8.8681839163	7.0868549070
H	13.0041547013	8.7236241239	7.2168986687
H	11.5011150612	9.3329654278	7.9771043191
H	11.7400912043	9.4852541075	6.2146573986
N	9.4192200739	9.2839719774	5.3280609872
N	8.5136609476	10.1311823082	4.8554705683

N	6.8136224189	8.9580880128	6.1305591266
N	7.7493736374	8.1429716792	6.5981240931
N	9.8143127035	5.9561801762	6.6733132526
N	11.3054327614	7.5422452079	6.9008611039
O	6.2705755212	10.5085728843	4.5153357161
C	18.3881711144	9.8689469659	1.1276218524
C	16.7796946987	8.0172232696	2.1154044020
C	15.8087018540	7.0157321165	2.5514159473
C	14.8588534676	5.1098759663	3.2420583372
H	14.8303377831	4.0671960173	3.5322835471
C	13.8697891625	6.0364372605	3.0968080592
H	12.7980654362	5.9950975293	3.2376195500
C	13.7157404501	8.4366999883	2.3200689833
H	12.8210524782	8.1055116430	1.7881722562
H	14.3349697986	9.0159736131	1.6349667146
C	13.2949059416	9.2518138700	3.5505917794
H	14.1733768270	9.4676013812	4.1713478229
H	12.6003807315	8.6462758867	4.1442544040
C	12.6133058073	10.5629544282	3.1198849891
H	13.3570037559	11.2053802360	2.6332446373
H	11.8567899004	10.3291527310	2.3594004873
C	11.9415298755	11.3129707457	4.2743990188
H	11.5522148302	12.2789228685	3.9387332783
H	12.6493651114	11.5100826833	5.0877539950
H	11.1045794899	10.7358953907	4.6718564022
C	17.3821837847	5.0971195956	3.0866051315
H	17.2376239918	4.0238453243	3.2166489422
H	17.8469656243	5.5268854480	3.9768546838
H	17.9992541628	5.2879088183	2.2144071296
N	17.7979725614	7.6087802436	1.3278109981
N	18.6451822500	8.5143389651	0.8552203679
N	17.4720878768	10.2143775911	2.1303095589
N	16.6569718693	9.2786263055	2.5978739621
N	14.4701808329	7.2136880851	2.6730625241
N	16.0562449295	5.7225672406	2.9006109686
O	19.0225728373	10.7574238577	0.5150855284
C	7.1538294514	-1.3549463775	1.1276217175
C	8.7623052938	0.4967770592	2.1154037754
C	9.7332976884	1.4982679827	2.5514161497
C	10.6831470755	3.4041239858	3.2420584516
H	10.7116619746	4.4468039611	3.5322836687
C	11.6722105136	2.4775622332	3.0968075826
H	12.7439343672	2.5189025644	3.2376193620
C	11.8262467822	0.0772927071	2.3200712349
H	12.7209493122	0.4084891539	1.7881711391
H	11.2070311241	-0.5019726908	1.6349676745
C	12.2470947474	-0.7378144949	3.5505911660
H	11.3686229921	-0.9536011212	4.1713477264
H	12.9416192757	-0.1322759805	4.1442543101
C	12.9286976616	-2.0489527313	3.1198949306
H	12.1849953323	-2.6913810451	2.6332438479
H	13.6852106838	-1.8151525720	2.3593996724
C	13.6004696676	-2.7989706484	4.2743979915
H	13.9897853622	-3.7649227739	3.9387332833
H	12.8926347996	-2.9960826431	5.0877541528
H	14.4374205664	-2.2218952027	4.6718561918
C	8.1598160703	3.4168802740	3.0866050010
H	8.3043760939	4.4901547904	3.2166489793
H	7.6950344971	2.9871146573	3.9768546486
H	7.5427458270	3.2260912339	2.2144070172
N	7.7440280334	0.9052199146	1.3278114796
N	6.8968179401	-0.0003395186	0.8552202633
N	8.0699117545	-1.7003779102	2.1303098790
N	8.8850279918	-0.7646258285	2.5978743696
N	11.0718194918	1.3003116624	2.6730625664
N	9.4857551054	2.7914333440	2.9006113343
O	6.5194264095	-2.2434235980	0.5150854137
C	-1.3549477389	18.3881717139	2.8726273148
C	0.4967767106	16.7796947809	1.8848452419
C	1.4982679500	15.8087017565	1.4488350532
C	3.4041237484	14.8588534449	0.7581916977

H	4.4468039149	14.8303378243	0.4679667024
C	2.4775627868	13.8697894328	0.9034416080
H	2.5189025868	12.7980653576	0.7626300217
C	0.0772926952	13.7157512524	1.6801857317
H	0.4084887870	12.8210512680	2.2120783820
H	-0.5019721854	14.3349683958	2.3652818994
C	-0.7378133395	13.2949050886	0.4496575127
H	-0.9536015328	14.1733767497	-0.1710978307
H	-0.1322759637	12.6003809076	-0.1440045593
C	-2.0489575512	12.6133145436	0.8803714503
H	-2.6913792715	13.3570026092	1.3670047793
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N	2.5371544936	9.8108147928	5.3359769992
N	0.9067507910	11.2549420426	5.0874414070
O	-1.9166218369	6.1906516539	7.5686121934
C	9.8399046433	18.4622107912	6.9163948073
C	8.2779088879	16.5933042510	5.8883281994
C	7.3251500458	15.5726434406	5.4490985281
C	6.4238279353	13.6407744074	4.7469565636
H	6.4163041536	12.6030391453	4.4376675497
C	5.4084140700	14.5390675576	4.9026949215
H	4.3389736159	14.4707442364	4.7562208237
C	5.1784502098	16.9284607073	5.7057404766
H	4.2984928259	16.5630107735	6.2404615338
H	5.7811544391	17.5217877904	6.3956920046
C	4.7295727757	17.7378634795	4.4801545010

H	5.5971703869	17.9616083672	3.8444370768
H	4.0293123400	17.1233623357	3.9006527775
C	4.0455611813	19.0434917289	4.9327184889
H	4.7915595545	19.6779060410	5.4267931537
H	3.2924313746	18.7974202849	5.6931784255
C	3.3702873438	19.8261329625	3.7964407911
H	2.9960107210	20.7915547545	4.1541417824
H	4.0744349981	20.0318654237	2.9798132836
H	2.5224296556	19.2689164530	3.3923785770
C	8.9478011878	13.6791887355	4.9234087018
H	8.8134782418	12.6208205441	4.6943830332
H	9.4664479051	14.1854134249	4.1063198735
H	9.5113455046	13.7872899999	5.8447391954
N	9.3046034273	16.1929410905	6.6746295786
N	10.1328325015	17.1069644363	7.1609875032
N	8.9501902916	18.7990629764	5.8835351537
N	8.1495356613	17.8547646964	5.4013052006
N	5.9768452655	15.7311852867	5.3359767621
N	7.6072490906	14.2870583041	5.0874413288
O	10.4306216750	19.3513477795	7.5686122725

Gas-phase calculation

BLYP

```

31
scf done: -792.862842265
C 1.321463 3.195776 -0.795705
C -4.194099 -2.948631 -0.786886
C -2.717008 -0.943524 -0.148636
C -1.032399 3.184250 0.123998
C 2.872728 -1.647687 0.010334
C 0.984068 0.132151 -0.138306
C -3.421908 -2.230043 0.339529
C -0.012056 1.164196 0.042177
C -1.913215 2.257403 0.603960
C -1.957640 -0.242231 0.996187
H 1.599564 2.735864 -1.751406
H -3.517618 -3.240518 -1.608257
H -1.989573 -1.194907 -0.937805
H 1.046688 4.250899 -0.938151
H -4.980165 -2.300228 -1.212604
H -3.458702 -0.246066 -0.582401
H -4.680906 -3.864068 -0.411443
H -1.125602 4.257965 -0.000710
H 2.179569 3.111445 -0.116866
H -2.664770 -2.915647 0.761814
H -2.926085 2.364178 0.977822
H -4.117469 -1.983607 1.165111
H -1.186777 -0.908068 1.402160
H -2.643831 0.051171 1.808190
N 1.524528 -2.109775 -0.097601
N 0.588689 -1.185762 -0.085561
N 0.140571 2.512786 -0.223897
N 3.180101 -0.393833 -0.613695
N 2.230958 0.512325 -0.584912
N -1.283095 1.012812 0.562762
O 3.748208 -2.327314 0.546410

```

M062X

```

31
scf done: -792.805094787
C 1.304469 3.124548 -0.801727
C -4.035387 -2.939264 -0.766911
C -2.706651 -0.882805 -0.124285

