Cooperative effects, Strengths of Hydrogen-bonds in Open-chain Cis-triaziridine Clusters (*n*=2-8): A DFT Investigation

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Table 1. $\rho(\mathbf{r}_{cp})$ (au), $\nabla^2\rho(\mathbf{r}_{cp})$ (au) and $q_{n(N)\to\sigma^*}$ (e) of 84 N…H bonds

n	N...H*	$\rho(\mathbf{r}_{cp})$	$\nabla^2\rho(\mathbf{r}_{cp})$	$q_{n(N)\to\sigma^*}$	*n*	N...H*	$\rho(\mathbf{r}_{cp})$	$\nabla^2\rho(\mathbf{r}_{cp})$	$q_{n(N)\to\sigma^*}$
2	1a...2a	0.01224	0.03273	0.00502	7	1a...2a	0.01606	0.04267	0.00844
	1b...2b	0.01257	0.03348	0.00526		1b...2b	0.01609	0.04272	0.00846
	1c...2c	0.01280	0.03402	0.00541		1c...2c	0.01596	0.04237	0.00834
3	1a...2a	0.01485	0.03942	0.00715		2a...3a	0.01889	0.05062	0.01151
	1b...2b	0.01475	0.03916	0.00707		2b...3b	0.01887	0.05058	0.01150
	1c...2c	0.01468	0.03900	0.00702		2c...3c	0.01879	0.05032	0.01141
	2a...3a	0.01481	0.03886	0.00725		3a...4a	0.01983	0.05323	0.01269
	2b...3b	0.01414	0.03731	0.00671		3b...4b	0.01982	0.05320	0.01269
	2c...3c	0.01432	0.03774	0.00685		3c...4c	0.01976	0.05301	0.01262
4	1a...2a	0.01563	0.04155	0.00786		4a...5a	0.01980	0.05302	0.01268
	1b...2b	0.01555	0.04135	0.00781		4b...5b	0.01979	0.05301	0.01266
	1c...2c	0.01548	0.04114	0.00774		4c...5c	0.01975	0.05289	0.01262
	2a...3a	0.01698	0.04515	0.00938		5a...6a	0.01891	0.05034	0.01150
	2b...3b	0.01728	0.04594	0.00967		5b...6b	0.01891	0.05034	0.01153
	2c...3c	0.01698	0.04508	0.00937		5c...6c	0.01889	0.05027	0.01153
	3a...4a	0.01580	0.04132	0.00823		6a...7a	0.01568	0.04087	0.00823
	3b...4b	0.01497	0.03931	0.00753		6b...7b	0.01568	0.04085	0.00825
	3c...4c	0.01494	0.03926	0.00751		6c...7c	0.01566	0.04080	0.00823
5	1a...2a	0.01602	0.04266	0.00834	8	1a...2a	0.01621	0.04308	0.00856
	1b...2b	0.01597	0.04253	0.00828		1b...2b	0.01620	0.04303	0.00856
	1c...2c	0.01584	0.04205	0.00816		1c...2c	0.01621	0.04304	0.00856
	2a...3a	0.01827	0.04867	0.01082		2a...3a	0.01898	0.05089	0.01164
	2b...3b	0.01860	0.04966	0.01116		2b...3b	0.01899	0.05092	0.01166
	2c...3c	0.01696	0.04520	0.00956		2c...3c	0.01901	0.05095	0.01166
	3a...4a	0.01806	0.04806	0.01062		3a...4a	0.02013	0.05414	0.01304
	3b...4b	0.01830	0.04870	0.01085		3b...4b	0.02015	0.05420	0.01307
	3c...4c	0.01772	0.04688	0.01024		3c...4c	0.02014	0.05417	0.01306
	4a...5a	0.01557	0.04059	0.00809		4a...5a	0.02042	0.05494	0.01338
	4b...5b	0.01549	0.04048	0.00802		4b...5b	0.02046	0.05504	0.01342
	4c...5c	0.01531	0.04009	0.00788		4c...5c	0.02044	0.05499	0.01340
6	1a...2a	0.01616	0.04300	0.00848		5a...6a	0.02006	0.05377	0.01300
	1b...2b	0.01615	0.04297	0.00848		5b...6b	0.02007	0.05381	0.01302
	1c...2c	0.01604	0.04267	0.00837		5c...6c	0.02006	0.05377	0.01300
	2a...3a	0.01863	0.04988	0.01123		6a...7a	0.01926	0.05145	0.01191
	2b...3b	0.01863	0.04986	0.01123		6b...7b	0.01927	0.05148	0.01191
	2c...3c	0.01845	0.04936	0.01105		6c...7c	0.01925	0.05141	0.01202
	3a...4a	0.01911	0.05102	0.01178		7a...8a	0.01584	0.04133	0.00836
	3b...4b	0.01909	0.05098	0.01176		7b...8b	0.01586	0.04138	0.00838
	3c...4c	0.01907	0.05093	0.01175		7c...8c	0.01579	0.04120	0.00830
	4a...5a	0.01859	0.04946	0.01117					
	4b...5b	0.01863	0.04958	0.01121					
	4c...5c	0.01864	0.04960	0.01123					
	5a...6a	0.01569	0.04098	0.00822					
	5b...6b	0.01578	0.04120	0.00502					
	5c...6c	0.01572	0.04107	0.00526					

