"Knock-Out" Analogues as a Tool to quantify Supramolecular Processes: a Theoretical Study of Molecular Interactions in Guanidiniocarbonyl Pyrrole Carboxylate Dimers

*Sebastian Schlund, Carsten Schmuck and Bernd Engels**

Prof. Dr. B. Engels, Prof. Dr. C. Schmuck, Dipl.-Chem. S. Schlund, Institute for Organic Chemistry, University of Wuerzburg, Am Hubland, 97074 Wuerzburg (Germany)

E-mail: bernd@chemie.uni-wuerzburg.de

Supporting Material

Table 1 Electronic energies (RI-DFT/B-LYP/TZVPP) in gas phase (BSSE corrected).

		E [a.u.]	ΔE [a.u.]			E [a.u]	ΔE(cp) [a.u]	ΔE(corr.) [a.u.]	ΔE [kJ/mol]
1	dimer	-1432,8778511900	-0,1686323184	**1**	mon. opt. dim[1]	-716,3390155747	0,0019200202	-0,1667122982	-437,7027481513
	monomer	-716,3546094358			ghost[2]	-716,3399755848			
2	dimer	-1707,9812887630	-0,0470467196	**2**	mon. opt. dim[1]	-853,9611713395	0,0027230788	-0,0443236408	-116,3716150259
	monomer	-853,9671210217			ghost[2]	-853,9625328789			
3a	dimer	-1400,7058247970	-0,1310778786	**3a**	mon. opt. dim[1]	-700,2727543991	0,0014746732	-0,1296032054	-340,2729119882
	monomer	-700,2873734592			ghost[2]	-700,2734917357			
3b	dimer	-1400,7203663640	-0,1705282170	**3b**	mon. opt. dim[1]	-700,2599225888	0,0017830726	-0,1687451444	-443,0399810841
	monomer	-700,2749190735			ghost[2]	-700,2608141251			
4	dimer	-1400,6871922560	-0,1398531782	**4**	mon. opt. dim[1]	-700,2588715357	0,0012147212	-0,1386384570	-363,9949438845
	monomer	-700,2736695389			ghost[2]	-700,2594788963			
5	dimer	-1400,6725803210	-0,1396165288	**5**	mon. opt. dim[1]	-700,2448893611	0,0008989344	-0,1387175944	-364,2027189434
	monomer	-700,2664818961			ghost[2]	-700,2453388283			
6	dimer	-1472,5894392310	-0,1328440154	**6**	mon. opt. dim[1]	-736,2090772015	0,0014433444	-0,1314006710	-344,9921537072
	monomer	-736,2282976078			ghost[2]	-736,2097988737			

[1] Energy of a monomer in the geometry within the dimer

[2] Energy of a monomer in the geometry within the dimer including ghost orbitals of the second monomer

Table 2 Electronic energies (RI-DFT/B-LYP/TZVPP/COSMO) in solvent (BSSE corrected).

		E [a.u.]	ΔE [a.u.]			E [a.u]	ΔE(cp) [a.u]	ΔE(corr.) [a.u.]	ΔE [kJ/mol]
1	dimer	-1432,9273575030	-0,0395524068	**1**	mon. opt. dim[1]	-716,4215347890	0,0014994990	-0,0380529078	-99,9078202328
	monomer	-716,4439025481			ghost[2]	-716,4222845385			
2	dimer	-1708,0038400860	-0,0213026474	**2**	mon. opt. dim[1]	-853,9742205960	0,0028568564	-0,0184457910	-48,4293810335
	monomer	-853,9912687193			ghost[2]	-853,9756490242			
3a	dimer	-1400,7571263300	-0,0225886472	**3a**	mon. opt. dim[1]	-700,3478303729	0,0011389892	-0,0214496580	-56,3160268008
	monomer	-700,3672688414			ghost[2]	-700,3483998675			
3b	dimer	-1400,7620871470	-0,0401307648	**3b**	mon. opt. dim[1]	-700,3381967539	0,0012858176	-0,0388449472	-101,9873178211
	monomer	-700,3609781911			ghost[2]	-700,3388396627			
4	dimer	-1400,7466418290	-0,0201955360	**4**	mon. opt. dim[1]	-700,3460029081	0,0012102906	-0,0189852454	-49,8457172963
	monomer	-700,3632231465			ghost[2]	-700,3466080534			
5	dimer	-1400,7269717680	-0,0236576578	**5**	mon. opt. dim[1]	-700,3292696029	0,0011918632	-0,0224657946	-58,9838910632
	monomer	-700,3516570551			ghost[2]	-700,3298655345			
6	dimer	-1472,6450377570	-0,0189448076	**6**	mon. opt. dim[1]	-736,2920386119	0,0012075088	-0,0177372988	-46,5692364233
	monomer	-736,3130464747			ghost[2]	-736,2926423663			

[1] Energy of a monomer in the geometry within the dimer

[2] Energy of a monomer in the geometry within the dimer including ghost orbitals of the second monomer

Table 3 Electronic energies (RI-DFT/B3-LYP/TZVPP/COSMO// RI-DFT/B-LYP/TZVPP/COSMO) in solvent (BSSE corrected).

		E [a.u.]	ΔE [a.u.]			E [a.u]	ΔE(cp) [a.u]	ΔE(corr.) [a.u.]	ΔE [kJ/mol]
1	dimer	-1432,5308453220	-0,0425915822	**1**	mon. opt. dim[1]	-716,2198058372	0,0013727348	-0,0412188474	-108,2199872321
	monomer	-716,2441268699			ghost[2]	-716,2204922046			
2	dimer	-1707,5595242320	-0,0206422116	**2**	mon. opt. dim[1]	-853,7491793136	0,0024121870	-0,0182300246	-47,8628868565
	monomer	-853,7694410102			ghost[2]	-853,7503854071			
3a	dimer	-1400,3802353600	-0,0253610148	**3a**	mon. opt. dim[1]	-700,1562766458	0,0010490916	-0,0243119232	-63,8308973739
	monomer	-700,1774371726			ghost[2]	-700,1568011916			
3b	dimer	-1400,3855688110	-0,0433368602	**3b**	mon. opt. dim[1]	-700,1463668763	0,0011899334	-0,0421469268	-110,6566575213
	monomer	-700,1711159754			ghost[2]	-700,1469618430			
4	dimer	-1400,3699462730	-0,0221669498	**4**	mon. opt. dim[1]	-700,1546044551	0,0011186142	-0,0210483356	-55,2623557804
	monomer	-700,1738896616			ghost[2]	-700,1551637622			
5	dimer	-1400,3522039980	-0,0256353912	**5**	mon. opt. dim[1]	-700,1388810730	0,0011056510	-0,0245297402	-64,4027753975
	monomer	-700,1632843034			ghost[2]	-700,1394338985			
6	dimer	-1472,2212807420	-0,0207620732	**6**	mon. opt. dim[1]	-736,0775275786	0,0011469992	-0,0196150740	-51,4993308094
	monomer	-736,1002593344			ghost[2]	-736,0781010782			

[1] Energy of a monomer in the geometry within the dimer

[2] Energy of a monomer in the geometry within the dimer including ghost orbitals of the second monomer

Table 4 Thermodynamic corrections (RI-DFT/B-LYP/TZVP) in gas-phase.

		E (corr.) [kJ/mol]	H (corr.) [kJ/mol]	S (corr.) [kJ/mol/K]	ΔH (corr.) [kJ/mol]	ΔS (corr.) *T [kJ/mol]	ΔE (elec.) [kJ/mol]]	ΔG [kJ/mol]
1	dimer	896,03	898,5089682	0,73458	8,851031825	-85,080084	-437,7027481513	-343,7716323
	monomer	442,35	444,8289682	0,50997				
2	dimer	1211,71	1214,188968	0,84718	10,43103183	-61,084972	-116,3716150259	-44,8556112
	monomer	599,40	601,8789682	0,52603				
3a	dimer	951,52	953,9989682	0,72390	11,08103183	-71,520222	-340,2729119882	-257,6716582
	monomer	468,98	471,4589682	0,48189				
3b	dimer	953,71	956,1889682	0,69615	11,29103183	-73,8249215	-443,0399810841	-357,9240278
	monomer	469,97	472,4489682	0,47188				
4	dimer	961,02	963,4989682	0,75329	20,98103183	-67,8499955	-363,9949438845	-275,1639166
	monomer	468,78	471,2589682	0,49043				
5	dimer	953,83	956,3089682	0,76495	10,93103183	-80,4259625	-364,2027189434	-272,8457246
	monomer	470,21	472,6889682	0,51735				
6	dimer	829,49	831,9689682	0,77808	5,811031825	-66,803489	-344,9921537072	-272,3776329
	monomer	410,60	413,0789682	0,50107				

Table 5 Thermodynamic corrections (RI-DFT/B-LYP/TZVPP/COSMO) in solvent (1): Contributions of enthalpy and entropy corrections.