```

```

C -1.042096 3.188768 0.075396
C 2.701884 -1.737510 -0.059235
C 0.917277 0.137844 -0.064721
C -3.262139 -2.227481 0.339682
C -0.059172 1.188298 0.076861
C -1.937149 2.292556 0.547686
C -1.978533 -0.171560 1.009328
H 1.606221 2.579745 -1.694940
H -3.392716 -3.116563 -1.634674
H -1.995868 -1.042870 -0.940809
H 1.032399 4.149719 -1.054916
H -4.889876 -2.339605 -1.097798
H -3.516843 -0.242428 -0.498753
H -4.414370 -3.906327 -0.426523
H -1.117634 4.252435 -0.082379
H 2.131073 3.106545 -0.093904
H -2.425045 -2.854573 0.669090
H -2.953754 2.412001 0.886581
H -3.912555 -2.080288 1.212132
H -1.215773 -0.819702 1.440799
H -2.672083 0.127829 1.801372
N 1.335820 -2.085086 -0.222314
N 0.475026 -1.138903 -0.160534
N 0.117584 2.498289 -0.217317
N 3.099465 -0.406997 -0.354124
N 2.201477 0.502728 -0.286065
N -1.316885 1.059632 0.557334
O 3.516056 -2.567666 0.271279

```

ωB97xD

```

31
scf done: -792.883533192
C 1.292357 3.138308 -0.809039
C -4.081654 -2.924086 -0.766402
C -2.704067 -0.893403 -0.124070
C -1.047214 3.171748 0.083678
C 2.732390 -1.713404 -0.027749
C 0.942942 0.141862 -0.086095
C -3.301634 -2.220556 0.342138
C -0.043762 1.182514 0.064935
C -1.927804 2.264570 0.557545
C -1.946463 -0.199774 1.002001
H 1.605398 2.597400 -1.701107
H -3.434352 -3.133528 -1.624685
H -2.001888 -1.075882 -0.943513
H 1.008381 4.159547 -1.067870
H -4.916189 -2.305896 -1.117016
H -3.496306 -0.230093 -0.497669
H -4.492555 -3.875803 -0.416234
H -1.137914 4.235343 -0.065361
H 2.119799 3.137444 -0.101166
H -2.488265 -2.870519 0.687247
H -2.942741 2.373946 0.903733
H -3.959422 -2.050242 1.205522
H -1.174626 -0.856999 1.402395
H -2.618053 0.083771 1.818639
N 1.386270 -2.074776 -0.272706
N 0.511715 -1.134035 -0.222689
N 0.117294 2.495795 -0.223760
N 3.131961 -0.392674 -0.347014
N 2.226360 0.516764 -0.291426
N -1.296200 1.037366 0.555055
O 3.530464 -2.523399 0.388292

```

Molecule 2

Periodic calculation

BLYP

216			
E =	-879.8534198930		
C	9.2392847640	5.6326287860	1.0063144007
C	10.1549604627	3.7037960778	2.5323619195
C	10.6398207165	2.5396135049	3.2607099455
C	10.7839751047	0.5118914383	4.2274320016
H	10.3999388797	-0.4364314709	4.5744051179
C	12.0070357574	1.0928958110	4.3128139752
H	12.9306001238	0.7894835373	4.7817389300
C	8.5317982432	1.1224382718	3.3238992655
C	7.6003091312	1.4849484482	4.3090844170
C	6.2738540249	1.0908549577	4.1178950989
H	5.5437122396	1.3447944630	4.8805255227
C	5.8806135261	0.3608250458	2.9905644526
C	6.8421932577	0.0321365849	2.0265446138
H	6.5489202536	-0.5426776659	1.1493730289
C	8.1903091640	0.3796845622	2.1841913691
C	8.0100231485	2.2385455252	5.5490884939
H	7.1519998991	2.3767419988	6.2080734924
H	8.4095833204	3.2244468140	5.2834493118
H	8.7836848419	1.6954985962	6.1057506314
C	4.4567804080	-0.1209383143	2.8675657395
H	3.7846409342	0.4887757265	3.4782474858
H	4.3743741996	-1.1559795502	3.2221259608
H	4.1137670057	-0.1104788752	1.8280064532
C	9.2268806630	-0.1111633269	1.2018947986
H	8.7741591319	-0.2879025398	0.2239817121
H	9.6560178013	-1.0593348447	1.5499452798
H	10.0552292822	0.5922522629	1.0682930310
C	13.0321878639	3.2830170822	3.7391232063
C	13.1628758564	4.1337395108	4.8456989131
C	14.3597985775	4.8468593354	4.9651941721
H	14.4903659232	5.4944447358	5.8261356433
C	15.3937107827	4.7229666625	4.0289811326
C	15.1929658650	3.8953574330	2.9194869981
H	15.9841589224	3.7962320579	2.1808111903
C	14.0168215358	3.1612683010	2.7503070241
C	12.0802688241	4.2506728486	5.8947736005
H	11.1014214857	4.4602638539	5.4460625012
H	12.3104920260	5.0542246507	6.5998291580
H	11.9906664322	3.3223315799	6.4736194623
C	16.6950713523	5.4464885289	4.1944064738
H	17.0274027415	5.4361911070	5.2390520084
H	16.6077534804	6.5009823416	3.8943931408
H	17.4889068442	5.0019549681	3.5857211194
C	13.8198508738	2.2867094639	1.5399760236
H	13.5694197812	1.2547842069	1.8108203466
H	14.7271477493	2.2668798798	0.9320719057
H	13.0018959143	2.6777195877	0.9233098082
N	11.0317348671	4.2976440397	1.6836532783
N	10.6050759230	5.3092474965	0.9491432656
N	8.4654039715	5.1960662052	2.0973552334
N	8.9303514912	4.1979689038	2.8360211395
N	9.9382036116	1.4109568199	3.5758243355
N	11.9122614249	2.3544624711	3.7185164487
O	8.7342326829	6.3642265539	0.1314936772
C	8.2438391257	13.3191935120	4.9147880020
C	7.3279208777	11.3902040413	3.3890222758
C	6.8429151475	10.2261066220	2.6607341422
C	6.6987466001	8.1984917805	1.6939391593
H	7.0822674642	7.2497417445	1.3476772155
C	5.4758048400	8.7796723597	1.6082348965
H	4.5525983832	8.4769623452	1.1380914403

C	8.9511741568	8.8092534610	2.5973138782
C	9.8826151632	9.1713758331	1.6119615501
C	11.2091382127	8.7774858008	1.8033664687
H	11.9393097441	9.0310052417	1.0405686077
C	11.6024989174	8.0476506022	2.9308235759
C	10.6408751363	7.7190466052	3.8947797402
H	10.9337904790	7.1439299789	4.7718700022
C	9.2928804669	8.0668955245	3.7370858350
C	9.4724662477	9.9234471675	0.3712373411
H	10.3303363377	10.0614521418	-0.2880235131
H	9.0720831425	10.9093757100	0.6356531049
H	8.6990683595	9.3791091759	-0.1845626391
C	13.0263504607	7.5657586444	3.0537094769
H	13.6984982490	8.1754188910	2.4430186154
H	13.1086840509	6.5307814730	2.6989838299
H	13.3697213680	7.5759881876	4.0931317846
C	8.2563009189	7.5764805581	4.7194010334
H	8.7088949557	7.3994428765	5.6973105205
H	7.8267432894	6.6286035806	4.3711874708
H	7.4283527789	8.2803123002	4.8531298182
C	4.4503618241	10.9693505729	2.1822115964
C	4.3202932306	11.8202192444	1.0757290513
C	3.1236846182	12.5337318002	0.9558365720
H	2.9934193461	13.1814812993	0.0949549882
C	2.0895165584	12.4097607091	1.8917183174
C	2.2895940501	11.5821077872	3.0010974998
H	1.4979694878	11.4830381650	3.7392392574
C	3.4654312105	10.8477809395	3.1707482794
C	5.4033079519	11.9364375852	0.0270848599
H	6.3819267200	12.1461781963	0.4761061270
H	5.1736969636	12.7394728754	-0.6786881941
H	5.4931177768	11.0076614047	-0.5508889161
C	0.7881448899	13.1333045650	1.7262923798
H	0.4559398746	13.1234467633	0.6816119033
H	0.8753856326	14.1877027578	2.0266679455
H	-0.0058273862	12.6886169298	2.3347198123
C	3.6612923239	9.9730847476	4.3810882151
H	3.9107928192	8.9409143009	4.1103953958
H	2.7537998578	9.9539562244	4.9887182563
H	4.4792395471	10.3632335890	4.9982639422
N	6.4514974717	11.9836256357	4.2380872705
N	6.8786091568	12.9946214703	4.9733479952
N	9.0169201785	12.8834602988	3.8226936922
N	8.5522147936	11.8846674937	3.0849219686
N	7.5445362125	9.0974323629	2.3458343491
N	5.5704120940	10.0410274603	2.2030014416
O	8.7490751087	14.0511006555	5.7892474785
C	2.3115354546	9.7408712567	10.8351441938
C	1.3958598448	11.6697037966	9.3090967795
C	0.9110014011	12.8338849769	8.5807480079
C	0.7668467486	14.8616082992	7.6140273940
H	1.1508798065	15.8099310785	7.2670528761
C	-0.4562144211	14.2806055329	7.5286432919
H	-1.3797820176	14.5840167556	7.0597192319
C	3.0190157875	14.2510612774	8.5175576140
C	3.9505081134	13.8885523242	7.5323755500
C	5.2769661310	14.2826446307	7.7235633204
H	6.0071091642	14.0287054669	6.9609310901
C	5.6702078788	15.0126760555	8.8508936383
C	4.7086264572	15.3413628340	9.8149138530
H	5.0018999631	15.9161786784	10.6920869328
C	3.3605091770	14.9938137172	9.6572646855
C	3.5407968027	13.1349550007	6.2923703109
H	4.3988202447	12.9967575009	5.6333836840
H	3.1412355321	12.1490529096	6.5580090126
H	2.7671345513	13.6780016187	5.7357069829
C	7.0940402996	15.4944386811	8.9738924455
H	7.7661776518	14.8847244856	8.3632110264
H	7.1764450925	16.5294786944	8.6193323539
H	7.4370521280	15.4839787821	10.0134506169
C	2.3239395596	15.4846631798	10.6395633144