* In this column, the N and H are labeled in terms of figure 1 in article, for example, 1b...2b means the HB in the chain "b" constitutes N on unit 1 and H on unit2.

Cartesian coordinates (in angstroms) for optimized geometries

Isolated molecule:

N	-0.2971734083	0.7947385102	-0.1013655153
N	-0.1289207962	-0.3846653396	0.7520830065
N	0.0796125509	-0.4913017878	-0.6946074366
H	0.5447210338	1.3826159907	-0.0234332519
H	0.7890140246	-0.3303274072	1.2157000913
H	1.0916365165	-0.4836882631	-0.8850372213

Dimer (*n*=2):

N	1.0569895164	0.0213823736	1.6613967725
N	-0.2026153091	-0.7141208382	1.8263895855
N	-0.2066729883	0.75367155	1.8089081584
H	1.2961357931	0.0095257752	0.6600057787
H	-0.4998995349	-1.0384517866	0.8954729142
H	-0.5049711122	1.054009026	0.8703338093
N	-0.6072731359	-0.7500574753	-1.477146688
N	-0.6078124296	0.7135830543	-1.4839078455
N	0.6519267481	-0.0184131893	-1.6234937277
H	-0.9119077848	-1.0994299383	-2.395350759
H	-0.9127444246	1.0547366762	-2.4050749091
H	0.9415902526	-0.022708079	-2.6104106195

Trimer (*n*=3):

N	0.1255465075	-0.4579872112	0.6867732183
N	0.0384777441	0.8639719302	0.0585351705
N	0.1656319803	-0.336273521	-0.773803342
H	-0.8223264952	-0.7500192241	0.9623365193
H	-0.9484026613	1.1570754736	0.0560862657
H	-0.7648155108	-0.5740809761	-1.1445868947
N	-3.0892032995	-0.7238952906	0.5754395936
N	-3.1786582313	0.594214378	-0.0528860673
N	-3.0541316129	-0.6044437619	-0.8821734506
H	-4.0225951568	-1.0307330396	0.8785850902
H	-4.1548432068	0.9172525354	-0.0497120234
H	-3.9709144671	-0.8539903945	-1.2752569185
N	3.3590418262	-0.2355431514	0.8377228777
N	3.2918967703	1.0919183117	0.2135841135
N	3.4141168141	-0.1077074915	-0.6240403468
H	2.396995213	-0.5069977344	1.0861784874
H	2.3022191995	1.3773201407	0.2007331761
H	2.475653593	-0.3256061266	-0.9884260702

Tetramer (*n*=4):

N	-1.4498841983	-0.6006589848	0.6348764495
N	-1.534433415	0.7181982055	0.0011405899
N	-1.4091870063	-0.4856105169	-0.8258171396
H	-2.3970779536	-0.8916371924	0.914439459
H	-2.5192665598	1.0182548419	-0.0030125735
H	-2.3383678545	-0.7241844466	-1.199677942
N	-4.6378215708	-0.855491332	0.529010392

N	-4.7243841642	0.4626580353	-0.1003820799
N	-4.6009017447	-0.7370917746	-0.9289887428
H	-5.5714985602	-1.1609305199	0.8322423232
H	-5.6995621764	0.7882866582	-0.0984916843
H	-5.5169170127	-0.9859370345	-1.3239989174
N	1.7053662596	-0.3244977807	0.7387635588
N	1.613703719	0.991066726	0.0965092007
N	1.746270891	-0.2176607398	-0.7236581854
H	0.7551981379	-0.6146887366	1.0112441841
H	0.6229288221	1.2734476144	0.091157627
H	0.813269931	-0.4612489176	-1.0864780236
N	4.9069637331	-0.078087038	0.9190559998
N	4.841085101	1.2323218876	0.2591606064
N	4.9746614349	0.0107490534	-0.5453744167
H	3.9425987883	-0.3452661052	1.1641521377
H	3.8497237701	1.511191438	0.2289071068
H	4.0388973918	-0.2185577861	-0.9105573263

Pentamer (*n*=5):