	H (corr.) [KJ/mol]	S (corr.) [J/(mol K)]	S (trans) [J/(mol K)]	S (rot) [J/(mol K)]	S (vib) [J/(mol K)]	G (corr.) [KJ/mol]	ΔH (corr.) (KJ/mol)	T*ΔS (corr.) (KJ/mol)
1	907,76	748,52	183,22	151,82	413,49	684,58	-1,28	-62,235831
	454,52	478,63	174,58	134,51	169,54	311,82		
2	1217,56	853,20	186,00	157,85	509,35	963,18	5,66	-61,675309
	605,95	530,03	177,36	141,73	210,94	447,92		
3a	967,14	744,70	183,16	152,16	409,39	745,11	3,12	-66,213152
	482,01	483,39	174,51	134,57	174,31	337,89		
3b	966,97	763,10	183,16	151,79	428,15	739,46	4,07	-49,993792
	481,45	465,39	174,51	134,57	156,31	342,70		
4	971,23	756,92	183,16	151,72	422,04	745,55	3,83	-58,944255
	483,70	477,31	174,51	134,79	168,00	341,39		
5	962,54	749,14	183,16	151,85	414,13	739,18	-1,02	-57,858989
	481,78	471,60	174,51	134,79	162,29	341,17		
6	839,54	750,68	183,28	151,67	415,73	615,73	-2,02	-55,986607
	420,78	469,23	174,64	134,27	160,32	280,88		

Table 6 Thermodynamic corrections in solvent (2): Non-electrostatic interaction (B-LYP/TZVPP/COSMO).

	E (n.e.) [kcal/mol]	ΔE (n.e.) [kcal/mol]	E (n.e.) [kJ/mol]
1	15,87 9,03	-2,1900	-9,1630
2	22,53 11,62	-0,7100	-2,9706
3a	17,57 9,51	-1,4500	-6,0668
3b	17,17 9,70	-2,2300	-9,3303
4	18,19 9,58	-0,9700	-4,0585
5	17,80 9,54	-1,2800	-5,3555
6	17,24 9,14	-1,0400	-4,3514

Table 7 Comparison of dissociation energies (all values given in kJ mol^{-1}) obtained in a polar solvent. All calculations employ the TZVPP basis set augmented with diffuse functions (see text).

	1	**2**	**3a**	**3b**	**4**	**5**	**6**
[1]BLYP//BLYP	+100/	+48	+56	+102	+50	+59	+47
[2]B3LYP//B3LYP	+109	--	--	--	--	--	--
[3]B3LYP//BLYP	+108	+48	+64	+111	+55	+64	+51

[1] Dissociation energies and geometries are obtained with the BLYP functional.

[2] Dissociation energies and geometries are obtained with the B3LYP functional.

[3] Dissociation energies obtained with B3LYP, geometries obtained with BLYP functional

The BLYP functional employed in our study is known to somehow underestimate dissociation energies.[1] However, its main advantage compared to more correct functionals such as B3LYP lies in the up to tenfold speed up of calculations by using the RI-approximation for two-electron-four-centre integrals. Especially for the number and size of systems as the ones we studied here, this is an important aspect to consider. Furthermore, the main focus of our study is the comparison of relative data for the various "knock-out" analogues shown above. Even if the absolute values calculated using the BLYP functional might be a little lower than the correct data, as long as this applies for all compounds our analysis will not be affected. However, to calibrate the dependency of the calculated dissociation energy on the theoretical method we calculated the dissociation energy of **1** employing the functionals BLYP and B3LYP. Additionally we used the MP2 approach for calculations in the gas phase.[2] All computations were performed with the augmented TZVPP basis described above. For gas phase we obtained dissociation energies of +438 kJ/mol (BLYP), +465 kJ/mol (B3LYP) and +502 kJ/mol (MP2) showing that BLYP indeed underestimates absolute dissociation energies considerably. For polar environment (see Table 7) dissociation energies of 100 kJ/mol (BLYP) and 109 kJ/mol (B3LYP) are computed. Again, with BLYP smaller absolute dissociation energies are obtained than with B3LYP. The dissociation energy of **1** calculated with the B3LYP functional for the geometry obtained using BLYP is +464 kJ/mol, *i.e.* the energy is in fact identical with the value calculated using the B3LYP geometry (+465 kJ/mol). This shows that both geometries are virtually identical. Therefore, to benefit from the higher accuracy of B3LYP without losing the speed we computed improved stabilities for solvent conditions employing the B3LYP functional based on previously optimized BLYP geometries. The thermodynamic corrections are also taken from BLYP calculations. Since we are more interested in solvent data the BLYP functional was employed for gas phase calculations throughout.

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[1] (a) Xu, X.; Goddard III, W. A. *J. Phys. Chem. A* **2004**, *108*, 2305-2313. (b) Xu, X.; Zhang, Q.; Muller, R. P.; Goddard III, W. A. *J. Chem. Phys.* **2005**, *122*, 014105.

[2] MP2 computations employing the COSMO approach were not possible.

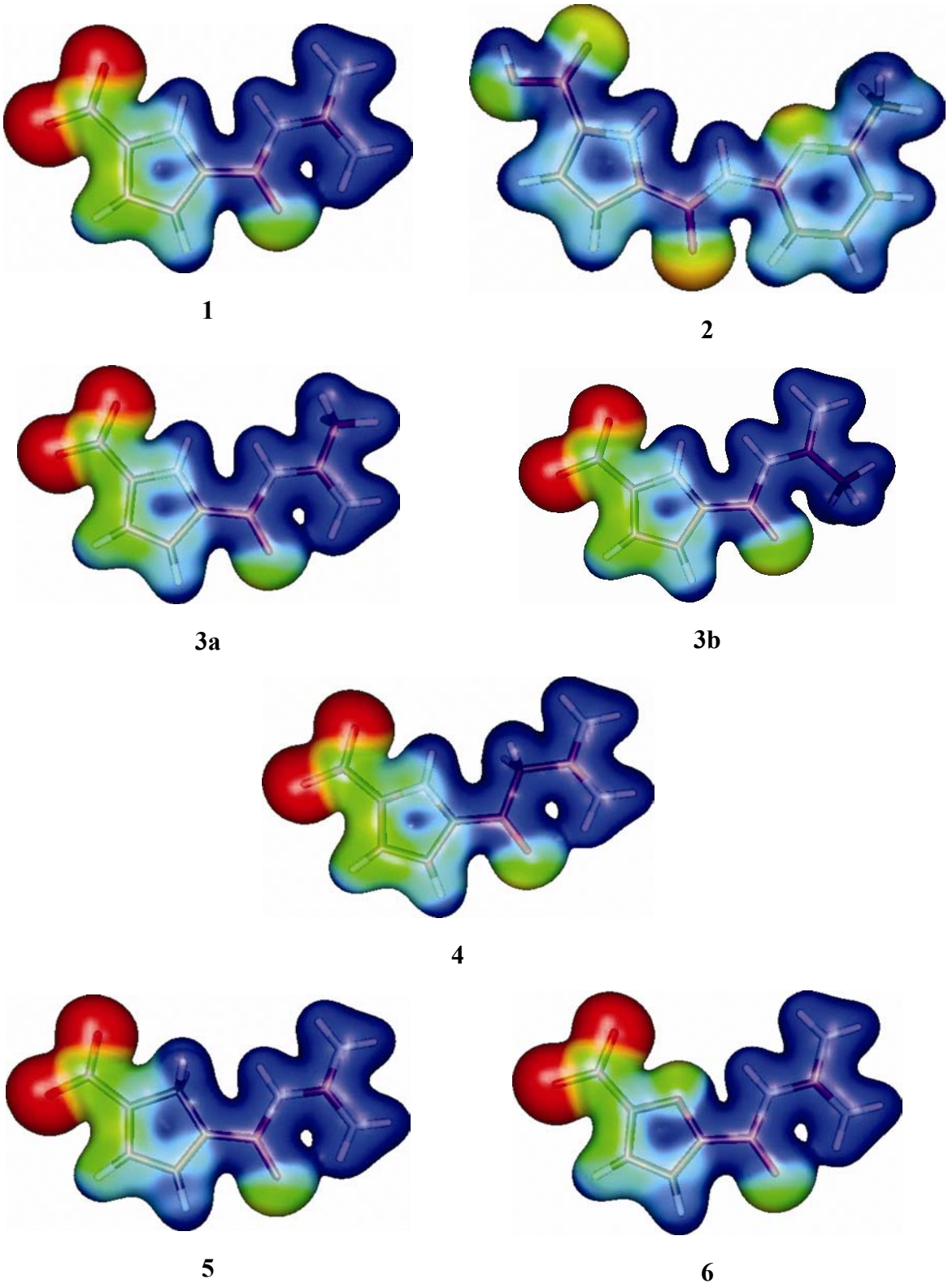
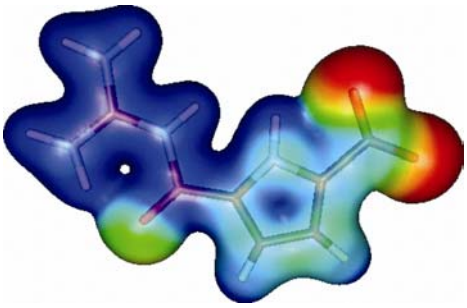


Chart 1: Electrostatic potential (contour value = 0.02) mapped on the electron density (contour value = 0.015) of the monomers 1-6 in solvent.