H	2.7766613131	15.6614026935	11.6174774022
H	1.8948019595	16.4328354225	10.2915125644
H	1.4955901397	14.7812474015	10.7731654797
C	-1.4813693712	12.0904830870	8.1023343351
C	-1.6120609470	11.2397588127	6.9957607173
C	-2.8089822109	10.5266390441	6.8762658471
H	-2.9395453001	9.8790574332	6.0153243589
C	-3.8428918140	10.6505352542	7.8124789947
C	-3.6421460374	11.4781406276	8.9219699259
H	-4.4333375216	11.5772684371	9.6606456468
C	-2.4660028487	12.2122306441	9.0911495559
C	-0.5294529194	11.1228278806	5.9466884760
H	0.4493959353	10.9132367621	6.3953916970
H	-0.7596690517	10.3192792377	5.2416310105
H	-0.4398442395	12.0511642251	5.3678392083
C	-5.1442524512	9.9270098732	7.6470504427
H	-5.4765839173	9.9373031529	6.6024054033
H	-5.0569400116	8.8725184591	7.9470672827
H	-5.9380912851	10.3715459350	8.2557332052
C	-2.2690313224	13.0867878600	10.3014784119
H	-2.0186012260	14.1187118895	10.0306414695
H	-3.1763227145	13.1066212602	10.9093844324
H	-1.4510798522	12.6957832983	10.9181473289
N	0.5190848231	11.0758564060	10.1578043159
N	0.9457434604	10.0642534116	10.8923143264
N	3.0854136179	10.1774330210	9.7441029018
N	2.6204671574	11.1755299791	9.0054363540
N	1.6126153359	13.9625425750	8.2656343659
N	-0.3614401188	13.0190377346	8.1229440176
O	2.8165869004	9.0092727178	11.7099649978
C	3.3069796188	2.0543073170	6.9266705446
C	4.2228995672	3.9832966206	8.4524353650
C	4.7079054584	5.1473935145	9.1807241017
C	4.8520734786	7.1750080345	10.1475193026
H	4.4685513649	8.1237583796	10.4937812389
C	6.0750153580	6.5938270365	10.2332234335
H	6.9982210133	6.8965381517	10.7033668344
C	2.5996432832	6.5642472333	9.2441444988
C	1.6682035639	6.2021238334	10.2294977892
C	0.3416815738	6.5960140123	10.0380920559
H	-0.3884897137	6.3424950284	10.8008888890
C	-0.0516781672	7.3258489598	8.9106344466
C	0.9099451174	7.6544536109	7.9466783456
H	0.6170298464	8.2295698191	7.0695889069
C	2.2579387986	7.3066050540	8.1043718189
C	2.0783534541	5.4500527361	11.4702211601
H	1.2204835751	5.3120480421	12.1294816050
H	2.4787360882	4.4641245420	11.2058051508
H	2.8517511467	5.9943904074	12.0260207051
C	-1.4755301114	7.8077414199	8.7877486875
H	-2.1476789645	7.1980809680	9.3984397946
H	-1.5578648718	8.8427193044	9.1424744293
H	-1.8189018420	7.7975120193	7.7483258231
C	3.2945187930	7.7970193215	7.1220573759
H	2.8419249446	7.9740572319	6.1441482455
H	3.7240762592	8.7448959573	7.4702708482
H	4.1224667964	7.0931879509	6.9883283178
C	7.1004577783	4.4041502589	9.6592470635
C	7.2305260257	3.5532799534	10.7657295852
C	8.4271352753	2.8397680763	10.8856214814
H	8.5574003183	2.1920180695	11.7465034027
C	9.4613023832	2.9637391386	9.9497406519
C	9.2612240538	3.7913940946	8.8403582143
H	10.0528515404	3.8904615144	8.1022178028
C	8.0853865592	4.5257212912	8.6707084029
C	6.1475095776	3.4370620963	11.8143752158
H	5.1688914896	3.2273209025	11.3653498216
H	6.3771247881	2.6340251871	12.5201474014
H	6.0577023011	4.3658408918	12.3923474897
C	10.7626737356	2.2401960650	10.1151648069
H	11.0948803092	2.2500525656	11.1598475163

H	10.6754341578	1.1857965499	9.8147899635
H	11.5566474015	2.6848823805	9.5067390940
C	7.8895271878	5.4004167633	7.4603678556
H	7.6400265645	6.4325859071	7.7310642168
H	8.7970216235	5.4195435131	6.8527394222
H	7.0715794399	5.0102650774	6.8431949157
N	5.0993216703	3.3898744623	7.6033713595
N	4.6722098945	2.3788789738	6.8681105577
N	2.5338986339	2.4900407781	8.0187635454
N	2.9986045493	3.4888326099	8.7565359335
N	4.0062832634	6.2760676753	9.4956239635
N	5.9804087253	5.3324729056	9.6384568894
O	2.8017445730	1.3223995567	6.0522108007

BLYP+D3

216

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C	10.7623314896	0.5192941003	4.2398965232
H	10.3863521522	-0.4336660491	4.5793577205
C	11.9867152439	1.0996091044	4.3177099395
H	12.9161536072	0.7931169075	4.7729752614
C	8.4934209588	1.1211881987	3.3710413952
C	7.5593000152	1.4881329636	4.3514457823
C	6.2368159391	1.0680382699	4.1690688187
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C	5.8531845315	0.3010518727	3.0594383936
C	6.8204845429	-0.0315597057	2.0993677882
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H	8.3921560377	3.2465425530	5.2774215098
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C	13.1692984699	4.1249950542	4.8761107966
C	14.3730815796	4.8315167152	4.9868693816
H	14.5243070193	5.4567136240	5.8620069170
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H	15.9533612726	3.8056361911	2.1625758311
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C	8.2531882048	13.3301620928	4.9201395456
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H	4.5678028091	8.4802196076	1.1468144272
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H	10.9457762925	7.0546624297	4.6870142366
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C	3.0573940738	14.2523112457	8.4704171201
C	3.9915204855	13.8853671899	7.4900150488
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H	6.0484005359	14.0472275881	6.9150682506
C	5.6976353066	15.0724511165	8.7820185556
C	4.7303356489	15.4050606312	9.7420911871
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N	3.1074513804	10.1514171052	9.7489432586
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N	1.6436972990	13.9476348429	8.2349269310
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C	4.1864377694	3.9673709703	8.4724581107
C	4.6736701384	5.1250546902	9.2099454611
C	4.8293214773	7.1673329090	10.1610708585
H	4.4533443894	8.1201853100	10.5006884138
C	6.0537370907	6.5872318061	10.2389193511
H	6.9830163914	6.8932789618	10.6946420242
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C	2.2295164600	7.3319322833	8.1636826080
C	2.0413878175	5.4107540460	11.4911512963
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H	2.8086688506	5.9515957390	12.0609348307
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H	2.8367181574	7.9675926609	6.1935713820
H	3.7182919867	8.7479827832	7.5194052229
H	4.0989712830	7.0842976018	7.0609551887
C	7.0809603497	4.3929661301	9.6753117652
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H	6.4014258184	2.6752328382	12.5863621033
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H	7.6286352950	6.4354809967	7.7589062117
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Gas-phase calculation