N	-2.9886225829	-0.7514510866	0.5763865565
N	-3.0751166479	0.5564700229	-0.0790997945
N	-2.9776206455	-0.6626787146	-0.8865604453
H	-3.931601288	-1.0283766557	0.8834153092
H	-4.0566210312	0.8673271158	-0.0666841094
H	-3.9168095401	-0.8998416251	-1.236141833
N	-6.1680324884	-0.9693444289	0.55413665
N	-6.2556820273	0.3357797412	-0.1016693678
N	-6.1609002264	-0.8825501267	-0.9065543479
H	-7.0973641003	-1.2595858096	0.8842877849
H	-7.2271738101	0.6717058793	-0.0866237396
H	-7.0868687803	-1.1313482497	-1.277467748
N	0.1293192046	-0.4735313435	0.6927275487
N	0.0359233305	0.8316127735	0.0307860428
N	0.1726315704	-0.3887485799	-0.77054854
H	-0.8204772107	-0.7630497521	0.968769531
H	-0.9548036548	1.1151206111	0.0171436993
H	-0.7569816674	-0.6410727011	-1.1363726152
N	3.2581320241	-0.1835524808	0.7908159052
N	3.1600223839	1.1172037774	0.1195292137
N	3.3073183516	-0.1081578549	-0.6734577772
H	2.3067658256	-0.4728906504	1.061816051
H	2.1659756517	1.3888648198	0.1011242176
H	2.3770052142	-0.3653015251	-1.0348513521
N	6.4635395322	0.1173647782	0.9470372745
N	6.3686704832	1.4200549281	0.2749225098
N	6.5211041834	0.193507189	-0.5187888817
H	5.5054847286	-0.1652209931	1.1998351011
H	5.371416366	1.6777471799	0.248416891
H	5.5872481795	-0.0579278039	-0.8743050143

Hexamer (*n*=6):

N	-4.5451498892	-0.7925759986	0.5397958531

N	-4.6129249413	0.5295067064	-0.0890969817
N	-4.5067779108	-0.672429343	-0.9203099233
H	-5.4951428594	-1.0709426455	0.8232528747
H	-5.5931932154	0.8448114012	-0.089089208
H	-5.4393406607	-0.8966475955	-1.294990866
N	-7.7189190525	-0.9988475631	0.4419614475
N	-7.7861898663	0.3178733697	-0.1927848556
N	-7.6829435081	-0.8869232173	-1.0164552029
H	-8.6560188782	-1.2888479735	0.7495908042
H	-8.7555774382	0.6601661129	-0.1907479552
H	-8.6027837787	-1.1231614105	-1.4100537008
N	-1.4322111899	-0.583967888	0.6432064459
N	-1.500656605	0.7408676851	0.0195577796
N	-1.3903990908	-0.4581683793	-0.8170627709
H	-2.3865246959	-0.8620859794	0.9159087722
H	-2.485020272	1.0466507652	0.0174323662
H	-2.3262705699	-0.6810906472	-1.1867447839
N	4.7941501615	-0.1602191327	0.8569907672
N	4.7246081677	1.1661592661	0.2334070338
N	4.835122197	-0.0335440672	-0.604058449
H	3.8364015221	-0.4340043042	1.1231047588
H	3.7370718392	1.462413438	0.231615606
H	3.8950875912	-0.2533722748	-0.9657400603
N	1.6728621686	-0.373783503	0.7514545946
N	1.604586272	0.952225787	0.1281250729
N	1.715229325	-0.2470246334	-0.7090426597
H	0.7161358926	-0.6492468554	1.0196716899
H	0.6182474898	1.2525581659	0.1256734296
H	0.777113573	-0.4678986693	-1.0752171298
N	8.0051822885	0.0628797739	0.9635577714
N	7.9330241772	1.3913490213	0.3409556384
N	8.0448613014	0.1917951831	-0.499020259
H	7.0438072592	-0.2057878003	1.2193803769
H	6.9417938176	1.6728537399	0.338464228
H	7.1000353484	-0.0225789353	-0.8497803187

Heptamer (*n*=7):

N	9.2835074483	-0.6702438982	-0.5236523504
N	9.2834217149	0.7799528322	-0.3290109729
N	9.2886694906	-0.1137911222	0.8295807953
H	10.2271269201	-0.9912056435	-0.7755374323
H	10.2270465459	1.155910669	-0.4873579855
H	10.2348457178	-0.1672657051	1.22802269
N	2.9840939033	-0.6677043689	-0.5153210116
N	2.9843466863	0.7844875405	-0.3124144098
N	2.9848434596	-0.1173342706	0.8436938178
H	3.9451233688	-0.9616848146	-0.7451556979
H	3.9455205086	1.1296988002	-0.4529478743
H	3.9461023638	-0.1688484296	1.2125738313
N	6.0989366481	-0.6687486582	-0.516184254
N	6.0995335442	0.7830744638	-0.3163835244
N	6.1018392217	-0.1158841294	0.8410142531