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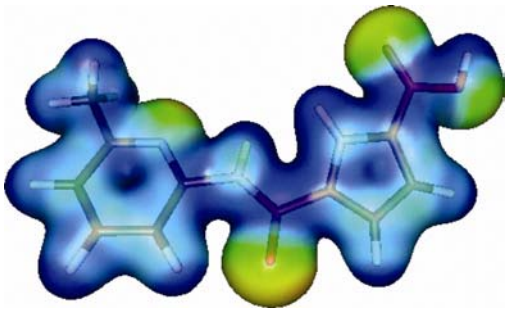

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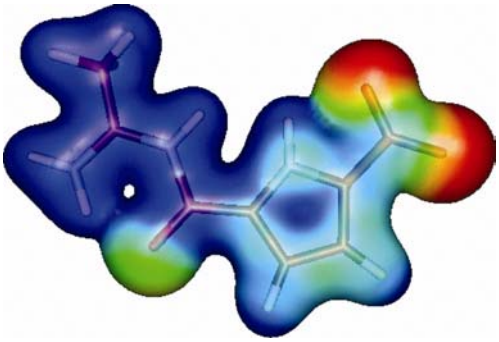

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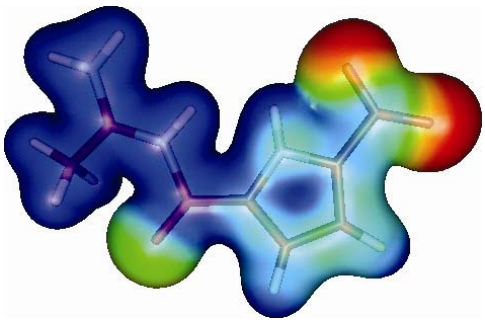

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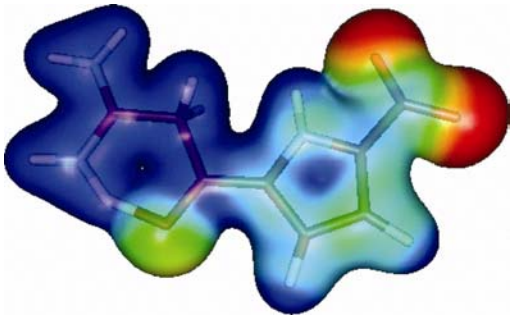

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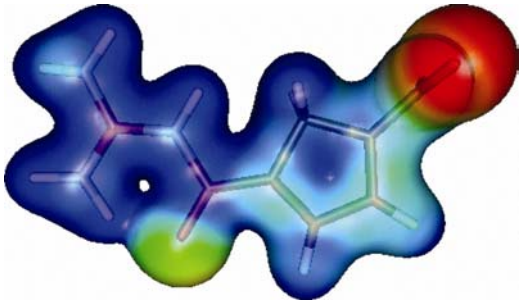

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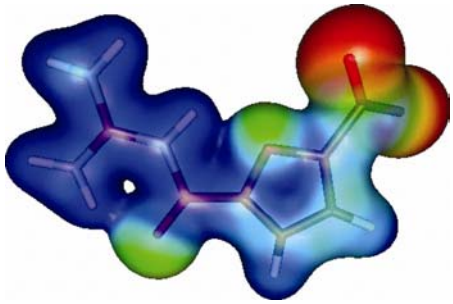

6

Chart 2: Electrostatic potential (contour value = 0.02) mapped on the electron density (contour value = 0.015) of the monomers 1-6 in gas phase.

Geometries

RI-DFT/B-LYP/TZVPP (all structures are zwitterionic except marked ones)

1 monomer gas phase (neutral structure)
FINAL HEAT OF FORMATION = -716.403386

O	-0.016537	-2.005205	-3.105985
C	-0.003848	-0.792414	-3.283467
O	0.007528	-0.218401	-4.528828
C	0.001084	0.192413	-2.203455
N	-0.003646	-0.258503	-0.899182
C	0.000930	0.815751	-0.032714
C	0.007957	1.979313	-0.815984
C	0.008471	1.592444	-2.169895
C	-0.000956	0.761496	1.448015
N	0.013989	-0.497488	2.023113
C	0.004033	-0.866913	3.401295
N	-0.007196	0.177458	4.282775
O	-0.015650	1.811783	2.107220
N	0.010143	-2.140183	3.614959
H	0.012867	2.982984	-0.412808
H	0.013630	2.237412	-3.038237
H	-0.015833	-1.250743	-0.688353
H	0.032780	-1.330055	1.443588
H	0.004797	-2.360232	4.614108
H	-0.033473	-0.012806	5.273632
H	-0.021611	1.129651	3.920478
H	0.003001	-0.956701	-5.170119
O	-0.016537	-2.005205	-3.105985

1 dimer gas phase (neutral structure)
FINAL HEAT OF FORMATION = -1432.869100

N	0.013309	-1.551601	-1.573039
C	0.006715	-2.655681	-0.752646
C	-0.015066	-3.796540	-1.572297
C	-0.020770	-3.349488	-2.908216
C	-0.004281	-1.941442	-2.890943
C	0.023175	-2.407296	0.692851
O	-0.000661	-3.448820	1.506205
C	-0.004835	-1.019501	-4.051453
N	-0.006895	0.340830	-3.745399
C	0.000953	1.435694	-4.621114
N	0.006561	1.147298	-5.949367
O	0.058112	-1.224781	1.104518
O	-0.003383	-1.456720	-5.213246
N	0.001776	2.625949	-4.071577
O	-0.028309	1.225007	-1.104281

C	-0.009326	2.407741	-0.692497
O	0.003405	3.449554	-1.505948
C	-0.001390	2.656211	0.753009
N	-0.003832	1.551839	1.573127
C	0.001971	1.941435	2.891130
C	0.007280	3.349589	2.908879
C	0.005976	3.796964	1.573080
C	-0.001216	1.019230	4.051454
N	0.010454	-0.340985	3.745162
C	-0.004755	-1.436143	4.620473
N	-0.017867	-1.148442	5.948897
O	-0.014987	1.456161	5.213301
N	-0.002175	-2.625931	4.070154
H	0.011177	3.952873	3.806917
H	0.008846	4.821265	1.224285
H	-0.002683	0.599073	1.197845
H	0.030411	-0.649881	2.761043
H	-0.010935	-3.372080	4.767251
H	-0.046813	-1.894538	6.628632
H	-0.026529	-0.164659	6.224548
H	-0.035409	-3.952965	-3.806032
H	-0.024256	-4.820667	-1.223098
H	0.021511	-0.598760	-1.198113
H	-0.016708	0.649803	-2.761306
H	0.006616	3.372038	-4.768929
H	0.017444	1.893079	-6.629920
H	0.005321	0.163467	-6.224637
H	0.003620	-3.104938	2.504080
H	0.000349	3.105770	-2.503280

1 monomer gas phase
FINAL HEAT OF FORMATION = -716.354610

C	0.065016	1.676480	-2.257047
C	0.041916	2.123265	-0.934240
C	-0.007521	0.979092	-0.087657
N	-0.005454	-0.128928	-0.941251
C	0.022194	0.259322	-2.233840
C	-0.003571	0.909880	1.325203
N	0.119101	-0.468980	1.849233
C	0.030691	-0.828392	3.146016
N	-0.092323	0.108731	4.089719
C	-0.029222	-0.902748	-3.252755
O	-0.122687	-2.031383	-2.664468
O	-0.084588	1.846122	2.142273
O	0.027099	-0.594555	-4.459853
N	0.061281	-2.144870	3.472764
H	0.073497	3.145643	-0.576458
H	0.106611	2.275488	-3.157033

H	-0.138499	-1.150835	-0.856540
H	0.148670	-2.856744	2.758762
H	0.350197	-1.196121	1.179206
H	0.204009	-2.432337	4.432269
H	-0.327675	-0.133300	5.043227
H	-0.128801	1.079407	3.722817

1 dimer gas phase
FINAL HEAT OF FORMATION = -1432.877851

C	0.006842	3.374357	2.795565
C	0.001967	1.962526	2.799893
N	-0.004186	1.553869	1.477793
C	-0.000737	2.641989	0.651198
C	0.006954	3.796270	1.455508
C	-0.000127	1.084155	3.963298
O	-0.015853	1.524825	5.128025
C	-0.010526	2.432138	-0.828391
O	0.021653	3.422698	-1.611022
N	0.016382	-0.311840	3.699566
C	-0.004251	-1.298407	4.641496
N	-0.024128	-2.568938	4.222673
O	-0.054467	1.199859	-1.200871
N	0.003757	-0.977040	5.948056
O	0.056623	-1.199770	1.200840
C	0.016427	-2.432208	0.828248
O	-0.015132	-3.422654	1.611063
C	0.008566	-2.642052	-0.651307
C	0.001827	-3.796414	-1.455485
C	-0.000589	-3.374554	-2.795541
C	0.002322	-1.962739	-2.800135
N	0.008948	-1.553951	-1.478004
C	-0.000933	-1.084063	-3.963262
O	0.008035	-1.524630	-5.128135
N	-0.014761	0.311731	-3.699238
C	-0.003853	1.298462	-4.641266
N	0.021854	2.569014	-4.222827
N	-0.027149	0.977293	-5.947795
H	0.010316	3.991493	3.684571
H	0.010631	4.812043	1.082989
H	-0.003327	0.588750	1.120934
H	-0.019145	-2.858031	3.195726
H	0.036128	-0.680476	2.696740
H	-0.008174	-3.308804	4.913699
H	-0.084032	-1.688525	6.660372
H	-0.017358	0.029840	6.157258
H	-0.004306	-3.991802	-3.684488
H	0.000568	-4.812292	-1.083184
H	0.005406	-0.589023	-1.120627

H	0.022724	2.857950	-3.195685
H	-0.030261	0.680446	-2.696399
H	-0.005535	3.308709	-4.913671
H	0.059743	1.688602	-6.660439
H	-0.003713	-0.029520	-6.157170