BLYP

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C -3.304124 -0.395720 1.295334
C -4.668609 -0.098263 1.125518
C 6.673048 -0.017739 0.073324
C -0.795623 -2.516189 0.543065
C 0.565947 -2.578372 0.448860
C 5.193160 -0.363132 0.094841
C -6.766826 0.201163 -0.286857
C 2.444388 -0.934128 0.115113
C -5.300844 -0.169073 -0.131689
C -2.577060 -0.789347 0.148974
C 0.410201 3.545146 -0.343480
C -0.050205 -0.433207 0.056837
C 0.018545 0.983043 -0.216871
C 4.532574 -0.780211 -1.077339
C 3.154734 -1.065797 -1.100347
C -4.532442 -0.562553 -1.244019
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M062X

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ωB97xD

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Molecule 3

Periodic calculation

BLYP

	192		
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BLYP+D3

192

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C	-1.5173524843	15.0877238189	16.4480077829
H	-2.0722133400	14.2746435398	16.9021749913
C	-0.3098843136	15.5110349547	17.0125717950
H	0.0511746469	15.0404976269	17.9212536574
C	0.4058626965	16.5541852043	16.4149006515
H	1.3395223654	16.8959805216	16.8533194744
C	-0.1059336053	17.1809755652	15.2743056965
H	0.4373034114	18.0056445575	14.8242595413
N	1.1460775343	15.0980593290	12.3482133823
N	1.1632453197	13.7736994183	12.3449143356
N	-0.8772952692	18.0048069802	12.5860309452
O	-0.0327725117	11.8399824660	12.0250584840
C	0.5789931680	19.3286392319	11.5517278586
H	1.1693960002	20.1581048613	11.1961823973
C	1.9778361252	17.5029608776	10.3629679118
H	2.5987082103	16.8018658101	10.9303510101
C	2.8429705612	18.6709503923	9.8604200266
H	2.2514972412	19.3800265817	9.2722859364
H	3.6070021921	18.2500627496	9.2008391654
H	3.3356015235	19.2128859368	10.6712311083
C	1.3398810595	16.7616646317	9.1894744448
C	2.0297110273	15.6920961111	8.5996201505
H	2.9553941434	15.3346795026	9.0415246728
C	1.5186827066	15.0834200476	7.4489509259
H	2.0657606246	14.2672736978	6.9903599299
C	0.3131339342	15.5184247056	6.8896266206
H	-0.0546431806	15.0543258203	5.9802137897
C	-0.3914653785	16.5667089713	7.4921064458
H	-1.3238231413	16.9164517184	7.0576566982
C	0.1270129313	17.1837032517	8.6357682823
H	-0.4086090216	18.0108062218	9.0903662282
N	-1.1482348216	15.1073761354	11.6008378509
N	-1.1850437913	13.7841917502	11.6191139343
N	0.9198068741	17.9949939161	11.3174926767

C	3.0809046290	3.7673175527	11.9835502878
C	3.0782275728	6.3997830381	12.0153554986
C	3.0783782224	7.8563069100	12.0128418218
C	3.6147341977	9.9838260080	11.5804999991
H	4.1955252349	10.8150021227	11.2158314037
C	5.0328689206	8.1720217884	10.4136123109
H	5.6601049548	7.4759221520	10.9798748085
C	5.8878526720	9.3460190999	9.9060036971
H	5.2902474679	10.0456736525	9.3130037674
H	6.6557700075	8.9284491776	9.2487114889
H	6.3744393600	9.8962254240	10.7145188544
C	4.4024745379	7.4267549190	9.2365973644
C	5.1160331528	6.3736621671	8.6427058357
H	6.0458970353	6.0289230032	9.0863832794
C	4.6241242683	5.7679105006	7.4810739146
H	5.1902638287	4.9679058757	7.0166998877
C	3.4118454042	6.1836445466	6.9207462676
H	3.0566335263	5.7205248704	6.0059138517
C	2.6807952879	7.2080786915	7.5328967454
H	1.7426277310	7.5423514105	7.0989273832
C	3.1837088028	7.8303324435	8.6805147163
H	2.6300761738	8.6429352537	9.1395236348
N	1.9380867056	5.7850909285	11.6134824958
N	1.9102639446	4.4610911696	11.6171579293
N	3.9753200274	8.6591366536	11.3700029286
O	3.0916635792	2.5192624958	11.9364028433
C	2.5019293785	9.9984216264	12.3655040707
H	1.9087956056	10.8335775546	12.7025955731
C	1.1143189913	8.1820302602	13.5851426221
H	0.4875427153	7.4873568749	13.0162161892
C	0.2572057052	9.3514623839	14.0952223576
H	0.8570808576	10.0613220530	14.6730257864
H	-0.4977826001	8.9325860821	14.7659347445
H	-0.2449819894	9.8907369544	13.2892863385
C	1.7489826314	7.4300525431	14.7523827575
C	1.0358445166	6.3768124862	15.3459089128
H	0.1007836474	6.0399475718	14.9075930769
C	1.5373159014	5.7597089232	16.4961101411
H	0.9734518771	4.9574489558	16.9590651254
C	2.7558342768	6.1678932417	17.0481663194
H	3.1172959683	5.6990712850	17.9575998020
C	3.4856887614	7.1940725797	16.4373640829
H	4.4281975562	7.5218699732	16.8667702441
C	2.9759064710	7.8227283457	15.2967208791
H	3.5300919571	8.6338692810	14.8363931073
N	4.2093773298	5.7800892593	12.4349060642
N	4.2338822941	4.4557877338	12.4149044997
N	2.1736591940	8.6703078135	12.6330163848

Gas-phase calculation

BLYP

```

48
scf done: -1215.46147559
C -1.894859 -0.463835 -3.490962
C -0.294383 1.628524 -2.137658
C -1.803352 -0.449133 -1.950419
C 0.637461 2.250552 -1.355356
C -3.122337 -0.065885 -1.266507
C -3.768689 -1.009187 -0.440205
C 5.126192 0.508957 -0.967741
C 3.937078 1.205981 -0.699751
C -3.724628 1.196099 -1.463253
C 0.030318 0.342793 -0.308680
C -4.996516 -0.699290 0.171324
C -4.947836 1.507639 -0.848144
C -5.588457 0.558585 -0.030526

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C 2.139184 3.226387 1.003355
C 5.597384 -0.457624 -0.060384
C -0.065439 -0.739929 0.666285
C 3.199989 0.943906 0.475870
C 1.914972 1.711227 0.813932
C 4.870510 -0.725349 1.111521
C 3.676661 -0.031258 1.377092
C -0.240335 -2.717577 2.447111
H -0.923626 -0.716603 -3.947037
H -2.622316 -1.237654 -3.780917
H -2.253899 0.490018 -3.911268
H -0.713171 1.920823 -3.092615
H -1.503001 -1.445067 -1.602806
H 1.164712 3.184612 -1.504701
H -3.303765 -1.983459 -0.266116
H 5.685228 0.721017 -1.884024
H 3.582449 1.952625 -1.417646
H -3.237554 1.946946 -2.093807
H 2.624721 3.702778 0.135769
H -5.483073 -1.440646 0.811461
H 1.191664 3.747277 1.217990
H 6.523740 -1.000474 -0.269559
H -5.401185 2.490508 -1.007857
H -6.541321 0.801698 0.448556
H 2.810512 3.365610 1.864748
H 1.489892 1.296916 1.736203
H 5.224709 -1.480487 1.818934
H 3.105727 -0.255571 2.282291
N -0.671489 0.450029 -1.494437
N 0.840366 1.459425 -0.224984
N -0.475795 -1.968387 0.215569
N -0.574997 -2.964126 1.063592
N 0.261386 -0.455989 1.967520
N 0.188628 -1.404668 2.870401
O -0.321051 -3.630295 3.268993

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M062X

