Table S1. Selected bond lengths [Å] and angles [°] for **6** (for atom numbering see Fig. 1).

N(1)-C(2)	1.364(2)	N(3)-C(2)-O(2)	123.49(17)
C(2)-N(3)	1.343(2)	N(3)-C(4)-C(41)	110.80(14)
N(3)-C(4)	1.472(2)	C(5)-C(4)-C(41)	110.94(15)
C(4)-C(5)	1.504(3)	C(4)-C(5)-C(51)	117.78(15)
C(5)-C(6)	1.346(3)	C(6)-C(5)-C(51)	124.56(16)
C(6)-N(1)	1.398(2)	C(5)-C(51)-O(51)	116.25(16)
C(2)-O(2)	1.2502(19)	C(5)-C(51)-O(52)	120.46(16)
C(4)-C(41)	1.530(3)	O(51)-C(51)-O(52)	123.29(15)
C(5)-C(51)	1.495(2)	C(5)-C(6)-C(61)	129.06(15)
C(51)-O(51)	1.271(2)	N(1)-C(6)-C(61)	112.11(15)
C(51)-O(52)	1.262(2)	N(1)-C(2)-N(3)-C(4)	15.9(2)
C(6)-C(61)	1.487(3)	C(2)-N(3)-C(4)-C(5)	-41.0(2)
C(6)-N(1)-C(2)	122.14(15)	N(3)-C(4)-C(5)-C(6)	35.4(2)
N(1)-C(2)-N(3)	116.41(15)	C(4)-C(5)-C(6)-N(1)	-7.2(2)
C(2)-N(3)-C(4)	120.52(16)	C(5)-C(6)-N(1)-C(2)	-22.0(2)
N(3)-C(4)-C(5)	109.14(14)	C(6)-N(1)-C(2)-N(3)	17.6(2)
C(4)-C(5)-C(6)	117.43(15)	C(6)-N(1)-C(2)-O(2)	-160.70(15)
C(5)-C(6)-N(1)	118.81(17)	C(2)-N(3)-C(4)-C(41)	81.5(2)
N(1)-C(2)-O(2)	120.08(16)	N(3)-C(4)-C(5)-C(51)	-149.77(14)

Table S2 Results (electronic excitation energies ν (cm^{-1}), oscillator strengths f, and rotational strength R (in cgs units ($*10^{40}$)) of semiempirical INDO/S calculations for different geometries (AM1, HF/3-21G, B3LYP/3-21G, HF/6-31G*, and B3LYP/6-31G*) of **(*S*) – 1a**.

ν	f	R	ν	f	R	ν	f	R	ν	f	R
s-trans			s-cis			s-trans			s-cis		
AM1						HF/3-21G					
26671	0.000	-2.136	26374	0.001	0.764	27719	0.001	-6.872	27394	0.001	-2.388
30204	0.000	-6.312	30197	0.000	-7.698	32365	0.001	16.485	32343	0.001	16.648
34061	0.417	36.358	34049	0.397	7.050	35916	0.413	27.430	35849	0.412	-1.202
43550	0.196	-11.764	43285	0.112	-11.831	45611	0.228	-18.447	45841	0.130	-38.622
45892	0.163	-33.240	46916	0.177	-44.605	46668	0.049	-33.582	47341	0.082	-30.314
B3LYP/3-21G						HF/6-31G*					
27163	0.001	-9.689	26736	0.001	-1.338	28310	0.001	-11.034	28343	0.001	-10.636
31811	0.002	19.773	31784	0.002	19.111	32537	0.002	23.126	32508	0.002	21.899
34779	0.443	31.137	34702	0.436	-3.817	36442	0.418	35.946	36353	0.400	10.981

44629	0.219	-27.251	44652	0.106	-34.660	46127	0.191	-39.324	46167	0.093	-38.137
45544	0.050	-27.393	46536	0.104	-31.221	47148	0.049	-27.800	48065	0.089	-43.162
B3LYP/6-31G*											
27683	0.002	-13.572	27722	0.001	-10.182						
31936	0.003	24.121	31921	0.002	23.016						
35302	0.450	36.506	35190	0.422	3.911						
45082	0.173	-42.679	45003	0.082	-35.626						
46183	0.064	-22.769	47294	0.103	-43.410						

Table S3. Results (electronic excitation energies ν (cm^{-1}), oscillator strengths f, and rotational strength R (in cgs units ($*10^{40}$)) of semiempirical INDO/S calculations for different geometries (AM1, HF/3-21G, B3LYP/3-21G, HF/6-31G*, and B3LYP/6-31G*) of **(*R*) – 2a**.

s-cis			s-trans			s-cis			s-trans		
ν	f	R	ν	f	R	ν	f	R	ν	f	R
AM1						HF/3-21G					
26558	0.001	-8.148	26761	0.000	0.752	27577	0.001	-10.891	27694	0.001	1.771
30168	0.000	-2.107	30189	0.000	-1.487	32370	0.001	-26.581	32426	0.002	-28.941
33816	0.376	-63.666	33816	0.396	-116.253	35517	0.368	-38.837	35608	0.371	-110.547
36600	0.008	1.995	36648	0.008	1.902	37343	0.007	1.212	37445	0.011	2.484
41956	0.128	43.196	40588	0.092	50.776	43178	0.146	31.779	42259	0.093	44.076
B3LYP/3-21G						HF/6-31G*					
26797	0.001	-1.395	27026	0.001	10.264	28522	0.001	-9.037	28360	0.001	-3.386
31804	0.003	-33.575	31879	0.004	-32.286	32559	0.001	-18.954	32606	0.002	-24.065
34766	0.381	-56.460	34646	0.406	-107.954	36028	0.364	-19.660	36019	0.367	-85.533

36816	0.019	5.272	36844	0.016	2.521	37457	0.003	-2.918	37428	0.004	0.569
43646	0.049	-42.423	41608	0.039	43.171	44155	0.181	26.008	42706	0.136	36.448
B3LYP/6-31G*											
27864	0.001	-4.690	27652	0.001	5.670						
31959	0.001	-19.524	32002	0.003	-28.029						
34899	0.390	-44.490	35065	0.407	-94.374						
36879	0.003	-2.193	36868	0.009	2.096						
43119	0.144	32.081	41701	0.074	42.121						

Table S4. Results (electronic excitation energies ν (cm^{-1}), oscillator strengths f, and rotational strength R (in cgs units ($*10^{40}$)) of semiempirical INDO/S calculations for ***(R)* – 3a** (AM1 geometry).

s-cis -3aA			s-trans-3aA			s-cis -3aB			s-trans -3aB		
ν	f	R	ν	f	R	ν	f	R	ν	f	R
26548	0.001	-6.824	26771	0.000	-0.071	26543	0.001	-6.088	26720	0.000	-3.120
30155	0.000	-4.508	30182	0.000	-3.322	30157	0.000	-1.989	30227	0.000	-1.000
31380	0.003	2.096	31431	0.002	1.889	31361	0.003	-2.718	31341	0.007	-5.717
33388	0.271	-170.579	33331	0.295	-236.128	33689	0.424	-76.065	33610	0.450	-161.459
36305	0.243	79.578	36301	0.244	56.390	36296	0.122	-10.433	35974	0.094	16.919

Table S5. Results (electronic excitation energies ν (cm^{-1}) and oscillator strengths f of semiempirical INDO/S calculations for different geometries (AM1 and HF/6-31G*) of **4**.