1 monomer solvent
FINAL HEAT OF FORMATION = -716.443902

C	0.014692	1.597492	-2.225690
C	0.011979	2.008014	-0.882387
C	-0.002010	0.850635	-0.080614
N	-0.006635	-0.235546	-0.944765
C	0.001883	0.192784	-2.243896
C	-0.002547	0.805796	1.369516
N	0.021436	-0.485087	1.956949
C	0.007310	-0.780710	3.299190
N	-0.021351	0.188109	4.205649
C	-0.005562	-0.806864	-3.377059
O	-0.035822	-2.033381	-3.036002
O	-0.021903	1.825985	2.075852
O	0.019821	-0.337949	-4.554913
N	0.022727	-2.068143	3.649663
H	0.021660	3.020152	-0.503375
H	0.025143	2.230595	-3.100874
H	-0.034401	-1.226754	-0.730253
H	0.039822	-2.806243	2.957881
H	0.058444	-1.290135	1.342768
H	0.017223	-2.338814	4.625092
H	-0.030324	-0.027440	5.194846
H	-0.027505	1.151989	3.875807

1 dimer solvent
FINAL HEAT OF FORMATION = -1432.927357

C	0.033246	3.350674	2.834631
C	0.007012	1.941835	2.835999
N	-0.019209	1.533194	1.516234
C	-0.008679	2.624665	0.688581
C	0.024962	3.775296	1.494759
C	0.000502	1.072229	4.014168
O	-0.019460	1.542820	5.165927
C	-0.045600	2.441230	-0.793069
O	0.026557	3.454327	-1.548585
N	0.015236	-0.313603	3.776838
C	-0.018136	-1.303790	4.731612
N	-0.022329	-2.568769	4.305824
O	-0.159241	1.227951	-1.203487
N	-0.049717	-1.002538	6.029161

O	0.172118	-1.227332	1.204037
C	0.065876	-2.440849	0.792822
O	0.007891	-3.455268	1.547868
C	0.019720	-2.623597	-0.688654
C	-0.022562	-3.774335	-1.494273
C	-0.042550	-3.350260	-2.834215
C	-0.013202	-1.941562	-2.836025
N	0.027075	-1.532361	-1.516730
C	-0.016934	-1.072884	-4.014929
O	-0.016507	-1.543621	-5.166734
N	-0.018140	0.312905	-3.776563
C	0.012105	1.303210	-4.731380
N	0.039577	2.567466	-4.304432
N	0.021257	1.003145	-6.029515
H	0.054382	3.970875	3.719144
H	0.036971	4.793573	1.133553
H	-0.026068	0.568867	1.162906
H	0.003268	-2.829035	3.301904
H	0.065877	-0.676876	2.794837
H	-0.034022	-3.318599	4.986230
H	-0.077634	-1.731608	6.730206
H	-0.047528	-0.018293	6.289670
H	-0.073674	-3.970521	-3.718385
H	-0.033897	-4.792477	-1.132603
H	0.030884	-0.567379	-1.164062
H	0.020833	2.827774	-3.300185
H	-0.059626	0.677648	-2.793609
H	0.036984	3.317521	-4.984735
H	0.053978	1.732615	-6.730012
H	0.006398	0.019333	-6.291058

2 monomer gas phase
FINAL HEAT OF FORMATION = -853.967121

C	-0.264192	-3.130601	-1.287312
C	0.006851	-2.297755	-0.185586
N	0.193760	-2.758138	1.064581
C	0.120305	-4.085242	1.292794
C	-0.147190	-4.993387	0.256102
C	-0.337229	-4.500542	-1.039263
N	0.103830	-0.891266	-0.259207
C	0.016033	-0.054407	-1.367817
O	-0.109308	-0.461279	-2.524342
C	0.333356	-4.533046	2.720573
C	0.081600	1.399629	-1.072037
C	0.317038	2.431361	-1.991411
C	0.296883	3.652082	-1.286814
C	0.038815	3.356618	0.057492
N	-0.079747	1.984245	0.167605

C	-0.135259	4.174495	1.256363
O	-0.380687	3.720349	2.368762
O	0.002089	5.517419	1.012682
H	-0.201176	-6.060590	0.460928
H	-0.543226	-5.184341	-1.861333
H	-0.453019	-4.127157	3.370448
H	0.325550	-5.624518	2.806471
H	1.289860	-4.154964	3.101571
H	-0.395611	-2.709044	-2.276102
H	-0.363006	1.545344	1.037284
H	0.350384	-0.491760	0.641968
H	0.449953	4.644452	-1.689367
H	0.492644	2.278945	-3.047822
H	-0.131751	5.964626	1.871924

2 dimer gas phase
FINAL HEAT OF FORMATION = - 1707.981289

C	-0.050728	-1.206857	6.165138
C	0.035187	-0.494740	4.950737
N	0.114217	0.861906	4.914426
C	0.124744	1.560668	6.075726
C	0.044394	0.918239	7.316307
C	-0.046515	-0.477192	7.349451
N	0.054797	-1.106092	3.689091
C	-0.164053	-2.451716	3.376264
O	-0.387874	-3.322679	4.220372
C	0.223360	3.066548	5.968936
C	-0.149682	-2.800939	1.929127
N	0.152135	-1.960123	0.885014
C	-0.005551	-2.626628	-0.312217
C	-0.410647	-3.940157	-0.021273
C	-0.493723	-4.049774	1.378092
C	0.227641	-1.896810	-1.552375
O	0.653534	-0.722030	-1.547150
O	-0.056562	-2.543395	-2.685337
O	-0.051348	2.546535	2.684279
C	0.232923	1.899320	1.551243
O	0.658865	0.724734	1.546347
C	-0.000550	2.629686	0.311357
N	0.154100	1.961910	-0.885493
C	-0.149455	2.801726	-1.929918
C	-0.490800	4.051522	-1.379325
C	-0.404665	3.943450	0.019961
C	-0.168578	2.450037	-3.376334
O	-0.398612	3.318958	-4.220944
N	0.057659	1.105469	-3.688688
C	0.036607	0.493254	-4.949740
C	-0.051434	1.204655	-6.164404

C	-0.047416	0.474738	-7.348509
C	0.046128	-0.920553	-7.315037
C	0.128375	-1.562463	-6.074362
N	0.117889	-0.863360	-4.913191
C	0.229709	-3.068163	-5.967269
H	0.052516	1.502491	8.232943
H	-0.110408	-1.000159	8.301995
H	1.136685	3.361630	5.436421
H	0.235593	3.530084	6.960103
H	-0.624041	3.476923	5.404945
H	-0.119598	-2.286505	6.148077
H	0.429776	-0.974472	0.938577
H	0.249615	-0.444657	2.926582
H	0.065278	-1.895120	-3.471791
H	0.054337	-1.505098	-8.231480
H	-0.113179	0.997350	-8.301113
H	-0.616646	-3.479998	-5.402765
H	0.242182	-3.531839	-6.958363
H	1.143849	-3.361495	-5.435204
H	-0.122532	2.284172	-6.147586
H	0.429225	0.975534	-0.938534
H	0.250951	0.443964	-2.925507
H	0.066216	1.897354	3.469637
H	-0.778733	-4.916038	1.959837
H	-0.617065	-4.708541	-0.754720
H	-0.608900	4.712818	0.752979
H	-0.776098	4.917535	-1.961314

2 monomer solvent
FINAL HEAT OF FORMATION = -853.991269

C	-0.024877	-3.147922	-1.308672
C	0.011978	-2.307349	-0.182551
N	0.035467	-2.771290	1.082312
C	0.020712	-4.103754	1.296090
C	-0.016903	-5.016064	0.230239
C	-0.039819	-4.523607	-1.077428
N	0.035795	-0.895916	-0.241180
C	-0.013649	-0.056079	-1.336225
O	-0.064962	-0.460181	-2.507948
C	0.038388	-4.558146	2.737926
C	0.005514	1.397483	-1.046696
C	0.064789	2.427565	-1.999314
C	0.067054	3.653111	-1.309794
C	0.007198	3.359741	0.060059
N	-0.026729	1.988535	0.195879
C	-0.022805	4.208296	1.248762
O	-0.071139	3.782953	2.401844
O	0.012160	5.535828	0.945099

H	-0.026527	-6.083509	0.424378
H	-0.066736	-5.208151	-1.920100
H	-0.881536	-4.247014	3.247594
H	0.123035	-5.645097	2.812670
H	0.876025	-4.099729	3.274570
H	-0.039144	-2.734121	-2.306167
H	-0.101702	1.536130	1.100139
H	0.093655	-0.485931	0.685878
H	0.109574	4.644063	-1.738057
H	0.106723	2.276468	-3.068216
H	-0.007690	6.036235	1.785752

2 dimer solvent
FINAL HEAT OF FORMATION = -1708.003840

C	0.095109	-1.236309	6.146070
C	0.104745	-0.515233	4.939214
N	0.195624	0.838835	4.908202
C	0.292492	1.530206	6.070704
C	0.289841	0.874745	7.307500
C	0.189060	-0.518595	7.335679
N	0.046909	-1.113296	3.666897
C	-0.288261	-2.418016	3.336085
O	-0.594276	-3.281099	4.172654
C	0.398090	3.034535	5.973388
C	-0.298535	-2.748264	1.888455
N	0.109909	-1.931439	0.862181
C	-0.107764	-2.556938	-0.346190
C	-0.665413	-3.818691	-0.083277
C	-0.776808	-3.940467	1.313208
C	0.217698	-1.845861	-1.578506
O	0.798658	-0.738366	-1.559235
O	-0.161403	-2.434191	-2.711120
O	-0.130626	2.452656	2.710062
C	0.231780	1.854603	1.575750
O	0.799849	0.741061	1.558144
C	-0.098317	2.563248	0.343805
N	0.104983	1.931218	-0.863409
C	-0.305475	2.746867	-1.889841
C	-0.768617	3.945796	-1.316080
C	-0.647059	3.828784	0.079992
C	-0.308869	2.408989	-3.335981
O	-0.641659	3.261660	-4.172999
N	0.049069	1.110188	-3.665056
C	0.108731	0.512535	-4.937573
C	0.109859	1.233985	-6.143949
C	0.210648	0.516511	-7.333193
C	0.308219	-0.877154	-7.305029
C	0.298867	-1.533367	-6.068710