```

48
scf done: -1215.42799621
C -2.081151 0.026177 -3.602028
C -0.231209 1.835823 -2.368930
C -1.659634 -0.273275 -2.167732
C 0.652107 2.477957 -1.568446
C -2.831325 -0.198156 -1.205521
C -3.320491 -1.357772 -0.606718
C 4.714482 -0.146709 -0.721407
C 3.663466 0.760699 -0.650626
C -3.440636 1.028729 -0.934242
C 0.069353 0.588443 -0.553055
C -4.412628 -1.290986 0.255751
C -4.530694 1.094996 -0.073909
C -5.018808 -0.067023 0.521592
C 2.363072 3.372796 0.550389
C 5.061803 -0.897165 0.400604
C -0.055603 -0.484061 0.410444
C 2.951142 0.922406 0.539381
C 1.833825 1.944951 0.630192
C 4.351319 -0.741600 1.586903
C 3.294704 0.163668 1.656844
C -0.558370 -2.343768 2.140609
H -1.231536 -0.013878 -4.290542
H -2.802891 -0.735799 -3.903473
H -2.576927 0.998130 -3.686363
H -0.628417 2.113087 -3.330286
H -1.218775 -1.268834 -2.117742
H 1.160109 3.417125 -1.705396
H -2.826442 -2.308690 -0.787065

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H 5.260456 -0.271540 -1.651299
H 3.387787 1.338949 -1.531148
H -3.052165 1.939576 -1.387247
H 2.961068 3.537351 -0.351230
H -4.774483 -2.195876 0.732748
H 1.553271 4.107644 0.593008
H 5.879078 -1.609334 0.345389
H -4.996008 2.052701 0.137501
H -5.863654 -0.014989 1.200949
H 3.018199 3.533861 1.409066
H 1.300318 1.802023 1.569333
H 4.606583 -1.336324 2.457970
H 2.715126 0.260259 2.570896
N -0.590581 0.665924 -1.731124
N 0.833976 1.698416 -0.443512
N -0.276450 -1.728096 -0.066380
N -0.470430 -2.683066 0.766277
N 0.215876 -0.215773 1.703772
N 0.041753 -1.136320 2.578839
O -1.089156 -3.094213 2.928125

```

ωB97xD

```

48
scf done: -1215.53541087
C -2.034086 -0.114465 -3.593308
C -0.201001 1.770174 -2.377239
C -1.646753 -0.330372 -2.134677
C 0.677712 2.419712 -1.578671
C -2.826892 -0.194538 -1.187519
C -3.278800 -1.302151 -0.472435
C 4.862624 0.067211 -0.764300
C 3.792739 0.945797 -0.645105
C -3.459507 1.038201 -1.015050
C 0.078819 0.551566 -0.543854
C -4.345873 -1.178139 0.413328
C -4.529081 1.161091 -0.136273
C -4.972615 0.051901 0.581273
C 2.265686 3.360367 0.667090
C 5.146193 -0.827998 0.265249
C -0.073226 -0.510237 0.430008
C 2.996099 0.937378 0.501668
C 1.830555 1.899230 0.644171
C 4.353189 -0.843313 1.407519
C 3.278731 0.034714 1.525141
C -0.801154 -2.317889 2.095954
H -1.168463 -0.200451 -4.258068
H -2.752283 -0.890731 -3.867348
H -2.523348 0.851782 -3.753438
H -0.588525 2.036579 -3.345444
H -1.213400 -1.325289 -2.026257
H 1.190858 3.354536 -1.725469
H -2.775098 -2.258824 -0.575839
H 5.474327 0.077923 -1.661409
H 3.571610 1.634389 -1.458176
H -3.105545 1.913367 -1.556531
H 2.867029 3.631914 -0.206594
H -4.666341 -2.041728 0.986698
H 1.405570 4.033633 0.739713
H 5.979389 -1.517735 0.171225
H -5.011563 2.124804 -0.003457
H -5.798257 0.151101 1.279173
H 2.892585 3.510334 1.549215
H 1.295606 1.669525 1.565760
H 4.559331 -1.548617 2.206400
H 2.641104 0.000488 2.403983
N -0.570302 0.612148 -1.725892
N 0.844447 1.657016 -0.441262
N -0.139754 -1.773784 -0.036654

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N -0.418080 -2.717062 0.796400
N 0.027920 -0.206124 1.738536
N -0.244346 -1.122514 2.602473
O -1.537425 -3.006481 2.770453
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Molecule 4

Periodic calculation

BLYP

212			
E =	-857.1653597054		
C	2.3151682195	3.4193386325	11.4272936292
C	4.5270056273	2.2818086560	10.6177103733
C	5.7717727870	1.5458729866	10.3516930662
C	7.8949271927	0.6165998945	10.6575532607
H	8.0779596172	-0.2081650223	11.3501369905
H	8.8216541024	1.1846760749	10.5340210242
C	7.2974645505	0.1129235846	9.3249987644
H	7.8976059790	0.3962526957	8.4624360100
H	7.1507879150	-0.9683630318	9.3337924383
C	5.2757764413	0.9607284140	7.9849259842
C	4.3427225651	-0.0125197155	7.5928545528
C	3.7032124940	0.1566426548	6.3613817444
H	2.9854718909	-0.5917539847	6.0377719539
C	3.9611180630	1.2599785763	5.5397364312
C	4.9261567077	2.1889091423	5.9486335994
H	5.1626960213	3.0309650676	5.3040736711
C	5.6144132149	2.0496124224	7.1602826635
C	4.0286959162	-1.1948984584	8.4725253111
H	3.3441272749	-1.8758769355	7.9600376525
H	3.5581010084	-0.8628239768	9.4044175382
H	4.9299077679	-1.7490158044	8.7558442806
C	3.2124582378	1.4414148527	4.2420665604
H	3.7412020745	2.1410660327	3.5887904871
H	2.2019614634	1.8367379775	4.4154669180
H	3.0938763296	0.4873710440	3.7179270528
C	6.7116066657	3.0220396784	7.5353608099
H	7.6954890669	2.5380210199	7.5142903168
H	6.5866184518	3.4350355130	8.5415087033
H	6.7458935441	3.8539371489	6.8291981684
C	6.7932697625	2.0581420896	12.5840576235
H	6.3918518782	3.0713556541	12.4929394132
C	8.2210664917	2.1573663953	13.1362888583
H	6.6883742705	1.1707312013	13.2698553479
H	8.1783660189	2.6364571002	14.1191086715
H	8.8790285590	2.7532993681	12.4968330917
C	5.8709069093	1.2566332550	13.4977342607
C	5.5793424672	-0.0952727697	13.2693604804
H	5.9780737734	-0.6186648182	12.4057074506
C	4.7543586628	-0.7957642600	14.1512457579
H	4.5414344663	-1.8394316734	13.9542767018
C	4.2037409014	-0.1607342268	15.2666940555
H	3.5660348807	-0.7078739806	15.9539065486
C	4.4916716856	1.1864004112	15.4949062497
H	4.0913099207	1.6915884846	16.3647091724
C	5.3180379938	1.8889861460	14.6186329405
H	5.5445826302	2.9303286853	14.8254678697
N	3.3645445009	1.6767971528	10.2743861334
N	2.2298657132	2.2679525073	10.6166040323
N	3.4911766688	4.1927214530	11.3596850608
N	4.6128749669	3.5731866542	11.0193848610
N	5.9741222110	0.8079840977	9.2479439252
N	6.8137109402	1.5090493806	11.1948974105
O	1.3475830883	3.8001379406	12.1055821025
C	12.3359310096	10.4484616208	3.9917937067
C	10.1240916391	11.5859892345	3.1822124853
C	8.8793227750	12.3219250228	2.9161992575
C	6.7561741659	13.2512022804	3.2220523853
H	6.5731398368	14.0759693951	3.9146378943
H	5.8294506077	12.6831281633	3.0985215504
C	7.3536378880	13.7548766713	1.8895010558
H	6.7534984926	13.4715496741	1.0269354757