s-cis		s-trans		s-cis		s-trans	
ν	f	ν	f	ν	f	ν	f
AM1				HF/6-31G*			
26599	0.001	26956	0.000	28474	0.001	28382	0.001
30664	0.000	30664	0.000	32654	0.001	32619	0.001
34034	0.381	34046	0.391	36367	0.384	36516	0.404
43645	0.147	43882	0.224	46336	0.097	46511	0.179
46707	0.187	45668	0.173	48837	0.129	47757	0.096

Table S6. Results (electronic excitation energies ν (cm^{-1}), oscillator strengths f, and rotational strength R (in cgs units ($*10^{40}$)) of semiempirical INDO/S calculations for ***(R)* – 5a** (AM1 geometry).

s-cis -5aA			s-trans-5aA			s-cis -5aB			s-trans -5aB		
ν	f	R	ν	f	R	ν	f	R	ν	f	R
20382	0.000	-7.244	20412	0.000	-6.614	20432	0.000	-6.559	20472	0.000	-5.955
26545	0.001	-13.495	26879	0.000	-0.868	26593	0.001	-16.616	26922	0.000	-4.931
31447	0.518	-54.587	31535	0.526	-78.960	31564	0.515	-52.384	31662	0.521	-73.309
35138	0.042	23.385	35006	0.052	40.897	35248	0.018	6.254	35141	0.044	27.878
35740	0.087	24.021	35434	0.045	5.966	35656	0.112	53.321	35336	0.066	30.115

Table S7 Basis set dependence of calculated (RPA) electronic transition energies ν (cm^{-1}), oscillator strengths f and rotational strengths R (10^{-40} esu^2 cm^2) for ***(S)* – 1a** (AM1 geometry) and ***(R)* – 1a** (HF/6-31G* geometry). CIS results are given in parentheses.

	***(S)* – 1** (AM1 geometry)			***(R)* – 1** (HF/6-31G* geometry)		
s-cis	ν	f	R	ν	f	R
6-31G*	45357	0.298	-0.200	48808	0.332	16.208
	50380	0.001	-1.384	54477	0.004	6.781
	55376	0.002	-14.495	62527	0.001	7.377
	66458	0.230	35.167	70761	0.163	-5.841
6-311++G**	44361	0.321	2.843	47956	0.351	15.132
	50680	0.000	-1.560	54589	0.004	6.945
	54742	0.003	-1.335	56314	0.005	-2.753
	55714	0.004	-19.640	61897	0.009	-6.938
aug-cc-pVDZ	44056	0.314	4.563	47360	0.350	16.351
	50603	0.000	-1.422	54146	0.003	3.892
	52794	0.002	-2.092	54322	0.004	1.065

	55731	0.004	-21.713	58859	0.004	-2.339
s-trans						
6-31G*	45466 (47639)	0.336 (0.448)	11.290	48657	0.352	-8.380
	51021 (52352)	0.002 (0.003)	-16.036	55039	0.003	22.738
	55384 (56625)	0.002 (0.004)	-12.959	62377	0.001	7.088
	65879 (67500)	0.240 (0.337)	35.694	69844	0.190	15.059
6-311++G**	44741 (46581)	0.355 (0.459)	12.018	47878	0.374	-4.936
	51349 (52388)	0.001 (0.002)	-15.553	55218	0.003	20.391
	54933 (53794)	0.002 (0.002)	-1.205	55531	0.004	-2.883
	55770 (56793)	0.004 (0.006)	-17.600	61863	0.007	-8.525
aug-cc-pVDZ	44245 (46282)	0.358 (0.444)	12.620	47355 (49424)	0.377 (0.468)	-3.463
	51205 (52477)	0.001 (0.002)	-15.337	53341 (53411)	0.003 (0.004)	-2.156
	52906 (52990)	0.001 (0.002)	-1.900	54937 (56209)	0.002 (0.003)	18.717
	55735 (56935)	0.005 (0.006)	-20.571	58782 (58840)	0.003 (0.005)	-1.315

Table S8 Geometry dependence of calculated (RPA/6-31G*) electronic transition energies ν (cm^{-1}), oscillator strengths f and rotational strengths R (10^{-40} esu^2 cm^2) for ***(S)* – 1a**.

RPA/6-31G*	s-cis			s-trans		
geometry	ν	f	R	ν	f	R
AM1	45357	0.298	-0.200	45466	0.336	11.290
	50380	0.001	-1.384	51021	0.002	-16.036
	55376	0.002	-14.495	55384	0.002	-12.959
	66458	0.230	35.167	65879	0.240	35.694
	70451	0.015	14.363	70135	0.056	-15.524
HF/3-21G	48156	0.338	-12.794	48642	0.375	13.439
	52638	0.001	-4.201	53054	0.004	-24.743
	61461	0.000	-2.563	61565	0.000	-2.335
	69218	0.178	-9.920	68526	0.199	-35.448
	74335	0.021	17.622	74473	0.029	-10.403
B3LYP/3-21G	46229	0.334	-14.415	46576	0.371	14.078
	50916	0.001	-3.641	51287	0.004	-27.111
	59331	0.000	-3.362	59438	0.000	-3.068
	67397	0.182	-3.877	66668	0.201	-29.893
	72068	0.033	31.045	72084	0.054	-25.926
HF/6-31G*	48433	0.311	-16.948	48660	0.352	8.400
	54715	0.003	-3.077	55037	0.003	-22.748
	62294	0.001	-7.307	62379	0.001	-7.076
	70629	0.176	13.370	69843	0.190	-15.123
	74537	0.004	-7.965	74461	0.005	-0.285

B3LYP/6-31G*	46581	0.309	-18.412	46728	0.352	9.192
	52664	0.002	-3.255	52955	0.004	-26.177
	60012	0.001	-7.340	60060	0.001	-7.350
	68717	0.181	20.769	67927	0.194	-6.710
	73035	0.015	15.429	73011	0.035	-6.192

Table S9 Geometry dependence of calculated (RPA/6-31G*) electronic transition energies ν (cm^{-1}), oscillator strengths f and rotational strengths R (10^{-40} esu^2 cm^2) for ***(R)* – 2a** .

RPA/6-31G*	s-cis			s-trans		
	ν	f	R	ν	f	R
AM1	44786	0.285	-123.193	44972	0.326	-127.386
	48258	0.001	1.185	48260	0.002	1.750
	48646	0.019	28.141	48555	0.013	22.405
	50372	0.000	-1.898	51076	0.001	7.517
	55013	0.002	10.953	55028	0.003	9.830
HF/3-21G	47406	0.288	-147.400	47784	0.305	-146.159
	49101	0.001	0.151	49136	0.001	-0.377
	49745	0.051	40.569	49758	0.053	19.711
	52709	0.000	-1.973	53201	0.002	17.840
	61397	0.017	9.835	61278	0.324	81.904
B3LYP/3-21G	45730	0.278	-31.949	45902	0.325	-84.314
	48320	0.008	-5.072	48322	0.006	-4.834
	48642	0.013	15.360	48579	0.012	19.781
	50733	0.000	-0.367	51496	0.002	21.648
	59003	0.007	1.097	59062	0.026	9.500
HF/6-31G*	47853	0.280	-143.621	47820	0.297	-160.432
	49032	0.005	-3.335	48985	0.002	0.237
	49584	0.050	41.271	49585	0.059	28.042
	54813	0.000	-0.718	54988	0.001	14.166
	61900	0.900	116.158	61645	0.820	124.283

B3LYP/6-31G*	46067	0.293	-139.745	45946	0.313	-124.308
	48234	0.004	0.046	48252	0.001	0.332
	48607	0.027	41.557	48599	0.021	28.018
	52727	0.000	-0.501	53159	0.002	17.168
	59840	0.002	6.466	59793	0.063	24.622
	60834	0.858	114.373	60623	0.655	105.915

Table S10. Main configurations for the first few excited singlet electronic states of compounds **1a – 3a, 4** and **5a** obtained by ab initio CIS/6-31G* calculations[a].