N	0.194538	-0.841804	-4.907029
C	0.398532	-3.037996	-5.970638
H	0.367834	1.448236	8.224935
H	0.189384	-1.048642	8.283799
H	1.258489	3.325448	5.360249
H	0.509492	3.480436	6.964034
H	-0.496773	3.458000	5.502659
H	0.022298	-2.313690	6.134155
H	0.496480	-0.986872	0.936891
H	0.274081	-0.460742	2.909157
H	0.029963	-1.803583	-3.513089
H	0.391594	-1.450306	-8.222163
H	0.219966	1.046907	-8.281076
H	-0.505615	-3.459245	-5.515860
H	0.525803	-3.483608	-6.959486
H	1.247275	-3.331658	-5.342770
H	0.040717	2.311697	-6.132397
H	0.479568	0.981480	-0.936417
H	0.288174	0.459776	-2.908475
H	0.051229	1.818014	3.507521
H	-1.169606	-4.780587	1.867303
H	-0.950691	-4.548880	-0.826899
H	-0.921405	4.563788	0.822983
H	-1.156900	4.787618	-1.870759

3a monomer gas phase
FINAL HEAT OF FORMATION = -700.287373

C	0.003764	1.674961	-2.243163
C	-0.000652	0.254633	-2.226096
N	-0.001198	-0.141025	-0.937262
C	-0.000998	0.962506	-0.077073
C	0.001627	2.113268	-0.919665
C	-0.005394	-0.902677	-3.251889
O	0.021552	-0.583166	-4.457102
C	0.001471	0.901350	1.335336
O	-0.017873	1.845547	2.148189
O	-0.032850	-2.036565	-2.668326
N	0.032575	-0.476100	1.881511
C	0.018150	-0.810511	3.176736
C	0.003456	-2.265886	3.556947
N	-0.014587	0.131349	4.111550
H	0.005901	3.133884	-0.555887
H	0.008957	2.277371	-3.141936
H	-0.027874	-1.173426	-0.862427
H	0.530988	-2.874440	2.815882
H	0.073191	-1.244959	1.219115
H	0.471895	-2.417069	4.534777
H	-0.023822	-0.120354	5.091814

H	-0.030739	1.109109	3.765191
H	-1.034087	-2.621394	3.613520

3a dimer gas phase
FINAL HEAT OF FORMATION = -1400.705824

N	0.004978	-1.484078	-1.471160
C	0.005611	-2.566334	-0.642990
C	-0.002424	-3.731234	-1.438719
C	-0.008456	-3.326824	-2.775653
C	-0.004441	-1.910981	-2.794251
C	0.012958	-2.446464	0.854474
O	0.013868	-3.497078	1.527956
C	-0.008028	-1.095532	-3.984660
N	0.004807	0.341544	-3.828846
C	0.007134	1.204098	-4.856426
N	-0.011877	0.780953	-6.119637
O	0.017479	-1.235062	1.323195
O	-0.020136	-1.595835	-5.127498
C	0.037938	2.683012	-4.591316
O	-0.003526	1.235682	-1.323461
C	-0.004497	2.446996	-0.854490
O	-0.003585	3.497812	-1.527732
C	-0.006348	2.566598	0.643018
N	-0.003938	1.484160	1.470881
C	-0.004610	1.910679	2.794075
C	-0.008937	3.326508	2.775917
C	-0.009801	3.731351	1.439121
C	-0.001765	1.095225	3.984456
N	-0.001529	-0.341941	3.828773
C	-0.000081	-1.204388	4.856465
N	0.011760	-0.781002	6.119679
O	-0.000918	1.595572	5.127357
C	-0.016668	-2.683563	4.591486
H	-0.011482	3.948865	3.661053
H	-0.013235	4.739425	1.047046
H	0.002247	0.501729	1.146129
H	0.033558	-2.927252	3.521144
H	0.002478	-0.784166	2.839115
H	0.827864	-3.155760	5.110363
H	0.008294	-1.455988	6.873916
H	0.011378	0.239352	6.267936
H	-0.015111	-3.949568	-3.660483
H	-0.002194	-4.739168	-1.046327
H	0.004959	-0.501502	-1.146699
H	-0.015888	2.927600	-3.521321
H	0.006649	0.784059	-2.839385
H	-0.798168	3.164349	-5.115412
H	-0.007752	1.456039	-6.873792

H	-0.023018	-0.239334	-6.267988
H	-0.940586	-3.112157	5.003991
H	0.969054	3.101401	-4.998115

3a monomer solvent
FINAL HEAT OF FORMATION = -700.367268

C	0.003120	1.595003	-2.215967
C	0.001646	0.188370	-2.225945
N	-0.000322	-0.233286	-0.926900
C	-0.001840	0.858227	-0.067553
C	0.000437	2.012675	-0.877208
C	-0.000545	-0.816943	-3.355898
O	0.009217	-0.351442	-4.534614
C	-0.003390	0.820344	1.376859
O	-0.016993	1.831896	2.092740
O	-0.012267	-2.041316	-3.007957
N	0.014438	-0.479393	1.979432
C	0.013619	-0.764736	3.303815
C	-0.007194	-2.204824	3.707602
N	0.007151	0.183490	4.210568
H	0.001578	3.027021	-0.503674
H	0.005745	2.222436	-3.095183
H	-0.008574	-1.223912	-0.707433
H	0.614279	-2.802691	3.036781
H	0.031186	-1.291222	1.371822
H	0.342354	-2.321028	4.734753
H	0.011049	-0.055537	5.195944
H	-0.007768	1.161308	3.915721
H	-1.036957	-2.576152	3.641959

3a dimer solvent
FINAL HEAT OF FORMATION = -1400.705824

N	0.004978	-1.484078	-1.471160
C	0.005611	-2.566334	-0.642990
C	-0.002424	-3.731234	-1.438719
C	-0.008456	-3.326824	-2.775653
C	-0.004441	-1.910981	-2.794251
C	0.012958	-2.446464	0.854474
O	0.013868	-3.497078	1.527956
C	-0.008028	-1.095532	-3.984660
N	0.004807	0.341544	-3.828846
C	0.007134	1.204098	-4.856426
N	-0.011877	0.780953	-6.119637
O	0.017479	-1.235062	1.323195
O	-0.020136	-1.595835	-5.127498
C	0.037938	2.683012	-4.591316
O	-0.003526	1.235682	-1.323461

C	-0.004497	2.446996	-0.854490
O	-0.003585	3.497812	-1.527732
C	-0.006348	2.566598	0.643018
N	-0.003938	1.484160	1.470881
C	-0.004610	1.910679	2.794075
C	-0.008937	3.326508	2.775917
C	-0.009801	3.731351	1.439121
C	-0.001765	1.095225	3.984456
N	-0.001529	-0.341941	3.828773
C	-0.000081	-1.204388	4.856465
N	0.011760	-0.781002	6.119679
O	-0.000918	1.595572	5.127357
C	-0.016668	-2.683563	4.591486
H	-0.011482	3.948865	3.661053
H	-0.013235	4.739425	1.047046
H	0.002247	0.501729	1.146129
H	0.033558	-2.927252	3.521144
H	0.002478	-0.784166	2.839115
H	0.827864	-3.155760	5.110363
H	0.008294	-1.455988	6.873916
H	0.011378	0.239352	6.267936
H	-0.015111	-3.949568	-3.660483
H	-0.002194	-4.739168	-1.046327
H	0.004959	-0.501502	-1.146699
H	-0.015888	2.927600	-3.521321
H	0.006649	0.784059	-2.839385
H	-0.798168	3.164349	-5.115412
H	-0.007752	1.456039	-6.873792
H	-0.023018	-0.239334	-6.267988
H	-0.940586	-3.112157	5.003991
H	0.969054	3.101401	-4.998115

3b monomer gas phase
FINAL HEAT OF FORMATION = -700.274918

C	0.085001	2.145414	-0.946940
C	0.017554	1.020944	-0.077026
N	-0.011179	-0.105016	-0.907834
C	0.011155	0.257039	-2.209149
C	0.088781	1.671586	-2.261336
C	0.037290	0.986773	1.341339
O	-0.025899	1.896929	2.158611
C	-0.070043	-0.923098	-3.203518
O	0.023013	-0.642713	-4.415435
N	0.181871	-0.437279	1.857193
C	0.033020	-0.869273	3.102191
N	0.272745	-2.162309	3.384801
O	-0.215174	-2.035405	-2.595306
C	-0.406412	0.020379	4.229266

H	0.146150	3.173566	-0.610171
H	0.142330	2.251203	-3.173430
H	-0.198658	-1.115494	-0.799480
H	0.551662	-2.833987	2.676448
H	0.494388	-1.113387	1.160687
H	0.147572	-2.506268	4.328300
H	-0.513346	-0.560529	5.150616
H	-1.358582	0.501627	3.984161
H	0.314534	0.830117	4.372906