H	7.5003153942	14.8361625074	1.8982958131
C	9.3753266113	12.9070721417	0.5494281061
C	10.3083792991	13.8803222819	0.1573578789
C	10.9478872658	13.7111609258	-1.0741146645
H	11.6656259403	14.4595580735	-1.3977244372
C	10.6899817738	12.6078246232	-1.8957593175
C	9.7249445572	11.6788918120	-1.4868633815
H	9.4884053811	10.8368357748	-2.1314223355
C	9.0366900162	11.8181863789	-0.2752140160
C	10.6224017960	15.0627015929	1.0370285729
H	11.3069679991	15.7436808812	0.5245401481
H	11.0929970609	14.7306284631	1.9689204891
H	9.7211892605	15.6168173896	1.3203479338
C	11.4386403008	12.4263895439	-3.1934308061
H	10.9098952647	11.7267388820	-3.8467079338
H	12.4491375365	12.0310645888	-3.0200318906
H	11.5572232950	13.3804343333	-3.7175699199
C	7.9394973354	10.8457595726	0.0998667987
H	6.9556149637	11.3297777416	0.0787971953
H	8.0644867829	10.4327646758	1.1060147339
H	7.9052108342	10.0138621699	-0.6062952914
C	7.8578260268	11.8096516560	5.1485560782
H	8.2592413604	10.7964354772	5.0574440491
C	6.4300435569	11.7104290954	5.7007952564
H	5.9827079286	12.6971042033	5.8343597723
H	6.4727400380	11.2313434293	6.6836131376
C	5.7720690094	11.1145005189	5.0613432214
C	8.7801778637	12.6111635098	6.0622342636
C	9.0717490604	13.9630682540	5.8338568945
H	8.6730209164	14.4864659741	4.9702048770
C	9.8967367270	14.6635673625	6.7157389681
H	10.1096666450	15.7072389708	6.5187680654
C	10.4473547299	14.0285401180	7.8311918855
H	11.0850651857	14.5756809183	8.5184032439
C	10.1594181735	12.6814055321	8.0594082020
H	10.5597790336	12.1762216016	8.9292167015
C	9.3330520622	11.9788190606	7.1831339999
H	9.1065081028	10.9374802575	7.3899748103
N	11.2865538973	12.1910021263	2.8388872770
N	12.4212337593	11.5998482410	3.1811042209
N	11.1599242005	9.6750770875	3.9241876365
N	10.0382247300	10.2946120877	3.5838894482
N	8.6769796156	13.0598162303	1.8124500064
N	7.8373835050	12.3587441420	3.7593999629
O	13.3035184773	10.0676658084	4.6700809233
C	7.4522318931	10.3532402720	10.8792063736
C	5.2403935834	9.2157092141	11.6887905272
C	3.9956254462	8.4797731783	11.9548059912
C	1.8724740644	7.5505042664	11.6489521119
H	1.6894402997	6.7257335746	10.9563637925
H	0.9457491771	8.1185759287	11.7724772666
C	2.4699329897	7.0468231132	12.9815007057
H	1.8697946352	7.3301566417	13.8440645168
H	2.6166119439	5.9655369808	12.9727093566
C	4.4916225683	7.8946279101	14.3215733456
C	5.4246787169	6.9213815583	14.7136446765
C	6.0641883719	7.0905437579	15.9451175786
H	6.7819286132	6.3421460812	16.2687272720
C	5.8062815689	8.1938799286	16.7667627587
C	4.8412429606	9.1228108328	16.3578658559
H	4.6047024323	9.9648680999	17.0024244486
C	4.1529876293	8.9835135691	15.1462159249
C	5.7387045097	5.7390020596	13.8339741671
H	6.4232735224	5.0580245752	14.3464621727
H	6.2092991587	6.0710753488	12.9020815238
H	4.8374935907	5.1848830190	13.5506549736
C	6.5549407438	8.3753172512	18.0644314549
H	6.0261961658	9.0749685443	18.7177059899
H	7.5654371497	8.7706405883	17.8910312045
H	6.6735219283	7.4212739918	18.5885711160
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Gas-phase calculation

BLYP

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H -3.006564 -0.624895 2.967536
H 0.652962 -3.076278 0.767712
H 1.759707 0.168119 2.601717
H -2.061160 0.899094 2.966901
H -1.252586 -2.241665 1.996733

```

```

H 3.099425 -0.770301 3.300411
H 1.626984 -1.597047 2.744636
N 1.418579 2.975130 -0.910392
N 1.206131 1.704440 -0.677660
N -0.156166 3.543620 0.879497
N -0.355341 2.261522 1.093368
N 0.739747 -1.061135 0.076143
N -1.334827 -0.518425 0.739222
O 0.209614 4.960563 -0.925567

```

M062X

```

53
scf done: -1255.92620025
C 4.644801 0.063245 2.321660
C 4.643199 -1.227843 1.800831
C 3.991712 1.085089 1.637501
C 0.296190 3.525659 -0.403155
C -1.729493 -0.843177 2.667164
C 3.982227 -1.498191 0.605270
C 3.328943 0.813219 0.444335
C -4.006383 -0.434468 1.642500
C -2.655591 -0.728407 1.488521
C -6.297907 0.106862 0.742478
C 3.308157 -0.483046 -0.080374
C 0.127110 0.951747 -0.580983
C -4.846959 -0.248373 0.542772
C -2.158544 -0.847205 0.188142
C 0.171205 -0.485501 -0.559844
C 2.529066 -0.746168 -1.359704
C -4.307871 -0.364181 -0.736667
C -2.960495 -0.663253 -0.941563
C -0.474429 -2.660449 -0.140285
C 0.981572 -2.636649 -0.616115
C 3.209731 -1.708002 -2.327431
C -2.389029 -0.739469 -2.335099
H 5.162271 0.274242 3.252180
H 5.164389 -2.025845 2.320660
H 3.999520 2.097868 2.027319
H -2.279176 -0.736235 3.604688
H -0.974888 -0.051464 2.609741
H -4.410682 -0.330127 2.646869
H -6.404731 1.171089 0.978468
H -1.204279 -1.804361 2.689148
H -6.733759 -0.458717 1.570893
H 4.013982 -2.506857 0.201365
H 2.837665 1.619671 -0.094534
H -6.884466 -0.095151 -0.157236
H 2.377016 0.199631 -1.878674
H -0.610335 -3.188266 0.806386
H -4.949207 -0.214013 -1.602146
H 1.678362 -2.852689 0.202265
H 4.175872 -1.290820 -2.619642
H 3.393402 -2.693083 -1.888539
H -1.150747 -3.098538 -0.883218
H -1.765651 0.135447 -2.553648
H 2.598116 -1.836289 -3.224734
H 1.168746 -3.330062 -1.437979
H -3.190315 -0.772773 -3.076325
H -1.760688 -1.625289 -2.480708
N -0.588823 2.828984 0.465339
N -0.610354 1.555030 0.385677
N 0.737844 2.885303 -1.592595
N 0.697046 1.605703 -1.620914
N -0.784407 -1.235044 0.011914
N 1.164483 -1.244597 -1.048838
O 0.639475 4.657040 -0.152052

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ωB97xD

```
53
scf done: -1256.05787849
C 4.582537 0.047773 2.362046
C 4.561376 -1.251960 1.864702
C 3.969856 1.070778 1.644438
C 0.452754 3.478586 -0.441829
C -1.691112 -0.790100 2.641970
C 3.919746 -1.529028 0.661005
C 3.327717 0.791675 0.442493
C -3.983829 -0.354671 1.672706
C -2.643855 -0.675857 1.484238
C -6.288937 0.222605 0.831482
C 3.284491 -0.512690 -0.058252
C 0.131021 0.939166 -0.628300
C -4.851855 -0.166907 0.596338
C -2.187004 -0.822342 0.172471
C 0.148902 -0.500340 -0.586378
C 2.515253 -0.784132 -1.342433
C -4.352406 -0.310928 -0.696154
C -3.018766 -0.638898 -0.935447
C -0.525140 -2.661913 -0.152337
C 0.933688 -2.660755 -0.618349
C 3.202419 -1.744564 -2.307935
C -2.491881 -0.745623 -2.344451
H 5.083661 0.263953 3.300649
H 5.051687 -2.052671 2.410480
H 3.990759 2.090772 2.014967
H -2.215185 -0.667441 3.593134
H -0.929487 -0.006874 2.561906
H -4.356959 -0.228548 2.686451
H -6.371068 1.301372 1.008047
H -1.175452 -1.757021 2.664943
H -6.701480 -0.285823 1.708518
H 3.936350 -2.546344 0.278621
H 2.867747 1.601497 -0.116617
H -6.916489 -0.020640 -0.030865
H 2.369233 0.158061 -1.869392
H -0.669662 -3.165751 0.806169
H -5.015753 -0.158850 -1.544447
H 1.619821 -2.900260 0.201616
H 4.169788 -1.324751 -2.594209
H 3.387104 -2.731909 -1.872951
H -1.199578 -3.117083 -0.886227
H -1.820620 0.088552 -2.579254
H 2.597525 -1.870672 -3.210802
H 1.113282 -3.351953 -1.444037
H -3.312498 -0.724682 -3.065781
H -1.927810 -1.670538 -2.511132
N -0.501288 2.854961 0.399414
N -0.582972 1.576926 0.329495
N 0.776135 2.846269 -1.666273
N 0.681551 1.563723 -1.695193
N -0.826986 -1.234189 -0.036381
N 1.147316 -1.272339 -1.039132
O 0.949870 4.541361 -0.140681
```