Compound	State	Main configurations
cis – 1a	S_1	0.68544 (45 → 46)
	S_2	0.52929 (42 → 46), 0.25570 (42 → 50)
	S_3	-0.38959 (43 → 46), 0.41270 (43 → 50)
	S_4	0.58958 (44 → 46), -0.24092 (44 → 50)
	S_5	0.56691 (45 → 47)
	S_6	0.31667 (39 → 46), -0.29986 (41 → 46), 0.35373 (45 → 50)
trans – 1a	S_1	0.68361 (45 → 46)
	S_2	0.55008 (42 → 46), -0.26332 (42 → 50)
	S_3	0.38879 (43 → 46), 0.43555 (43 → 50)
	S_4	0.61016 (44 → 46)
	S_5	0.54675 (45 → 47)
	S_6	0.43400 (39 → 46)
cis – 2a	S_1	-0.35593 (59 → 62), 0.49988 (61 → 62)
	S_2	0.35613 (60 → 63), -0.29734 (61 → 63), 0.28103 (61 → 64)
	S_3	-0.30905 (59 → 62), 0.30017 (60 → 64), -0.30399 (61 → 63)
	S_4	0.44660 (56 → 62)
	S_5	0.38698 (57 → 62), 0.34544 (57 → 68)
	S_6	0.32467 (59 → 62), -0.36980 (60 → 63), 0.34610 (61 → 62)
trans – 2a	S_1	0.45348 (59 → 62), -0.42991 (61 → 62)
	S_2	0.36115 (60 → 63), -0.32063 (61 → 63), 0.30964 (61 → 64)
	S_3	-0.33183 (59 → 62), 0.30224 (60 → 64), -0.30180 (61 → 63)

	S_4	0.48531 (56 → 62)
	S_5	0.39877 (57 → 62), 0.33916 (57 → 68)
	S_6	-0.31720 (60 → 63), 0.44007 (61 → 62)
cis – 3aA	S_1	-0.27667 (73 → 77),0.50202 (74 → 75), 0.32062 (74 → 76)
	S_2	0.39744 (73 → 75), 0.42736 (74 → 77)
	S_3	0.45624 (72 → 75), -0.38625 (72 → 76)
	S_4	0.32086 (69 → 75), -0.33138 (69 → 76)
	S_5	-0.23510 (68 → 79), -0.21107 (73 → 75), -0.22300 (74 → 76)
	S_6	0.21287 (68 → 75), -0.25150 (68 → 79), 0.20153 (74 → 76), -0.21097 (74 → 78)
cis – 3aB	S_1	0.28623 (73 → 77), -0.46951 (74 → 75), 0.35929 (74 → 76)
	S_2	0.36289 (73 → 75), 0.42878 (74 → 77)
	S_3	0.46761 (72 → 75), 0.36474 (72 → 76)
	S_4	0.32842 (69 → 75), 0.35460 (69 → 76)
	S_5	0.25857 (68 → 75), -0.26048 (68 → 79), 0.25519 (68 → 80)
	S_6	-0.25839 (73 → 75), 0.20043 (74 → 75), 0.26986 (74 → 76), 0.21502 (74 → 78)
trans – 3aA	S_1	-0.29537 (73 → 77), -0.41924 (74 → 75), 0.42235 (74 → 76)
	S_2	-0.32973 (73 → 75), 0.37296 (73 → 76), 0.43869 (74 → 77)
	S_3	0.53640 (72 → 75), 0.29892 (72 → 76)
	S_4	0.38501 (67 → 75), 0.25468 (67 → 76)
	S_5	-0.22898 (73 → 75), 0.25219 (74 → 75), 0.25268 (74 → 76)
	S_6	0.28335 (68 → 75), 0.22733 (68 → 79), -0.29032 (68 → 80)
trans – 3aB	S_1	-0.30128 (73 → 77), 0.39817 (74 → 75), 0.44465 (74 → 76)
	S_2	0.29861 (73 → 75), 0.36846 (73 → 76), 0.44803 (74 → 77)

	S_3	0.54452 (72 → 75), -0.29161 (72 → 76), 0.23600 (73 → 75)
	S_4	0.34927 (67 → 75), -0.28522 (67 → 76)
	S_5	-0.24812 (73 → 75), 0.31330 (74 → 75), -0.28449 (74 → 76)
	S_6	0.31795 (68 → 75), 0.32997 (68 → 80)
cis - 4	S_1	0.68638 (45 → 46)
	S_2	0.50702 (42 → 46), 0.28758 (42 → 49), 0.27596 (43 → 46)
	S_3	-0.38808 (43 → 46), 0.34511 (43 → 49)
	S_4	0.59067 (44 → 46)
	S_5	0.58759 (45 → 47)
	S_6	0.32907 (44 → 47), -0.26093 (44 → 48), -0.34264 (45 → 48)
trans - 4	S_1	0.68529 (45 → 46)
	S_2	0.53310 (42 → 46), -0.26601 (42 → 4)
	S_3	0.39710 (43 → 46), 0.39083 (43 → 49)
	S_4	0.60555 (44 → 46)
	S_5	0.57903 (45 → 47)
	S_6	0.31478 (44 → 47), 0.39151 (44 → 48), 0.33634 (45 → 48)
cis – 5aA[b]	S_1	0.44881 (67 → 70), -0.36657 (67 → 73)
	S_2	0.37550 (65 → 70), 0.49331 (69 → 70)
	S_3	-0.33105 (66 → 72), 0.32781 (68 → 71), -0.30799 (69 → 71)
	S_4	0.48441 (65 → 70)
	S_5	0.34930 (66 → 71), 0.31881 (68 → 72), -0.30268 (69 → 72)
	S_6	0.48058 (64 → 70)
cis – 5aB[b]	S_1	0.51047 (67 → 70), -0.41199 (67 → 73)
	S_2	0.37773 (65 → 70), 0.51750 (69 → 70)
	S_3	0.48965 (68 → 71)

	S_4	0.49213 (65 → 70)
	S_5	0.35402 (66 → 71), 0.38561 (68 → 72)
	S_6	0.48939 (64 → 70)
trans – 5aA[b]	S_1	0.49302 (67 → 70), -0.40500 (67 → 73)
	S_2	0.37577 (65 → 70), 0.40755 (69 → 70)
	S_3	-0.32378 (66 → 72), -0.30834 (68 → 71), 0.40612 (69 → 71)
	S_4	0.49756 (65 → 70)
	S_5	0.38636 (66 → 71), 0.36459 (69 → 72)
	S_6	0.40453 (63 → 70)
trans – 5aB[b]	S_1	0.50479 (67 → 70), -0.40608 (67 → 73)
	S_2	0.38219 (65 → 70), 0.42520 (69 → 70)
	S_3	-0.30318 (66 → 72), 0.37850 (68 → 71), -0.37148 (69 → 71)
	S_4	0.50720 (65 → 70)
	S_5	0.37688 (66 → 71), 0.32005 (68 → 72)
	S_6	0.36360 (63 → 70), 0.33307 (64 → 70)
cis – 5aA[c]	S_1	0.54694 (67 → 70), -0.39071 (67 → 73)
	S_2	-0.30998 (65 →70), 0.40090 (68 → 70), -0.38661 (69 → 70)
	S_3	0.45260 (69 → 71), 0.26668(66 → 72), -0.23660 (69 → 70)
	S_4	0.46422 (65 → 70)
	S_5	0.37560 (69 → 72), -0.24816 (66 → 71), 0.23821 (66 → 70)
	S_6	0.44036 (64 → 70), 0.27846 (64 → 73)
cis – 5aB[c]	S_1	0.55358 (67 → 70), -0.35043 (67 → 73)
	S_2	0.48924 (68 → 70), -0.31807 (65 → 70), -0.26547 (69 → 70)
	S_3	0.51245 (69 → 71), 0.24521 (69 → 70), -0.22107 (66 → 72)
	S_4	0.48920 (65 → 70), -0.22297 (69 → 72)