3b dimer gas phase
FINAL HEAT OF FORMATION = -700.274918

C	0.085001	2.145414	-0.946940
C	0.017554	1.020944	-0.077026
N	-0.011179	-0.105016	-0.907834
C	0.011155	0.257039	-2.209149
C	0.088781	1.671586	-2.261336
C	0.037290	0.986773	1.341339
O	-0.025899	1.896929	2.158611
C	-0.070043	-0.923098	-3.203518
O	0.023013	-0.642713	-4.415435
N	0.181871	-0.437279	1.857193
C	0.033020	-0.869273	3.102191
N	0.272745	-2.162309	3.384801
O	-0.215174	-2.035405	-2.595306
C	-0.406412	0.020379	4.229266
H	0.146150	3.173566	-0.610171
H	0.142330	2.251203	-3.173430
H	-0.198658	-1.115494	-0.799480
H	0.551662	-2.833987	2.676448
H	0.494388	-1.113387	1.160687
H	0.147572	-2.506268	4.328300
H	-0.513346	-0.560529	5.150616
H	-1.358582	0.501627	3.984161
H	0.314534	0.830117	4.372906
C	0.085001	2.145414	-0.946940
C	0.017554	1.020944	-0.077026
N	-0.011179	-0.105016	-0.907834
C	0.011155	0.257039	-2.209149
C	0.088781	1.671586	-2.261336
C	0.037290	0.986773	1.341339
O	-0.025899	1.896929	2.158611
C	-0.070043	-0.923098	-3.203518
O	0.023013	-0.642713	-4.415435
N	0.181871	-0.437279	1.857193
C	0.033020	-0.869273	3.102191
N	0.272745	-2.162309	3.384801
O	-0.215174	-2.035405	-2.595306

C	-0.406412	0.020379	4.229266
H	0.146150	3.173566	-0.610171
H	0.142330	2.251203	-3.173430
H	-0.198658	-1.115494	-0.799480
H	0.551662	-2.833987	2.676448
H	0.494388	-1.113387	1.160687
H	0.147572	-2.506268	4.328300
H	-0.513346	-0.560529	5.150616
H	-1.358582	0.501627	3.984161
H	0.314534	0.830117	4.372906

3b monomer solvent
FINAL HEAT OF FORMATION = -700.360979

C	0.014701	2.017154	-0.873874
C	0.017318	0.862879	-0.065604
N	0.002614	-0.227109	-0.926365
C	-0.003478	0.195760	-2.226712
C	0.001506	1.601138	-2.214320
C	0.026906	0.833052	1.384752
O	0.009491	1.839783	2.090423
C	-0.017287	-0.807981	-3.356499
O	0.009255	-0.342699	-4.535801
N	0.057229	-0.482171	1.971555
C	0.001863	-0.814672	3.280386
N	0.055134	-2.094030	3.593769
O	-0.052265	-2.032737	-3.010818
C	-0.118525	0.187469	4.382622
H	0.022468	3.031263	-0.499938
H	-0.002370	2.230472	-3.092276
H	-0.008644	-1.218109	-0.709770
H	0.137166	-2.828425	2.896245
H	0.134287	-1.265699	1.329165
H	0.009089	-2.383706	4.563963
H	-0.185469	-0.329230	5.341219
H	-1.002902	0.810926	4.231662
H	0.748218	0.853471	4.379645

3b dimer solvent
FINAL HEAT OF FORMATION = -1400.762080

C	0.035554	3.348534	2.849162
C	0.016428	1.938681	2.851095
N	-0.037266	1.530659	1.530536
C	-0.046896	2.622958	0.704586
C	-0.006093	3.773979	1.510372
C	0.038225	1.077214	4.035266
O	0.060464	1.536454	5.179699
C	-0.088589	2.439112	-0.777085

O	-0.050463	3.456482	-1.532267
N	0.031582	-0.326409	3.783329
C	-0.025943	-1.327495	4.695729
N	-0.011775	-2.567236	4.243961
O	-0.163889	1.225580	-1.188670
H	0.070869	3.967982	3.734043
H	-0.005012	4.792193	1.148823
H	-0.034605	0.566906	1.175817
H	0.028481	-2.826929	3.230507
H	0.084476	-0.658665	2.789372
H	-0.064393	-3.327074	4.913133
H	-0.186490	-2.059705	6.689190
H	-0.969932	-0.476017	6.416272
C	-0.106563	-1.100591	6.173969
H	0.780334	-0.565960	6.523791
O	0.168780	-1.225061	1.187457
C	0.086094	-2.438137	0.776142
O	0.052476	-3.455687	1.531378
C	0.031548	-2.622106	-0.705115
C	-0.030932	-3.773003	-1.509930
C	-0.066618	-3.348410	-2.848794
C	-0.031303	-1.938384	-2.851807
N	0.034500	-1.530552	-1.531920
C	-0.059600	-1.076547	-4.035116
O	-0.107662	-1.534376	-5.179069
N	-0.024350	0.326582	-3.783109
C	0.062933	1.325789	-4.694869
N	0.054774	2.566049	-4.244190
H	-0.114235	-3.967924	-3.733182
H	-0.043002	-4.791003	-1.147779
H	0.040299	-0.566751	-1.177417
H	-0.002108	2.826039	-3.231732
H	-0.081297	0.660012	-2.789625
H	0.132893	3.324797	-4.912123
H	0.295305	2.051882	-6.683902
H	1.017605	0.442094	-6.394127
C	0.171327	1.096202	-6.170881
H	-0.725747	0.593141	-6.540794

4 monomer gas phase
FINAL HEAT OF FORMATION = -700.273670

N	-0.005849	-0.171321	-0.985613
C	-0.002936	0.924721	-0.113449
C	0.009501	2.082419	-0.952452
C	0.013469	1.652794	-2.276721
C	0.003142	0.230386	-2.271292
C	-0.014631	0.811266	1.288149
O	-0.012074	1.800294	2.090131

C	0.001703	-0.896027	-3.329939
O	0.009197	-0.528551	-4.524329
C	-0.036092	-0.645355	1.856062
C	0.002884	-0.782524	3.360497
N	0.019906	-2.022493	3.879576
N	0.016727	0.309036	4.086072
O	-0.006545	-2.048754	-2.791452
H	0.014570	3.101379	-0.583302
H	0.022573	2.259039	-3.172957
H	-0.016474	-1.191091	-0.863571
H	0.011654	-2.832512	3.271065
H	0.810794	-1.210298	1.443361
H	0.043492	-2.188258	4.880131
H	0.046629	0.285479	5.101841
H	0.004967	1.206556	3.442535
H	-0.942802	-1.155131	1.498153

4 dimer gas phase
FINAL HEAT OF FORMATION = -1400.687192

N	-0.365545	-1.483070	-1.627923
C	-0.146562	-2.502165	-0.750430
C	0.344769	-3.610212	-1.473975
C	0.428289	-3.230408	-2.816532
C	-0.008595	-1.885530	-2.912755
C	-0.389671	-2.301679	0.717913
O	0.008931	-3.227448	1.506849
C	-0.054715	-1.064734	-4.097157
C	-0.666443	0.364245	-4.013192
C	0.219522	1.418722	-4.633407
N	0.721985	1.148969	-5.849885
O	-0.953039	-1.222434	1.062523
O	0.359542	-1.470154	-5.204618
N	0.439177	2.549566	-3.993671
C	-0.666547	-0.363797	4.013010
C	0.219070	-1.417911	4.633052
N	0.718515	-1.149586	5.851429
C	-0.053505	1.064697	4.097360
O	0.359648	1.469450	5.205509
C	-0.007208	1.886216	2.913786
C	0.428571	3.231361	2.815820
C	0.343997	3.609939	1.473122
C	-0.146797	2.500992	0.750245
N	-0.363904	1.482412	1.629014
C	-0.389098	2.301193	-0.718323
O	-0.950399	1.220862	-1.063795
O	0.006706	3.228295	-1.507015
N	0.441923	-2.547640	3.992615
H	0.760779	3.827778	3.655954

H	0.599448	4.565368	1.034273
H	-0.653615	0.536556	1.325835
H	0.136982	-2.770348	2.951376
H	-0.929954	-0.677049	2.998093
H	1.042477	-3.243205	4.430741
H	1.424098	-1.747259	6.268902
H	0.671208	-0.155776	6.123254
H	0.759567	-3.825837	-3.657703
H	0.600709	-4.565855	-1.035954
H	-0.656351	-0.538734	-1.319464
H	0.133156	2.770235	-2.953235
H	-0.930713	0.678456	-2.998720
H	1.041690	3.244860	-4.429499
H	1.426681	1.747190	-6.267966
H	0.674379	0.154845	-6.120931
H	-1.590979	0.320946	-4.608860
H	-1.591346	-0.319634	4.608086

4 monomer solvent
FINAL HEAT OF FORMATION = -700.363223

N	-0.004895	-0.230010	-0.969378
C	-0.002999	0.867765	-0.116899
C	0.006424	2.015098	-0.939679
C	0.010041	1.585172	-2.274380
C	0.002795	0.176988	-2.271797
C	-0.012674	0.794218	1.326787
O	-0.010502	1.824454	2.029757
C	0.002227	-0.834499	-3.395239
O	0.013494	-0.376145	-4.577584
C	-0.034047	-0.621055	1.940828
C	0.003287	-0.763690	3.447034
N	0.017738	-1.997207	3.936360
N	0.017043	0.295774	4.230288
O	-0.009599	-2.057912	-3.043016
H	0.009861	3.033520	-0.576949
H	0.016811	2.203642	-3.160116
H	-0.011149	-1.213392	-0.722617
H	0.009805	-2.800234	3.320119
H	0.811914	-1.193590	1.540343
H	0.040154	-2.176376	4.934699
H	0.040265	0.216936	5.241544
H	0.006376	1.212209	3.771654
H	-0.937203	-1.137390	1.590021