Molecule 5

Periodic calculation

BLYP

90			
E =	-437.6535756221		
C	-2.1882832589	1.3939660179	-1.1357216642
C	-1.4763515194	0.6266649509	1.2544469727
C	-0.9302287510	0.2313545988	2.5418828572
C	-0.4291863672	-0.9382046573	4.3719164397
C	-1.6839868346	-2.1786919351	2.5226360817
C	-0.8840195242	-3.2582582931	2.1515641045
H	0.1904455908	-3.2041432926	2.2761311343
C	-1.4975212280	-4.3965302057	1.6296660953
H	-0.8989181816	-5.2558977585	1.3505509142
C	-2.8860626398	-4.4337441668	1.4651047779
H	-3.3455581366	-5.3207508152	1.0398924708
C	-3.6705138821	-3.3362777186	1.8315282196
H	-4.7453891858	-3.3465485059	1.6912140050
C	-3.0700045040	-2.1992577769	2.3750766738
H	-3.6725499963	-1.3503563358	2.6793751357
C	0.2259197999	2.3497070252	3.3267856982
C	0.8107516371	2.8149075905	2.1462026627
H	0.8969189772	2.1769699208	1.2764451307
C	1.3283990615	4.1089510408	2.1272431079
H	1.7773320723	4.4868050159	1.2150161971
C	1.2748390880	4.9125777718	3.2682317365
H	1.6669035917	5.9214500866	3.2331730058
C	0.6786957323	4.4312788796	4.4328800013
H	0.6323463165	5.0558137384	5.3157884599
C	0.1529413007	3.1426816383	4.4733226576
H	-0.2817153552	2.7449323403	5.3833373330
C	-0.3282626610	-2.0053734929	5.3767447860
C	0.6967095264	-1.9100159499	6.3383347439
H	1.3922560461	-1.0793817538	6.3111729419
C	0.8160811584	-2.8714964044	7.3402598741
H	1.6029124957	-2.7746769862	8.0796654251
C	-0.0842841745	-3.9373436185	7.4008749435
H	0.0071942693	-4.6841350212	8.1813834168
C	-1.1107448369	-4.0337301569	6.4599809880
H	-1.8217090274	-4.8518655414	6.5178632056
C	-1.2412185415	-3.0766566813	5.4556334041
H	-2.0576069622	-3.1595837221	4.7511306061
N	-1.5113327772	-0.3226526936	0.2901095613
N	-1.9289591260	0.0350796839	-0.9104190545
N	-2.4897040788	2.2290001887	-0.0418676355
N	-2.0605440461	1.8489937809	1.1508791036
N	-1.0461180521	-1.0100182292	3.1190781545
N	-0.2472781994	0.9893944381	3.4239721035
N	0.0563678441	0.2748325092	4.5724292687
O	-2.2052787043	1.8312208274	-2.2994124480
C	5.8943574500	6.3962537614	11.9880143493
C	5.1824966195	7.1635759752	9.5978929309
C	4.6363876168	7.5589044550	8.3104626949
C	4.1353788689	8.7284580581	6.4804082589
C	5.3901743614	9.9689516658	8.3296902704
C	4.5901902282	11.0485088075	8.7007517349
H	3.5157243218	10.9943889618	8.5761880375
C	5.2036655707	12.1867957915	9.2226458357
H	4.6050458735	13.0461515554	9.5017688409
C	6.5922049991	12.2240352359	9.3872146973
H	7.0516713975	13.1110517745	9.8124387158
C	7.3766767706	11.1265809605	9.0208039102
H	8.4515464159	11.1368625875	9.1611482958
C	6.7761922513	9.9895470027	8.4772567301
H	7.3787641750	9.1406598382	8.1729812479
C	3.4802759908	5.4405372737	7.5255452888

C	2.8954499798	4.9753292740	8.7061279733
H	2.8093005997	5.6132667935	9.5758902429
C	2.3777976707	3.6812866356	8.7250845141
H	1.9288453708	3.3034568942	9.6373122590
C	2.4313527969	2.8776586275	7.5840952794
H	2.0392660150	1.8687941095	7.6191524999
C	3.0275030211	3.3589617004	6.4194518507
H	3.0738414038	2.7344381332	5.5365372203
C	3.5532608790	4.6475588347	6.3790097729
H	3.9879399641	5.0453010223	5.4690027642
C	4.0344622821	9.7956119692	5.4755746026
C	3.0094838598	9.7002601713	4.5139829571
H	2.3139138059	8.8696384975	4.5411545622
C	2.8901137555	10.6617481734	3.5120594011
H	2.1032718398	10.5649397042	2.7726563823
C	3.7904727442	11.7276054745	3.4514622172
H	3.6989762485	12.4744162987	2.6709743242
C	4.8169251831	11.8239905410	4.3923619943
H	5.5278619151	12.6421474435	4.3345083079
C	4.9474070236	10.8669049410	5.3966943857
H	5.7637896421	10.9498329523	6.1011989149
N	5.2175424050	8.1129139365	10.5622081026
N	5.6351800576	7.7551625054	11.7627227208
N	6.1959486143	5.5612739902	10.8941791966
N	5.7667575684	5.9412726006	9.7014362164
N	4.7522973631	8.8002739863	7.7332599810
N	3.9534510414	6.8008615350	7.4283663972
N	3.6498170529	7.5154158307	6.2799048000
O	5.9110315078	5.9589500411	13.1516847419

BLYP+D3

90

E =	-437.9757546538		
C	-2.1477674585	1.3969659393	-1.1603978186
C	-1.4370823529	0.6230398117	1.2434246458
C	-0.9086248117	0.2302641299	2.5405495879
C	-0.4185378052	-0.9310669316	4.3901041984
C	-1.6734521855	-2.1751777328	2.5381968941
C	-0.8806176238	-3.2784734785	2.2220617187
H	0.1883273466	-3.2417449618	2.3924618230
C	-1.4948168031	-4.4145264203	1.6926289741
H	-0.9001119412	-5.2905519719	1.4570896080
C	-2.8765921350	-4.4208632324	1.4595582510
H	-3.3360553312	-5.3013544733	1.0186757543
C	-3.6550956667	-3.3003313857	1.7762472836
H	-4.7251409905	-3.2944341373	1.5940532358
C	-3.0540343944	-2.1672951815	2.3341495246
H	-3.6481938214	-1.3001209020	2.6059127795
C	0.2352647876	2.3597778498	3.3296452797
C	0.8121946233	2.8390019477	2.1482506884
H	0.8906807304	2.2114175484	1.2704462833
C	1.3226850841	4.1379279610	2.1375828897
H	1.7635147224	4.5296787805	1.2258555895
C	1.2708610514	4.9320169077	3.2883633525
H	1.6676786361	5.9394254893	3.2619074240
C	0.6709849558	4.4422655047	4.4496850501
H	0.6216831005	5.0606931607	5.3378823764
C	0.1514624032	3.1493606573	4.4806252754
H	-0.2856586128	2.7472579471	5.3884803299
C	-0.3138436053	-1.9896395478	5.4038148099
C	0.7562453781	-1.9181425296	6.3198814508
H	1.4819360339	-1.1156540356	6.2545496962
C	0.8763187096	-2.8625314450	7.3392504157
H	1.6984155312	-2.7843936187	8.0418184203
C	-0.0716288265	-3.8821481153	7.4653824625
H	0.0152525659	-4.6124805089	8.2629953152
C	-1.1411926062	-3.9569271535	6.5684075693
H	-1.8855607180	-4.7392168023	6.6811306916