	S_5	0.26160 (64 → 70), 0.24647 (69 → 72)
	S_6	0.40259 (64 → 70), -0.25119 (64 → 72)
trans – 5aA[c]	S_1	0.51334 (67 → 70), -0.32945 (67 → 73)
	S_2	0.32918 (65 → 70), 0.25692 (66 → 70), 0.39607 (68 → 70), -0.33291 (69 → 70)
	S_3	0.46591 (69 → 71), 0.25053 (69 → 70)
	S_4	0.44202 (65 → 70), -0.25541 (68 → 70)
	S_5	-0.24368 (66 → 70), -0.24347 (66 → 71), -0.39665 (69 → 72)
	S_6	0.43683 (64 → 70), 0.23129 (64 → 73)
trans – 5aB[c]	S_1	0.54116 (67 → 70), -0.27874 (67 → 72), -0.29578 (67 → 73)
	S_2	-0.33316 (65 → 70), 0.22488 (66 → 70), 0.50021 (68 → 70)
	S_3	0.27428 (69 → 70), 0.52024 (69 → 71)
	S_4	0.46018 (65 → 70)
	S_5	0.24348 (65 → 70), 0.23716 (66 → 70), 0.24040 (66 → 71), -0.24962 (68 → 71), -0.23012 (69 → 72), 0.32597 (69 → 73)
	S_6	0.44928 (64 → 70), 0.31685 (64 → 72)

[a] HF/6-31G* geometries were used for **1a**, **2a** and **4** and AM1 geometries for **3a**.

[b]HF/3-21G(*) geometry. [c]AM1 geometry.

Table S11. Crystal data and structure refinement for **6**.

Crystal data	
Empirical formula	$C_{15}H_{21}N_3O_3$
Formula weight	291.35
Melting point	462 K
Crystal description	block, colourless
Crystal size	0.40 x 0.34 x 0.20mm
Crystal system, space group	monoclinic, P 2_1
Unit cell dimensions:	a 7.953(3)Å
b	7.196(4)Å
c	12.664(4)Å
β	94.84(3)°
Volume	722.2(4)Å^3
Z	2
Calculated density	1.340Mg/m^3
F(000)	312
Linear absorption coefficient μ	0.095mm-1
Absorption correction	none
Unit cell determination	$3.83 < \Theta < 15.87°$
	56 reflections used at 90K
Data collection	
Temperature	90(2)K
Diffractometer	Stoe 4-circle
Radiation source	fine-focus sealed tube

Radiation and wavelength	MoK_α, 0.71069Å
Monochromator	graphite
Scan type	ω
Standard reflections	3 every 100 reflections
Intensity decay	2.7%
Theta range for data collection	2.57 to 30.00°
Index ranges	-11<=h<=11, -3<=k<=10, -17<=l<=17
Reflections collected / unique	3899 / 2999
Significant unique reflections	2833 with $I>2\sigma(I)$
R(int), R(sigma)	0.0319, 0.0481
Completeness to theta = 30.00°	99.9%

Refinement

Refinement method	full-matrix least-squares on F^2
Data / parameters / restraints	2999 / 205 / 1
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.0989
R indices (all data)	R1 = 0.0420, wR2 = 0.1010
Absolute structure parameter	-1.1(10)
Extinction expression	none
Weighting scheme	$w=1/[\omega^2(F_o^2)+(0.0529P)^2+0.1354P]$ where $P=(F_o^2+2F_c^2)/3$
Largest delta/sigma in last cycle	0.000
Largest difference peak and hole	0.321 and -0.259e/Å^3
Structure Solution Program	SHELXS-97
Structure Refinement Program	SHELXL-97

Table S12. Hydrogen bonds for **6** [Å, °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1)···O(2)$^{\#1}$	0.95(3)	1.86(3)	2.806(2)	178(2)
N(3)-H(3)···O(2)$^{\#2}$	0.89(3)	2.17(3)	3.050(2)	169(2)
N(7)-H(71)···O(51)$^{\#3}$	0.91	2.05	2.925(2)	161.2
N(7)-H(72)···O(51)$^{\#4}$	0.91	1.95	2.842(2)	168.1
N(7)-H(73)···O(52)$^{\#5}$	0.91	2.06	2.825(3)	140.6

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1,y+1/2,-z $^{\#2}$ -x+1,y-1/2,-z $^{\#3}$ -x+1,y+1/2,-z+1

$^{\#4}$ x+1,y,z $^{\#5}$ -x+1,y-1/2,-z+1

Table S13. Atomic coordinates and equivalent isotropic displacement parameters (Å²) for **6**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
N(1)	0.35665(18)	0.9960(2)	0.09238(11)	0.0153(3)
C(2)	0.4237(2)	0.8304(3)	0.06442(13)	0.0144(3)
O(2)	0.52606(15)	0.8253(2)	-0.00523(9)	0.0170(3)
N(3)	0.37685(19)	0.6797(2)	0.11724(11)	0.0170(3)
C(4)	0.2288(2)	0.6866(3)	0.17950(13)	0.0153(3)
C(41)	0.0657(2)	0.6604(3)	0.10792(14)	0.0221(4)
C(5)	0.2278(2)	0.8690(3)	0.23749(13)	0.0140(3)
C(51)	0.1512(2)	0.8731(3)	0.34130(12)	0.0145(3)
O(51)	0.07831(15)	0.7251(2)	0.36758(9)	0.0175(3)
O(52)	0.16193(15)	1.0172(2)	0.39832(9)	0.0178(3)
C(6)	0.2836(2)	1.0197(3)	0.18808(12)	0.0140(3)
C(61)	0.2766(2)	1.2186(3)	0.21943(15)	0.0206(4)
C(7)	0.7052(2)	0.9066(3)	0.44687(13)	0.0154(3)
N(7)	0.86645(17)	0.8768(2)	0.51558(11)	0.0166(3)
C(8)	0.5700(2)	0.9742(3)	0.51563(14)	0.0203(4)
C(91)	0.73563(19)	1.0380(3)	0.35680(12)	0.0142(3)
C(92)	0.76655(19)	1.2261(3)	0.37421(13)	0.0157(3)
C(93)	0.7972(2)	1.3433(3)	0.29050(14)	0.0192(3)
C(94)	0.7957(2)	1.2720(3)	0.18857(14)	0.0216(4)
C(95)	0.7649(2)	1.0841(3)	0.17091(14)	0.0212(4)
C(96)	0.7356(2)	0.9671(3)	0.25453(14)	0.0177(3)

Table S14. Hydrogen coordinates and isotropic displacement parameters (Å²) for **6**.