4 dimer solvent
FINAL HEAT OF FORMATION = -1400.746641

N	-0.342590	-1.453223	-1.637878

C	-0.110848	-2.439144	-0.719941
C	0.470224	-3.533370	-1.391731
C	0.583205	-3.187422	-2.742520
C	0.078953	-1.875715	-2.895395
C	-0.468290	-2.270606	0.729636
O	-0.044177	-3.165113	1.534021
C	0.003871	-1.114829	-4.126347
C	-0.635942	0.293670	-4.112964
C	0.193133	1.342765	-4.817036
N	0.630369	1.095994	-6.047029
O	-1.166872	-1.255837	1.044441
O	0.410038	-1.585344	-5.205747
N	0.428164	2.488958	-4.203660
C	-0.635011	-0.292973	4.112332
C	0.191215	-1.342678	4.818521
N	0.624885	-1.096722	6.049943
C	0.006427	1.114845	4.125647
O	0.414240	1.584725	5.204645
C	0.080218	1.875909	2.894741
C	0.583141	3.188064	2.741557
C	0.468587	3.534149	1.390924
C	-0.112032	2.439439	0.719496
N	-0.342136	1.453271	1.637499
C	-0.469922	2.270300	-0.729955
O	-1.166863	1.254321	-1.044365
O	-0.047613	3.165470	-1.534489
N	0.427794	-2.488579	4.205129
H	0.976604	3.793443	3.546047
H	0.757308	4.465262	0.924914
H	-0.706522	0.524399	1.378725
H	0.129709	-2.675092	3.220855
H	-0.874926	-0.645823	3.108765
H	0.973515	-3.209293	4.668801
H	1.227674	-1.746616	6.543251
H	0.536205	-0.147228	6.404762
H	0.976742	-3.792451	-3.547230
H	0.760288	-4.464120	-0.925827
H	-0.707584	-0.524543	-1.379034
H	0.128420	2.675996	-3.219863
H	-0.877450	0.646194	-3.109652
H	0.975457	3.209116	-4.666313
H	1.234653	1.745448	-6.539052
H	0.541168	0.146642	-6.402156
H	-1.580606	0.196971	-4.665609
H	-1.580743	-0.194572	4.662873

5 monomer gas phase
FINAL HEAT OF FORMATION = -700.266483

C	-0.002685	-0.790997	0.003414
C	-0.038395	0.426042	0.921048
C	0.004292	-0.171183	2.313076
C	0.054311	-1.556660	2.192100
C	0.048215	-1.923285	0.825554
C	-0.003128	0.682203	3.548899
O	1.132899	1.088823	3.906911
C	-0.004633	-0.813764	-1.407157
O	0.036609	-1.794060	-2.184763
O	-1.144138	0.901324	4.031384
N	-0.065319	0.540122	-2.014518
C	-0.022129	0.816079	-3.330661
N	0.058826	2.111087	-3.746075
N	-0.047909	-0.184941	-4.217697
H	0.081904	-2.942056	0.448431
H	0.088543	-2.250434	3.026180
H	-0.953805	1.030361	0.813951
H	-0.015303	2.866077	-3.076281
H	-0.105174	1.321114	-1.367411
H	-0.149643	2.339676	-4.709937
H	0.169718	-0.022944	-5.192278
H	-0.012115	-1.127772	-3.772392
H	0.821961	1.101894	0.791768

5 dimer gas phase
FINAL HEAT OF FORMATION = -1400.672580

C	0.338093	-1.449617	-1.257665
C	0.144513	-2.607674	-0.322477
C	-0.240773	-3.703220	-1.049151
C	-0.311912	-3.346289	-2.452951
C	0.006169	-2.017301	-2.612127
C	0.313045	-2.437945	1.159947
O	-0.172749	-3.305388	1.952635
C	-0.002791	-1.284548	-3.880105
N	-0.048247	0.130200	-3.747739
C	0.090400	1.027775	-4.770729
N	0.185562	0.586355	-6.040019
O	0.910362	-1.363227	1.523903
O	0.033919	-1.834952	-4.995703
N	0.129106	2.326877	-4.468218
N	0.071113	-0.133841	3.751632
C	-0.065616	-1.028954	4.777184
N	-0.153137	-0.582938	6.045904
C	0.008622	1.280228	3.878154
O	-0.035374	1.834587	4.991901
C	-0.005703	2.011579	2.609017
C	0.308031	3.341705	2.450220
C	0.230409	3.700507	1.047367

C	-0.158263	2.605894	0.320837
C	-0.340973	1.445250	1.254478
C	-0.336483	2.442048	-1.161615
O	-0.925748	1.364162	-1.529894
O	0.130812	3.322342	-1.951772
N	-0.101779	-2.328413	4.476437
H	0.600757	4.011513	3.254279
H	0.458299	4.679428	0.637340
H	-1.364885	1.043582	1.199046
H	-0.090796	-2.706105	3.467609
H	0.376474	-0.584624	2.829898
H	-0.121662	-3.000425	5.234216
H	-0.432590	-1.206313	6.791166
H	-0.146376	0.438950	6.158120
H	-0.602802	-4.016567	-3.257243
H	-0.475161	-4.680330	-0.638510
H	-0.305578	-0.596664	-0.989786
H	0.094104	2.707460	-3.460434
H	-0.350940	0.578106	-2.825761
H	0.150526	2.999037	-5.225841
H	0.438512	1.217073	-6.788152
H	0.161546	-0.433748	-6.160942
H	0.307147	0.597690	0.981272
H	1.365174	-1.056760	-1.200041

5 monomer solvent
FINAL HEAT OF FORMATION = -700.351656

C	0.001144	-0.757174	0.016922
C	-0.004028	0.461506	0.915798
C	0.000761	-0.129187	2.305755
C	0.007342	-1.493799	2.202823
C	0.007168	-1.878337	0.810008
C	-0.002917	0.697483	3.574042
O	-0.024126	1.962515	3.428255
C	-0.001238	-0.790364	-1.440091
O	-0.008562	-1.826359	-2.123430
O	0.015364	0.067463	4.679672
N	0.005598	0.486952	-2.058639
C	0.002602	0.756625	-3.405428
N	0.020935	2.036338	-3.783069
N	-0.018082	-0.232240	-4.290732
H	0.011623	-2.900138	0.446515
H	0.011786	-2.186965	3.034990
H	-0.885763	1.100416	0.764503
H	0.030072	2.787955	-3.105844
H	0.020178	1.297034	-1.448226
H	0.017132	2.287172	-4.763891
H	-0.021281	-0.039851	-5.284646

H	-0.025270	-1.188329	-3.938096
H	0.869968	1.110709	0.762770

5 dimer solvent
FINAL HEAT OF FORMATION = -1400.726972

C	0.329337	-1.435547	-1.295012
C	0.142471	-2.604272	-0.366514
C	-0.253000	-3.690745	-1.099473
C	-0.341068	-3.323138	-2.499158
C	-0.023347	-1.995939	-2.649513
C	0.347500	-2.489006	1.116087
O	-0.119907	-3.393947	1.882239
C	-0.022472	-1.271987	-3.926842
N	-0.053805	0.134106	-3.817387
C	0.087060	1.035511	-4.850397
N	0.224379	0.612639	-6.107156
O	0.968135	-1.445060	1.524328
O	0.013887	-1.842767	-5.031446
N	0.084705	2.332482	-4.542592
N	0.047044	-0.133026	3.817444
C	-0.092049	-1.036438	4.848820
N	-0.241669	-0.615860	6.104906
C	0.004446	1.272573	3.927944
O	-0.044788	1.842121	5.032741
C	0.013238	1.997714	2.651320
C	0.336818	3.323757	2.502757
C	0.261355	3.690844	1.102190
C	-0.132777	2.605552	0.366753
C	-0.332134	1.438588	1.294542
C	-0.327790	2.488989	-1.117032
O	-0.966756	1.456779	-1.526713
O	0.165673	3.380705	-1.882310
N	-0.076719	-2.333281	4.540642
H	0.631557	3.992663	3.304047
H	0.489950	4.675389	0.711067
H	-1.363948	1.061463	1.251620
H	-0.044382	-2.683386	3.559907
H	0.320891	-0.567798	2.907423
H	-0.163927	-3.016446	5.283684
H	-0.386644	-1.276176	6.857990
H	-0.201557	0.385904	6.282189
H	-0.638615	-3.992848	-3.298718
H	-0.474545	-4.676348	-0.706986
H	-0.303611	-0.582735	-1.011095
H	0.069415	2.681492	-3.560789
H	-0.322704	0.571662	-2.907140
H	0.177824	3.014494	-5.285924
H	0.374037	1.270717	-6.861245