C	-1.2691449318	-3.0198973604	5.5421889521
H	-2.1182962284	-3.0779646221	4.8722191478
N	-1.4444158034	-0.3188487483	0.2700132406
N	-1.8415882601	0.0425718668	-0.9371000190
N	-2.4178346526	2.2450820127	-0.0599280229
N	-1.9957986420	1.8578445988	1.1320488269
N	-1.0316843758	-1.0069999294	3.1302094248
N	-0.2294369557	0.9938038608	3.4231707390
N	0.0702232187	0.2833629468	4.5793466773
O	-2.2310651506	1.8242694357	-2.3242184363
C	5.8539583836	6.3932846339	12.0127242401
C	5.1432757668	7.1672031733	9.6089037754
C	4.6148166618	7.5599841611	8.3117762105
C	4.1247302419	8.7213147332	6.4622233005
C	5.3796447687	9.9654251189	8.3141300269
C	4.5868097393	11.0687213847	8.6302652167
H	3.5178649950	11.0319923530	8.4598653772
C	5.2010088855	12.2047743934	9.1596981102
H	4.6063039766	13.0807997334	9.3952375711
C	6.5827840982	12.2111107922	9.3927689286
H	7.0422473330	13.0916020865	9.8336517826
C	7.3612878331	11.0905791832	9.0760801333
H	8.4313330648	11.0846818610	9.2582744430
C	6.7602267400	9.9575427166	8.5181777409
H	7.3543862871	9.0903683836	8.2464149344
C	3.4709274263	5.4304698270	7.5226813927
C	2.8939977920	4.9512458283	8.7040766016
H	2.8155112545	5.5788297854	9.5818806152
C	2.3835070852	3.6523194504	8.7147441901
H	1.9426774066	3.2605687177	9.6264713177
C	2.4353308224	2.8582308014	7.5639635841
H	2.0385132231	1.8508222379	7.5904192933
C	3.0352069447	3.3479821884	6.4026419756
H	3.0845091480	2.7295546586	5.5144446258
C	3.5547297815	4.6408871325	6.3717018457
H	3.9918508634	5.0429896250	5.4638466923
C	4.0200356574	9.7798874666	5.4485123763
C	2.9499469003	9.7083903820	4.5324461856
H	2.2242561484	8.9059018726	4.5977779637
C	2.8298737118	10.6527793186	3.5130769600
H	2.0077769258	10.5746413345	2.8105087871
C	3.7778209993	11.6723957642	3.3869450484
H	3.6909398656	12.4027281598	2.5893321378
C	4.8473849528	11.7471747828	4.2839198841
H	5.5917529423	12.5294644459	4.1711965951
C	4.9753373025	10.8101450048	5.3101382945
H	5.8244885956	10.8682122466	5.9801082126
N	5.1506098281	8.1090981226	10.5823118919
N	5.5477792044	7.7476742656	11.7894278316
N	6.1240276696	5.5451636411	10.9122560696
N	5.7019863832	5.9324059572	9.7202772991
N	4.7378767162	8.7972479664	7.7221175428
N	3.9356290666	6.7964438454	7.4291563654
N	3.6359689853	7.5068847492	6.2729804346
O	5.9372560688	5.9659771760	13.1765455107

Gas-phase calculation

BLYP

```

45
scf done: -1305.30811531
C 2.669914 1.985593 -2.779181
C -3.439925 1.860809 -2.315867
C 3.052419 3.164039 -2.111841
C 1.903573 1.015028 -2.115471
C -1.529818 0.575522 -1.132620

```

```

C 2.667537 3.374567 -0.776404
C 1.520703 1.243756 -0.782205
C -0.593766 -0.059717 -0.245462
C 1.897201 2.412632 -0.102350
C 3.783442 -0.479689 0.645777
C 5.060885 -0.620800 1.210504
C 1.255449 -0.677660 0.885559
C -2.098481 -1.737138 0.958389
C -3.216047 -0.970076 1.332497
C -2.136002 -3.141563 0.974968
C -4.398645 -1.628586 1.700913
C -3.323726 -3.786573 1.355014
C 2.631692 -0.757149 1.420283
C -4.456113 -3.034103 1.712562
C 5.209159 -1.039797 2.543819
C 2.789061 -1.187453 2.762192
C 4.068603 -1.326308 3.316167
H 2.962624 1.822270 -3.819663
H 3.646392 3.918598 -2.634486
H 1.590633 0.100451 -2.624664
H 2.959169 4.291302 -0.257220
H 3.687977 -0.171279 -0.395288
H 5.942832 -0.407219 0.600348
H 1.581547 2.569075 0.931611
H -3.163502 0.120129 1.330965
H -1.247884 -3.710667 0.694414
H -5.274379 -1.038547 1.982993
H -3.362467 -4.879169 1.364930
H -5.381203 -3.540565 2.000891
H 6.207316 -1.144685 2.978362
H 1.900278 -1.406368 3.357304
H 4.174638 -1.653575 4.354164
N -3.507695 0.431489 -2.296440
N -2.130595 2.452213 -2.319756
N -2.576531 -0.188159 -1.610473
N -1.209122 1.817743 -1.637186
N 0.756874 0.224952 -0.073697
N -0.849334 -1.087181 0.624361
N 0.293446 -1.483101 1.309510
O -4.453341 2.554908 -2.396293

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M062X

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45
scf done: -1305.22763121
C 2.487765 2.016492 -2.740026
C -3.336880 1.816881 -2.415753
C 3.023437 3.095520 -2.038333
C 1.715819 1.068500 -2.079012
C -1.524771 0.591416 -1.055961
C 2.783137 3.235004 -0.674202
C 1.485097 1.227595 -0.717539
C -0.594704 -0.058675 -0.179900
C 2.004335 2.297403 -0.002979
C 3.720642 -0.487844 0.599075
C 5.001586 -0.610121 1.126204
C 1.228439 -0.677179 0.909850
C -2.078757 -1.728898 0.970061
C -3.215718 -0.967764 1.219949
C -2.085543 -3.113749 1.074189
C -4.394316 -1.620876 1.556981
C -3.270846 -3.753046 1.422956
C 2.610646 -0.744247 1.411271
C -4.424380 -3.010474 1.658325
C 5.183245 -0.987520 2.454321
C 2.795027 -1.133329 2.742697
C 4.078567 -1.252915 3.260473
H 2.667183 1.914080 -3.804854
H 3.624899 3.832995 -2.559450

```

```

H 1.282632 0.224330 -2.606665
H 3.194739 4.078326 -0.130159
H 3.591181 -0.206357 -0.440248
H 5.860333 -0.413998 0.492781
H 1.799823 2.389504 1.058836
H -3.180607 0.113775 1.143287
H -1.174236 -3.670703 0.886732
H -5.290698 -1.039173 1.742428
H -3.290857 -4.834705 1.503733
H -5.348824 -3.513633 1.921810
H 6.185858 -1.077987 2.859995
H 1.925667 -1.338063 3.358866
H 4.215750 -1.550173 4.294915
N -3.392505 0.398759 -2.313956
N -2.099587 2.472582 -2.170744
N -2.516746 -0.173026 -1.580464
N -1.245300 1.858356 -1.443904
N 0.727481 0.225043 -0.015190
N -0.837338 -1.082238 0.655627
N 0.286595 -1.478762 1.315813
O -4.312477 2.446844 -2.749905

```

ωB97xD

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45
scf done: -1305.30980185
C 2.532944 1.955337 -2.748649
C -3.372238 1.803981 -2.324877
C 3.026355 3.066453 -2.068177
C 1.765603 1.011409 -2.077573
C -1.518600 0.574558 -1.050488
C 2.748715 3.241138 -0.715598
C 1.495792 1.205609 -0.728740
C -0.581757 -0.073083 -0.180392
C 1.974362 2.307495 -0.035980
C 3.730868 -0.508843 0.609440
C 5.009714 -0.607257 1.144572
C 1.238934 -0.686267 0.913150
C -2.072437 -1.730225 0.962878
C -3.170596 -0.959182 1.324945
C -2.129181 -3.116708 0.932744
C -4.362642 -1.599082 1.638664
C -3.324897 -3.745178 1.262094
C 2.617480 -0.741548 1.423151
C -4.441177 -2.989215 1.608176
C 5.187288 -0.939329 2.484672
C 2.798860 -1.083869 2.767472
C 4.080304 -1.181258 3.294030
H 2.741233 1.824586 -3.805288
H 3.624288 3.801799 -2.596827
H 1.365249 0.143697 -2.591930
H 3.127855 4.109824 -0.187713
H 3.606364 -0.259574 -0.438137
H 5.870163 -0.427476 0.508180
H 1.741866 2.429872 1.016538
H -3.098864 0.122999 1.347526
H -1.249581 -3.687483 0.656437
H -5.231014 -1.007448 1.908151
H -3.384186 -4.828412 1.238871
H -5.375450 -3.483663 1.854049
H 6.188622 -1.012082 2.897688
H 1.930252 -1.270606 3.390224
H 4.213755 -1.442838 4.338804
N -3.393962 0.386092 -2.297995
N -2.127379 2.458463 -2.142761
N -2.499182 -0.195274 -1.586770
N -1.248688 1.842451 -1.438732
N 0.739558 0.209934 -0.017925
N -0.826500 -1.091390 0.657422

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N 0.297202 -1.486421 1.323927
O -4.380506 2.435963 -2.547325