	x	y	z	U_{iso}
H(1)	0.394(3)	1.109(4)	0.0635(18)	0.019(6)
H(3)	0.415(3)	0.574(4)	0.0919(19)	0.022(6)
H(4)	0.2381	0.5837	0.2328	0.012(5)
H(41)	0.0689	0.5406	0.0713	0.029(4)
H(42)	0.0546	0.7609	0.0556	0.029(4)
H(43)	-0.0310	0.6629	0.1510	0.029(4)
H(61)	0.1841	1.2370	0.2648	0.051(5)
H(62)	0.2576	1.2959	0.1558	0.051(5)
H(63)	0.3836	1.2539	0.2583	0.051(5)
H(7)	0.6684	0.7842	0.4156	0.024(6)
H(73)	0.8472	0.7976	0.5693	0.048(5)
H(71)	0.9041	0.9875	0.5430	0.048(5)
H(72)	0.9456	0.8272	0.4760	0.048(5)
H(81)	0.5558	0.8833	0.5718	0.028(4)
H(82)	0.4631	0.9889	0.4720	0.028(4)
H(83)	0.6040	1.0940	0.5475	0.028(4)
H(92)	0.7668	1.2751	0.4439	0.032(3)
H(93)	0.8191	1.4715	0.3031	0.032(3)
H(94)	0.8157	1.3515	0.1311	0.032(3)
H(95)	0.7639	1.0353	0.1011	0.032(3)
H(96)	0.7156	0.8385	0.2420	0.032(3)

Table S15. Anisotropic displacement parameters (Å² x 104) for **6**. The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	203(6)	129(7)	136(6)	0(6)	74(5)	7(6)
C(2)	177(7)	133(8)	126(7)	-24(7)	36(5)	-17(7)
O(2)	211(5)	159(7)	154(5)	-28(5)	92(4)	-12(5)
N(3)	242(7)	111(7)	169(7)	-11(6)	95(5)	11(6)
C(4)	208(7)	114(8)	148(7)	4(6)	78(6)	-10(7)
C(41)	252(8)	212(10)	208(8)	-47(8)	72(7)	-69(8)
C(5)	181(7)	120(8)	122(7)	-3(6)	33(5)	8(6)
C(51)	142(6)	177(9)	117(6)	11(7)	17(5)	30(6)
O(51)	195(5)	193(7)	143(5)	31(5)	45(4)	-4(5)
O(52)	217(5)	183(7)	135(5)	-27(5)	35(4)	32(5)
C(6)	170(6)	128(8)	127(6)	-2(7)	49(5)	0(6)
C(61)	305(8)	137(8)	190(7)	-16(7)	100(7)	-11(8)
C(7)	173(7)	143(8)	146(7)	14(7)	22(6)	-11(6)
N(7)	170(6)	182(8)	153(6)	47(6)	44(5)	34(6)
C(8)	170(7)	256(10)	189(8)	23(8)	47(6)	-1(7)
C(91)	134(6)	152(8)	140(6)	21(7)	3(5)	12(7)
C(92)	159(6)	167(8)	144(7)	1(7)	5(5)	-6(7)
C(93)	206(7)	174(8)	191(8)	39(7)	-4(6)	-14(7)
C(94)	236(8)	247(10)	163(8)	74(8)	2(6)	-44(8)
C(95)	251(8)	255(11)	128(7)	7(7)	5(6)	-36(8)
C(96)	197(7)	171(9)	161(7)	-2(7)	6(6)	-15(7)

Table S16. Full list of bond lengths [Å] and angles [°] for **6** (for deposition).

N(1)-C(2)	1.364(2)	C(2)-N(3)	1.343(2)
N(3)-C(4)	1.472(2)	C(4)-C(5)	1.504(3)
C(5)-C(6)	1.346(3)	C(6)-N(1)	1.398(2)
N(1)-H(1)	0.95(3)	C(2)-O(2)	1.2502(19)
N(3)-H(3)	0.89(3)	C(4)-C(41)	1.530(3)
C(4)-H(4)	1.00	C(41)-H(41)	0.98
C(41)-H(42)	0.98	C(41)-H(43)	0.98
C(5)-C(51)	1.495(2)	C(51)-O(51)	1.271(2)
C(51)-O(52)	1.262(2)	C(6)-C(61)	1.487(3)
C(61)-H(61)	0.98	C(61)-H(62)	0.98
C(61)-H(63)	0.98	C(7)-N(7)	1.503(2)
C(7)-C(91)	1.516(2)	C(7)-C(8)	1.519(2)
C(7)-H(7)	1.00	N(7)-H(73)	0.91
N(7)-H(71)	0.91	N(7)-H(72)	0.91
C(8)-H(81)	0.98	C(8)-H(82)	0.98
C(8)-H(83)	0.98	C(91)-C(92)	1.390(3)
C(91)-C(96)	1.392(2)	C(92)-C(93)	1.392(3)
C(92)-H(92)	0.95	C(93)-C(94)	1.388(3)
C(93)-H(93)	0.95	C(94)-C(95)	1.389(3)
C(94)-H(94)	0.95	C(95)-C(96)	1.388(3)
C(95)-H(95)	0.95	C(96)-H(96)	0.95
C(6)-N(1)-C(2)	122.14(15)	N(1)-C(2)-N(3)	116.41(15)
C(2)-N(3)-C(4)	120.52(16)	N(3)-C(4)-C(5)	109.14(14)
C(4)-C(5)-C(6)	117.43(15)	C(5)-C(6)-N(1)	118.81(17)

N(1)-C(2)-O(2)	120.08(16)	N(3)-C(2)-O(2)	123.49(17)
C(2)-N(1)-H(1)	120.4(14)	C(6)-N(1)-H(1)	113.3(14)
C(2)-N(3)-H(3)	113.1(16)	C(4)-N(3)-H(3)	122.4(16)
N(3)-C(4)-C(41)	110.80(14)	C(5)-C(4)-C(41)	110.94(15)
N(3)-C(4)-H(4)	108.6	C(5)-C(4)-H(4)	108.6
C(41)-C(4)-H(4)	108.6	C(4)-C(41)-H(41)	109.5
C(4)-C(41)-H(42)	109.5	H(41)-C(41)-H(42)	109.5
C(4)-C(41)-H(43)	109.5	H(41)-C(41)-H(43)	109.5
H(42)-C(41)-H(43)	109.5	C(4)-C(5)-C(51)	117.78(15)
C(6)-C(5)-C(51)	124.56(16)	C(5)-C(51)-O(51)	116.25(16)
C(5)-C(51)-O(52)	120.46(16)	O(51)-C(51)-O(52)	123.29(15)
C(5)-C(6)-C(61)	129.06(15)	N(1)-C(6)-C(61)	112.11(15)
C(6)-C(61)-H(61)	109.5	C(6)-C(61)-H(62)	109.5
H(61)-C(61)-H(62)	109.5	C(6)-C(61)-H(63)	109.5
H(61)-C(61)-H(63)	109.5	H(62)-C(61)-H(63)	109.5
N(7)-C(7)-C(91)	110.01(13)	N(7)-C(7)-C(8)	108.92(14)
C(91)-C(7)-C(8)	113.39(16)	N(7)-C(7)-H(7)	108.1
C(91)-C(7)-H(7)	108.1	C(8)-C(7)-H(7)	108.1
C(7)-N(7)-H(73)	109.5	C(7)-N(7)-H(71)	109.5
H(73)-N(7)-H(71)	109.5	C(7)-N(7)-H(72)	109.5
H(73)-N(7)-H(72)	109.5	H(71)-N(7)-H(72)	109.5
C(7)-C(8)-H(81)	109.5	C(7)-C(8)-H(82)	109.5
H(81)-C(8)-H(82)	109.5	C(7)-C(8)-H(83)	109.5
H(81)-C(8)-H(83)	109.5	H(82)-C(8)-H(83)	109.5
C(92)-C(91)-C(96)	119.39(16)	C(92)-C(91)-C(7)	121.68(15)
C(96)-C(91)-C(7)	118.93(17)	C(91)-C(92)-C(93)	120.61(17)