H	7.0549586751	-0.970080094	-0.7520788671
H	7.0559080982	1.1357822748	-0.4624359273
H	7.0592111653	-0.1675958237	1.2166641056
N	-0.1113205164	-0.6673180435	-0.516456568
N	-0.1113322974	0.7850429541	-0.312097578
N	-0.1119551682	-0.1181154297	0.8434383173
H	0.8518514081	-0.9582595055	-0.7434714392
H	0.851863483	1.1272134533	-0.4500042349
H	0.8508566099	-0.1694889771	1.2097305971
N	-3.2112198343	-0.1188182587	0.8407358595
N	-3.2097206259	-0.6673130142	-0.5197099154
N	-3.2099053333	0.7851701802	-0.3144606299
H	-2.2476703179	-0.1700348361	1.205191627
H	-2.2454417436	-0.9561638874	-0.7448051818
H	-2.2456865201	1.1252327293	-0.4506316668
N	-6.3346125832	-0.1184845193	0.8365483816
N	-6.3326289719	-0.6667606419	-0.5244609283
N	-6.332794882	0.7860797154	-0.3187231587
H	-5.37023449	-0.1694209006	1.1979035804
H	-5.3673403909	-0.9529619604	-0.7470937825
H	-5.3675347308	1.1228259451	-0.4531683868
N	-9.5563575867	-0.1167122688	0.8346073312
N	-9.5542053274	-0.6654900845	-0.5279824536
N	-9.5542963223	0.7889335342	-0.3219656988
H	-8.5881193853	-0.1660660026	1.1837895065
H	-8.5851108424	-0.9420149591	-0.74308197
H	-8.5851751197	1.1142700819	-0.4516726062

Octamer (*n*=8):

N	-7.581256618	-0.9549216223	0.7114976015
N	-7.6634879727	0.3765639141	0.1054788006
N	-7.5938560811	-0.8132693584	-0.7467249032
H	-8.5216014708	-1.2340718744	1.0246688635
H	-8.6409157364	0.6979228465	0.1450552349
H	-8.5398474774	-1.0289322589	-1.091445389
N	-10.7550491981	-1.1446438504	0.7214411274
N	-10.8373498263	0.1831863497	0.112705818
N	-10.7674567121	-1.0070222458	-0.7348556609
H	-11.6823454526	-1.4378424946	1.0545689202
H	-11.8042666297	0.5300805736	0.1525714746
H	-11.7006778188	-1.2327225215	-1.1023135291
N	-4.4750906529	-0.768674394	0.7017879975
N	-4.557612705	0.5645842355	0.0977877482
N	-4.4882893929	-0.6243342751	-0.7569782156
H	-5.4202091798	-1.0437233389	1.008081912
H	-5.5390803134	0.8775054804	0.1374154286
H	-5.4391912938	-0.836055266	-1.094239072
N	1.6836004987	-0.3951636232	0.6819154997
N	1.5999219974	0.9394103251	0.0796525124
N	1.669766574	-0.2486742047	-0.7771817387
H	0.7356938611	-0.6684942519	0.9838902642
H	0.6156407299	1.2461664051	0.1196440236

H	0.7158531119	-0.4585432312	-1.1096412323
N	-1.3931925431	-0.5828094805	0.6924432831
N	-1.4761027879	0.7513162677	0.0894813141
N	-1.4066101643	-0.4371427182	-0.7665754982
H	-2.3403592634	-0.856512611	0.9958110532
H	-2.4594398256	1.0605201544	0.1291931274
H	-2.3595790903	-0.647449839	-1.1008983416
N	4.7701361208	-0.2061550874	0.6720368788
N	4.6861915219	1.1286079255	0.0700486928
N	4.7563470799	-0.0593162483	-0.7871087988
H	3.8217909237	-0.4788705488	0.9725867866
H	3.7015286172	1.4335608423	0.1099092531
H	3.8020531908	-0.2686708519	-1.1182520343
N	7.8781614703	-0.0152494046	0.6625650455
N	7.7939672374	1.3199602749	0.06004393
N	7.8646537875	0.1313458546	-0.7972182019
H	6.9285798442	-0.2863392186	0.960361423
H	6.8083338273	1.621497617	0.0993597633
H	6.9092508651	-0.0769365458	-1.1255968106
N	11.0889664493	0.1861347061	0.6553879493
N	11.0040292153	1.5214647069	0.0502807692
N	11.0767372755	0.33060499	-0.8061913329
H	10.135447749	-0.0790816232	0.942484336
H	10.0154401752	1.8096457466	0.0890538089
H	10.1180286414	0.12672555	-1.1243135902

Complete references

(20) Frisch, M. J; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K. Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision B.05; Gaussian, Inc.: Pittsburgh PA, 2003.