H	0.172816	-0.388824	-6.283401
H	0.298218	0.582225	1.015545
H	1.359382	-1.053092	-1.259293

6 monomer gas phase
FINAL HEAT OF FORMATION = -736.228297

O	0.002334	-0.081901	-0.793597
C	-0.063806	0.224777	-2.126412
C	-0.142157	1.614584	-2.258901
C	-0.118499	2.174880	-0.968972
C	-0.025877	1.111349	-0.071014
C	0.004205	-0.938491	-3.124866
O	-0.458491	-2.029356	-2.712133
C	0.011106	0.981397	1.344941
N	0.081345	-0.424684	1.746692
C	0.057760	-0.887766	3.009107
N	0.081325	-0.030521	4.036668
O	-0.020715	1.878667	2.204353
O	0.541167	-0.596459	-4.211099
N	0.007850	-2.226227	3.218942
H	-0.156065	3.222847	-0.696843
H	-0.187027	2.132438	-3.207519
H	0.039572	-2.871932	2.439376
H	0.082978	-1.086322	0.967900
H	0.145370	-2.609321	4.145094
H	-0.058098	-0.344433	4.987108
H	0.047152	0.967212	3.769991

6 dimer gas phase
FINAL HEAT OF FORMATION = -1472.589438

O	0.189120	-1.523811	-1.532515
C	0.096453	-2.610050	-0.702588
C	-0.131801	-3.750610	-1.452228
C	-0.173957	-3.350185	-2.810964
C	0.011413	-1.977660	-2.818597
C	0.227370	-2.376365	0.775665
O	-0.163145	-3.340770	1.518123
C	0.005475	-1.034055	-3.931802
N	-0.036604	0.332175	-3.590874
C	0.039995	1.358812	-4.501910
N	0.056458	1.078196	-5.821292
O	0.688696	-1.263729	1.154369
O	0.029737	-1.442468	-5.107676
N	0.084519	2.607637	-4.047954
H	-0.339971	-3.965816	-3.685298
H	-0.256038	-4.745667	-1.047331
H	0.093405	2.882867	-2.989899

H	-0.243193	0.640250	-2.581634
H	0.071552	3.359313	-4.727742
H	0.271936	1.803032	-6.492461
H	0.069065	0.081351	-6.068754
N	0.037387	-0.332623	3.590842
C	-0.037559	-1.359171	4.502556
N	-0.065236	-1.077581	5.821145
C	-0.007047	1.033478	3.931568
O	-0.034070	1.442280	5.107305
C	-0.012031	1.977438	2.818246
C	0.171736	3.350187	2.811132
C	0.128525	3.750944	1.452505
C	-0.096724	2.610114	0.702421
O	-0.187384	1.523404	1.532061
C	-0.226876	2.376799	-0.775830
O	-0.685795	1.263376	-1.154967
O	0.161263	3.342590	-1.517773
N	-0.070152	-2.608454	4.048862
H	0.331571	3.966646	3.686031
H	0.251159	4.746358	1.047943
H	-0.085616	-2.882990	2.990738
H	0.246409	-0.640686	2.582089
H	-0.066839	-3.359972	4.728860
H	-0.269759	-1.804701	6.493171
H	-0.077224	-0.080921	6.069128

6 monomer solvent
FINAL HEAT OF FORMATION = -736.313046

O	-0.007249	-0.162581	-0.840785
C	0.001128	0.211311	-2.167060
C	0.006205	1.590830	-2.250900
C	-0.000283	2.096879	-0.925985
C	-0.006486	0.998723	-0.089670
C	-0.003404	-0.879131	-3.217750
O	-0.076903	-2.075230	-2.809695
C	-0.007216	0.890285	1.361611
N	0.010439	-0.434910	1.842410
C	0.011920	-0.835016	3.157295
N	-0.007272	0.061619	4.135336
O	-0.021505	1.873643	2.112306
O	0.066432	-0.466105	-4.415116
N	0.033527	-2.144746	3.404264
H	0.001099	3.131771	-0.614228
H	0.012834	2.163100	-3.166494
H	0.043546	-2.825039	2.655093
H	0.026202	-1.172469	1.142995
H	0.034638	-2.492915	4.355220
H	-0.007073	-0.229513	5.105062

H	-0.020742	1.049319	3.889443

6 dimer solvent
FINAL HEAT OF FORMATION = -1472.645037

O	0.166289	-1.520875	-1.601491
C	0.071689	-2.627753	-0.789546
C	-0.146517	-3.751447	-1.562570
C	-0.181561	-3.325666	-2.914853
C	0.001303	-1.956448	-2.897899
C	0.212720	-2.431893	0.692965
O	-0.157940	-3.416433	1.415483
C	0.011392	-1.001328	-4.006841
N	-0.022345	0.356085	-3.663710
C	0.035854	1.403233	-4.566149
N	0.096663	1.165606	-5.876644
O	0.673429	-1.327775	1.106112
O	0.040764	-1.407616	-5.180613
N	0.029532	2.642907	-4.085041
H	-0.334374	-3.933977	-3.794783
H	-0.263492	-4.758902	-1.191446
H	0.046155	2.872291	-3.063494
H	-0.194724	0.636652	-2.667897
H	0.064809	3.416412	-4.738877
H	0.168159	1.931297	-6.534739
H	0.078282	0.199107	-6.195118
N	0.023654	-0.356341	3.663650
C	-0.029227	-1.403630	4.566337
N	-0.092824	-1.166113	5.876556
C	-0.015467	1.000935	4.006642
O	-0.048586	1.407090	5.180417
C	-0.006026	1.956259	2.897876
C	0.173041	3.325978	2.915620
C	0.139938	3.752045	1.563392
C	-0.073804	2.628040	0.789582
O	-0.167010	1.520628	1.600964
C	-0.211661	2.432372	-0.693312
O	-0.672728	1.328750	-1.107388
O	0.160793	3.416792	-1.414966
N	-0.014422	-2.643366	4.085567
H	0.322455	3.934436	3.796021
H	0.254980	4.759928	1.192897
H	-0.034702	-2.872703	3.064087
H	0.196534	-0.636352	2.667819
H	-0.045652	-3.416880	4.739578
H	-0.160796	-1.932135	6.534645
H	-0.081561	-0.199422	6.194769

RI-DFT/B3-LYP/TZVPP

1 monomer gas phase
FINAL HEAT OF FORMATION = -716.152255

C	0.019955	1.667468	-2.239095
C	0.010956	2.100375	-0.920305
C	-0.006841	0.957846	-0.089565
N	-0.005930	-0.133807	-0.943562
C	0.005935	0.260776	-2.219800
C	-0.001706	0.888113	1.316060
N	0.040615	-0.472704	1.838818
C	0.010255	-0.814475	3.133266
N	-0.019622	0.122536	4.065716
C	-0.007271	-0.892415	-3.238630
O	-0.029474	-2.011090	-2.655284
O	-0.024996	1.820331	2.120029
O	0.005797	-0.581815	-4.430765
N	0.005676	-2.117319	3.460947
H	0.020918	3.114678	-0.556408
H	0.035274	2.268641	-3.131529
H	-0.049375	-1.154813	-0.867397
H	0.045173	-2.832639	2.756167
H	0.115009	-1.221006	1.168966
H	0.079468	-2.407063	4.419597
H	-0.104167	-0.106373	5.039494
H	-0.030696	1.086094	3.705561

1 dimer gas phase
FINAL HEAT OF FORMATION = -1432.483111

C	0.014021	3.347179	2.776877
C	0.004482	1.948366	2.777213
N	-0.003462	1.541540	1.467627
C	0.002263	2.620561	0.650295
C	0.013386	3.767326	1.443264
C	0.001208	1.074425	3.936033
O	-0.000738	1.509126	5.086468
C	-0.005086	2.413391	-0.823126
O	0.016039	3.393870	-1.594385
N	0.000129	-0.306316	3.672737
C	-0.009330	-1.286122	4.606041
N	-0.008046	-2.544776	4.189326
O	-0.033644	1.195354	-1.191828
N	-0.023434	-0.973968	5.901966
O	0.025429	-1.195664	1.192124
C	0.012011	-2.413914	0.823205
O	0.003697	-3.394621	1.594323
C	0.007196	-2.620585	-0.650337
C	0.007821	-3.767353	-1.443422
C	0.005149	-3.347048	-2.776998
C	0.001529	-1.948226	-2.777188

N	0.003245	-1.541546	-1.467540
C	-0.001645	-1.074370	-3.936027
O	0.006879	-1.509067	-5.086393
N	-0.015304	0.306487	-3.672919
C	-0.007741	1.286378	-4.606028
N	0.005691	2.544838	-4.189099
N	-0.019492	0.974798	-5.902339
H	0.020268	3.959529	3.662215
H	0.019249	4.776838	1.070481
H	-0.004480	0.584275	1.112304
H	-0.000985	-2.829448	3.172876
H	0.010314	-0.667974	2.679731
H	-0.017642	-3.280880	4.873623
H	-0.017778	-1.688225	6.606342
H	-0.015245	0.020682	6.122789
H	0.005526	-3.959329	-3.662414
H	0.011584	-4.776928	-1.070785
H	-0.000730	-0.584289	-1.112269
H	0.008833	2.829548	-3.172582
H	-0.024060	0.667909	-2.679746
H	-0.008469	3.280922	-4.873377
H	0.038102	1.688188	-6.605372
H	-0.001106	-0.019706	-6.123028

Full Author List

[18] TURBOMOLE, Ahlrichs, R.; Bär, M.; Baron, H.-P.; Bauernschmitt, R.; Böcker, S.; Ehrig, M.; Eichkorn, K.; Elliott, S.; Haase, F.; Häser, M.; Horn, H.; Huber, C.; Huniar, U.; Kattannek, M.; Kölmel, C.; Kollwitz, M.; Ochsenfeld, C.; Öhm, H.; Schäfer, A.; Schneider, U.; Treutler, O.; von Arnim, M.; Weigend, F.; Weis, P.; Weiss, H. **since 1988**, *Quant. Chem. Group, University of Karlsruhe*, Germany.

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