C(91)-C(92)-H(92)	119.7	C(93)-C(92)-H(92)	119.7
C(94)-C(93)-C(92)	119.73(19)	C(94)-C(93)-H(93)	120.1
C(92)-C(93)-H(93)	120.1	C(93)-C(94)-C(95)	119.79(18)
C(93)-C(94)-H(94)	120.1	C(95)-C(94)-H(94)	120.1
C(96)-C(95)-C(94)	120.42(18)	C(96)-C(95)-H(95)	119.8
C(94)-C(95)-H(95)	119.8	C(95)-C(96)-C(91)	120.05(19)
C(95)-C(96)-H(96)	120.0	C(91)-C(96)-H(96)	120.0
N(1)-C(2)-N(3)-C(4)	15.9(2)	C(2)-N(3)-C(4)-C(5)	-41.0(2)
N(3)-C(4)-C(5)-C(6)	35.4(2)	C(4)-C(5)-C(6)-N(1)	-7.2(2)
C(5)-C(6)-N(1)-C(2)	-22.0(2)	C(6)-N(1)-C(2)-N(3)	17.6(2)
C(6)-N(1)-C(2)-O(2)	-160.70(15)	O(2)-C(2)-N(3)-C(4)	-165.77(15)
C(2)-N(3)-C(4)-C(41)	81.5(2)	C(41)-C(4)-C(5)-C(6)	-86.92(18)
N(3)-C(4)-C(5)-C(51)	-149.77(14)	C(41)-C(4)-C(5)-C(51)	87.87(18)
C(6)-C(5)-C(51)-O(51)	167.88(16)	C(4)-C(5)-C(51)-O(51)	-6.5(2)
C(6)-C(5)-C(51)-O(52)	-12.7(2)	C(4)-C(5)-C(51)-O(52)	172.88(15)
C(51)-C(5)-C(6)-N(1)	178.36(14)	C(51)-C(5)-C(6)-C(61)	-3.1(3)
C(4)-C(5)-C(6)-C(61)	171.33(16)	C(2)-N(1)-C(6)-C(61)	159.21(15)
N(7)-C(7)-C(91)-C(92)	-70.8(2)	C(8)-C(7)-C(91)-C(92)	51.5(2)
N(7)-C(7)-C(91)-C(96)	107.96(17)	C(8)-C(7)-C(91)-C(96)	-129.79(17)
C(96)-C(91)-C(92)-C(93)	0.1(2)	C(7)-C(91)-C(92)-C(93)	178.79(15)
C(91)-C(92)-C(93)-C(94)	0.5(3)	C(92)-C(93)-C(94)-C(95)	-0.5(3)
C(93)-C(94)-C(95)-C(96)	0.0(3)	C(94)-C(95)-C(96)-C(91)	0.5(3)
C(92)-C(91)-C(96)-C(95)	-0.5(2)	C(7)-C(91)-C(96)-C(95)	-179.32(16)

Table S17 Cartesian coordinates (Z-matrices for AM1))of calculated structures.

trans-5aA: HF/3-21G*; E = -1186.17192523

O,0,-3.4039010687,-1.046567379,0.1468498541

O,0,-1.7147262862,-2.3873710529,0.6935785844

S,0,1.3484635251,3.2617987967,2.1371211352

N,0,-0.7528096749,2.1953458683,0.9253750829

H,0,-1.0320278276,3.1516729344,0.8515537191

N,0,0.8320740852,0.7090132053,1.6036310781

H,0,1.6960041003,0.5265578926,2.0719493838

C,0,0.9113156837,-0.7046804819,-0.4254919035

C,0,1.6049721337,0.2870107607,-1.1081811907

H,0,1.6702696268,1.2793749361,-0.7157304081

C,0,2.2329355333,-0.015211235,-2.3001334377

H,0,2.7697855923,0.7490109171,-2.826127119

C,0,2.1845916889,-1.2957421784,-2.8204590844

H,0,2.6800407269,-1.5197929404,-3.7452779972

C,0,1.4998883841,-2.2810858763,-2.1371919298

O,0,1.4094649125,-3.5789570746,-2.5854990197

C,0,0.8665338989,-1.9860156045,-0.9427861569

H,0,0.3313816222,-2.7633268717,-0.4428003647

C,0,0.189516823,-0.4060204613,0.8924238492

H,0,0.2433862401,-1.2770456419,1.5258412977

C,0,-1.2756289777,-0.0740888501,0.6403502281

C,0,-2.1113832327,-1.2588581111,0.4975583312

H,0,-3.8844531429,-1.8855071531,0.0854064068

C,0,-1.6650285329,1.2005572259,0.5969755619

C,0,-3.0228998113,1.7654432966,0.2613066457

H,0,-2.9144558522,2.4525712935,-0.5723257601

H,0,-3.3961094555,2.3227853053,1.1143760436

H,0,-3.7156212924,0.991431202,0.0016448549

C,0,0.4530412542,1.9824093672,1.5330784683

H,0,1.8877028566,-3.7261691952,-3.4096229859

trans-5aB> HF/3-21G*; E = -1186.17186237

O,0,-3.4432057738,-1.3435007251,0.3924881547

O,0,-1.7058878217,-2.6519707813,0.859313918

S,0,1.3467142646,3.0700089967,2.0278970921

N,0,-0.8054309626,1.9496558918,0.9645628382

H,0,-1.1053763991,2.8999545566,0.8941800387

N,0,0.8508358198,0.5023531073,1.5528907382

H,0,1.7513181493,0.3447150509,1.9569767006

C,0,0.8176178856,-0.9879458874,-0.4228598106

C,0,0.8174224315,-2.3070612543,-0.8642148243

H,0,0.3595895121,-3.0660131528,-0.2670371569

C,0,1.3852168003,-2.6196015764,-2.0827058331

H,0,1.388338686,-3.6361688315,-2.422725046

C,0,1.9544485624,-1.6350702692,-2.8708024821

H,0,2.3948235753,-1.888801591,-3.815601946

C,0,1.9538693742,-0.3269987869,-2.4296819039

O,0,2.497639517,0.7097251659,-3.1525831869

C,0,1.3914070443,-0.0065879283,-1.2060462327

H,0,1.4312714407,1.0153140414,-0.8969456662

C,0,0.1759777045,-0.6421208525,0.9236393038

H,0,0.2773119351,-1.4888728423,1.5840105842

C,0,-1.3053909427,-0.3331893908,0.7486398217

C,0,-2.1289970519,-1.5313672374,0.6707107528

H,0,-3.9139235506,-2.1898996938,0.374797871

C,0,-1.7162739034,0.9354717456,0.7050519057

C,0,-3.0995073834,1.4734517806,0.4343233025

H,0,-3.4335244407,2.042105671,1.2961155136

H,0,-3.7936220974,0.6849242519,0.2279649346

H,0,-3.0470463458,2.1456073679,-0.4166798335

C,0,0.4425775802,1.767332125,1.4937762394

H,0,2.9070013196,0.4210241456,-3.976317024

cis-5aA: HF/3-21G*; E = -1186.17468559

O,0,-1.518349798,-2.4034454432,0.5828931812

O,0,-3.3241508295,-1.2581930888,-0.047905634

S,0,1.1461986932,3.3550243213,2.1464374272

N,0,-0.9520434077,2.2015618772,1.0143532693

H,0,-1.307507902,3.1351240808,1.0201048855

N,0,0.7717886647,0.8001690324,1.5187319525

H,0,1.6840891726,0.6689777422,1.9058197305

C,0,0.8790531263,-0.6698211185,-0.4532808229

C,0,1.2396857034,0.3578695467,-1.3176260393

H,0,1.0165335487,1.3755405889,-1.0734444451

C,0,1.8952432317,0.0627746535,-2.4937170718

H,0,2.1757075797,0.8531869149,-3.1609433032

C,0,2.2027349205,-1.2479170251,-2.8220434914

H,0,2.7159836516,-1.4653367449,-3.7385865623

C,0,1.8468904742,-2.2653672769,-1.9621794571

O,0,2.1144016096,-3.5921306552,-2.2115172402

C,0,1.1868663228,-1.9738108121,-0.7791034042

H,0,0.9088957089,-2.7833554251,-0.1405673375

C,0,0.1521182435,-0.3628120288,0.8570120027

H,0,0.2515467207,-1.2065830666,1.5194513078

C,0,-1.3218707776,-0.0872197069,0.6090472126

C,0,-2.1743950882,-1.2375267798,0.3313968548

H,0,-2.0708843708,-3.1702031986,0.3740101412

C,0,-1.7883498103,1.1627308938,0.6401619962

C,0,-3.1932281834,1.6198536359,0.3357397009

H,0,-3.6044418644,2.1143688632,1.2097361611

H,0,-3.8149227216,0.7916701374,0.0556868383

H,0,-3.1586137522,2.3377041879,-0.4779612238

C,0,0.3023397934,2.0442661054,1.5352267626

H,0,2.5884827452,-3.7315666126,-3.0394694936

cis-5aB: HF/3-21G*; E = -1186.17395444

O,0,-1.3783634429,-2.6863175915,0.8231967704

O,0,-3.2620755421,-1.6321736162,0.2674853866

S,0,1.1487560487,3.2238710776,2.0115895025

N,0,-0.9645770884,1.9510126234,1.0481871559

H,0,-1.3525909157,2.8714256215,1.0324610723

N,0,0.8383289027,0.6345942743,1.5042479542

H,0,1.7783432251,0.5545900338,1.8346902262

C,0,0.8912157888,-0.9462950268,-0.382424965

C,0,1.2991451973,-2.2498251865,-0.6258665128

H,0,1.1221076852,-3.0087155546,0.1066467873

C,0,1.9108417864,-2.5636867387,-1.8247426609

H,0,2.229568087,-3.5693458054,-2.0144451698

C,0,2.1175774726,-1.5908864711,-2.7845220675

H,0,2.5931838249,-1.8430889639,-3.7124144516

C,0,1.7085273897,-0.2928143793,-2.5405098042

O,0,1.8746848667,0.7290169637,-3.4457371231

C,0,1.1024733239,0.0263130024,-1.3400408517

H,0,0.8099104748,1.042624988,-1.1830147438

C,0,0.2219233788,-0.5817490716,0.9432429997

H,0,0.3830415108,-1.3827276757,1.6459405126

C,0,-1.270837907,-0.3650068752,0.7603231073

C,0,-2.0931432265,-1.5537546257,0.5741797942

H,0,-1.9178129103,-3.4768489322,0.6791322954

C,0,-1.7794390246,0.8694231566,0.7624455383

C,0,-3.213111975,1.2642443817,0.5093988923

H,0,-3.597261797,1.7879998557,1.3786420192

H,0,-3.8186015191,0.4033557289,0.302051792

H,0,-3.2438149148,1.9413892676,-0.3385839293

C,0,0.32346146,1.8608327426,1.4994090904

H,0,2.3317987297,0.4531804128,-4.2484998541

1a-anion: HF 6-31G*; E = -603.8736816

N,0,-1.8906868898,-0.1128848817,-0.2282859847

C,0,-1.9018447009,-0.1628478542,1.1180663259

N,0,-0.6623582809,-0.1196095898,1.686372127

C,0,0.5451324155,-0.2772654358,0.9619109645

C,0,0.554985286,-0.1005271484,-0.354126659

C,0,-0.7390980261,0.3031362717,-1.034204853

H,0,-2.7978783578,-0.0362429365,-0.6301134844

O,0,-2.9116979647,-0.2576893295,1.7829534972

H,0,-0.6613808601,-0.3162173631,2.660680076

C,0,1.6969438169,-0.6322438831,1.8586633438

C,0,1.7780472871,-0.2317328104,-1.2920938925

O,0,2.8600905305,-0.5417508541,-0.7910754504

O,0,1.5165788385,0.0025887296,-2.4752340401

H,0,-0.7934186856,-0.2281042352,-1.971408792

C,0,-0.7858918409,1.8052586181,-1.3328196112

H,0,1.4945004772,-1.5733928908,2.3699053563

H,0,1.816030351,0.1326945941,2.6261046136

H,0,2.5978055389,-0.7164962321,1.2772948497

H,0,0.0505132833,2.0658237053,-1.9664886352

H,0,-0.7338601927,2.3812045208,-0.4125789956

H,0,-1.7104120177,2.0703372228,-1.8455237493

trans-1a: HF/6-31G*; E = -604.4366628 au

6	0	2.216882	0.162447	-0.231742
6	0	0.235086	-1.327110	-0.171827

6	0	-0.601273	-0.063998	-0.070664
6	0	-0.003024	1.112838	0.175666
6	0	0.246759	-2.126935	1.134988
6	0	-0.654546	2.457462	0.393042
6	0	-2.043604	-0.269945	-0.235345
7	0	1.583896	-0.969339	-0.595097
7	0	1.372797	1.152838	0.243479
8	0	-2.540291	-1.345074	-0.397293
8	0	-2.797971	0.830103	-0.210163
8	0	3.396702	0.354789	-0.325383
1	0	-1.016572	2.855345	-0.546909
1	0	-1.493111	2.386900	1.066039
1	0	0.064912	3.154421	0.805329
1	0	0.846587	-3.026230	1.025233
1	0	0.666271	-1.535998	1.943086
1	0	-0.760032	-2.422919	1.402813
1	0	-0.183642	-1.948551	-0.950188
1	0	1.832815	2.018723	0.410958
1	0	2.200829	-1.703929	-0.863811
1	0	-3.700111	0.550646	-0.333224

trans-1a: AM1 geometry; DHf = -118.190677 KCAL

C	0.0000000	0	0.000000	0	0.000000	0	0	0	0	4.3423
C	2.4775000	0	0.000000	0	0.000000	0	1	0	0	3.7783
C	1.5131102	0	86.445869	0	0.000000	0	2	1	0	3.9887
C	1.3727690	0	121.183048	0	-5.095105	0	3	2	1	3.9676

C	1.5330145	0	114.404306	0	-109.813396	0	2	1	3	4.1547
C	1.4949869	0	122.491329	0	-178.464878	0	4	3	2	4.1972
C	1.4529680	0	113.872044	0	174.042652	0	3	2	1	4.0428
N	1.3954510	0	30.253273	0	-155.665982	0	1	2	3	5.0946
N	1.3860768	0	119.929953	0	0.966031	0	4	3	2	5.0467
O	1.2395411	0	127.994870	0	-2.305449	0	7	3	2	6.3189
O	1.3699315	0	117.062149	0	178.014286	0	7	3	2	6.0191
O	1.2510462	0	150.906647	0	176.880777	0	1	2	3	6.3718
H	1.1204492	0	109.095394	0	-59.648685	0	6	4	3	0.9136
H	1.1201883	0	109.170006	0	57.897104	0	6	4	3	0.9844
H	1.1171611	0	113.162557	0	179.151705	0	6	4	3	0.8998
H	1.1162653	0	110.647717	0	-87.081495	0	5	2	1	0.8698
H	1.1151557	0	111.340768	0	34.097624	0	5	2	1	1.0070
H	1.1176542	0	108.430423	0	153.924132	0	5	2	1	0.9405
H	1.1366327	0	127.803176	0	109.853381	0	2	1	3	1.0109
H	0.9950532	0	120.499811	0	179.008921	0	9	4	3	0.8340
H	0.9969802	0	114.881774	0	-146.812035	0	8	1	2	0.9549
H	0.9717105	0	108.882453	0	179.582552	0	11	7	3	1.0832

cis-1a: HF/6-31G*; E = -604.438056569

7	0	1.761561	0.658180	-0.453241
6	0	1.186144	1.868911	-0.310244
7	0	-0.164421	1.820296	-0.008650
6	0	-0.930326	0.677947	-0.034987
6	0	-0.315989	-0.517899	-0.051344
6	0	1.197828	-0.588636	0.052008

1	0	2.746802	0.701139	-0.594628
8	0	1.746528	2.918250	-0.457855
1	0	-0.606904	2.711330	-0.011891
6	0	-2.417119	0.927710	-0.048199
6	0	-1.092345	-1.757093	-0.136803
8	0	-2.281765	-1.855130	-0.215203
8	0	-0.319852	-2.847194	-0.125301
1	0	1.556365	-1.373180	-0.598957
6	0	1.677453	-0.880102	1.478653
1	0	-2.837476	0.635539	-1.001580
1	0	-2.620887	1.979005	0.116540
1	0	-2.915776	0.345171	0.710413
1	0	-0.894461	-3.603237	-0.192100
1	0	1.290114	-1.831130	1.824196
1	0	1.346514	-0.102309	2.159180
1	0	2.762556	-0.924090	1.514430

cis-1a: AM1 geometry; DHf = -119.006097 kcal

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3831
C	2.479858	1	0.000000	0	0.000000	0	1	0	0	0.0813
C	1.508312	1	86.332963	1	0.000000	0	2	1	0	-0.2837
C	1.375535	1	121.345535	1	5.211425	1	3	2	1	0.1647
C	1.533495	1	114.256839	1	109.860925	1	2	1	3	-0.2440
C	1.494082	1	121.690696	1	178.291995	1	4	3	2	-0.2106
C	1.451622	1	117.486631	1	-173.984917	1	3	2	1	0.3710
N	1.395991	1	30.220761	1	155.730288	1	1	2	3	-0.3385

N	1.384450	1	119.992942	1	-1.236584	1	4	3	2	-0.3210
O	1.240663	1	129.344117	1	183.417968	1	7	3	2	-0.3923
O	1.369573	1	115.443262	1	3.973765	1	7	3	2	-0.3184
O	1.251007	1	150.810479	1	-176.908147	1	1	2	3	-0.3727
H	1.120756	1	109.108530	1	-58.346618	1	6	4	3	0.1282
H	1.121071	1	109.082463	1	58.491832	1	6	4	3	0.1289
H	1.116676	1	113.170461	1	-179.943240	1	6	4	3	0.0895
H	1.117268	1	108.485128	1	-153.346007	1	5	2	1	0.1045
H	1.115246	1	111.320527	1	-33.600137	1	5	2	1	0.0820
H	1.116236	1	110.661501	1	87.580851	1	5	2	1	0.0781
H	1.136255	1	127.725544	1	-110.015152	1	2	1	3	0.1217
H	0.995081	1	120.595858	1	-178.885800	1	9	4	3	0.2625
H	0.996898	1	114.808208	1	146.825932	1	8	1	2	0.2409
H	0.971564	1	108.809532	1	-181.040161	1	11	7	3	0.2448
0	0.000000	0	0.000000	0	0.000000	0	0	0	0	

trans-2a: HF/6-31G*; E = -794.944186314

6	0	2.833161	-0.924490	1.454688
6	0	3.883374	-0.198781	0.910212
6	0	3.676369	0.545800	-0.236232
6	0	2.426379	0.564013	-0.839075
6	0	1.370981	-0.158443	-0.303254
6	0	1.588747	-0.903278	0.852669
1	0	2.985716	-1.507514	2.345507
1	0	4.851825	-0.216855	1.377468
1	0	4.483166	1.112777	-0.665400

1	0	2.269037	1.156990	-1.721394
6	0	0.002119	-0.132790	-0.983873
1	0	0.786952	-1.474323	1.286089
7	0	-0.505227	-1.473993	-1.241014
6	0	-1.395998	-2.138167	-0.480704
7	0	-2.070888	-1.346375	0.431407
8	0	-1.634747	-3.309836	-0.570040
6	0	-2.001375	0.028011	0.486109
6	0	-1.037665	0.658178	-0.204184
6	0	-3.070128	0.651340	1.353716
6	0	-0.888033	2.114252	-0.312941
8	0	-0.101072	2.642846	-1.039690
8	0	-1.703694	2.842224	0.450850
1	0	0.125861	0.346544	-1.943951
1	0	0.039631	-2.066792	-1.827865
1	0	-2.794655	-1.825510	0.916700
1	0	-2.630892	1.253698	2.134540
1	0	-3.676313	-0.121082	1.810300
1	0	-3.714432	1.291970	0.768168
1	0	-1.504569	3.756936	0.275343

cis-2a: HF/6-31G*; E = -794.945736189

6	0	1.004012	-3.082077	-0.405886
6	0	2.312461	-3.132312	-0.867509
6	0	2.943680	-1.966644	-1.259111
6	0	2.269540	-0.754913	-1.191257

6	0	0.963388	-0.693853	-0.731917
6	0	0.337168	-1.873421	-0.338525
1	0	0.506357	-3.984864	-0.099548
1	0	2.830876	-4.073012	-0.919283
1	0	3.957528	-1.994722	-1.616830
1	0	2.771079	0.148873	-1.489749
6	0	0.225393	0.644151	-0.694414
1	0	-0.676168	-1.849463	0.021622
7	0	-0.895468	0.660412	-1.628274
6	0	-2.193590	0.474816	-1.316703
7	0	-2.478605	0.577370	0.032441
8	0	-3.063256	0.266312	-2.114884
6	0	-1.577753	0.958925	0.998120
6	0	-0.271397	1.029001	0.690475
6	0	-2.199152	1.258303	2.339694
6	0	0.706451	1.473180	1.689842
8	0	0.493939	1.706034	2.843259
8	0	1.929104	1.620628	1.177936
1	0	0.916862	1.403770	-1.030771
1	0	-0.690919	0.487917	-2.588069
1	0	-3.450008	0.544588	0.243589
1	0	-1.805853	0.597006	3.098015
1	0	-3.274806	1.140167	2.288427
1	0	-1.970189	2.267355	2.650296
1	0	2.504249	1.893190	1.885792