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Structure of 4,4-Bisphenylsulfonyl-*N*,*N*-dimethylbutylamine: Interplay of Intramolecular C–H···N, C–H···O=S and π···π Interactions

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Supporting Information

Cartesian coordinates and total energies (in Hartrees) of MP2/6-31G* optimized geometries of BSDBA conformers and $AH^{\cdots}NH_3$ complexes (7 pages)

Conformer **a** (-1847.21591)

S	-0.04801	-2.09972	0.21235
S	0.19596	0.23814	-1.78983
O	-0.32076	-3.16750	-0.75676
O	0.65380	-2.38571	1.47986
O	-0.79153	-0.52658	-2.56726
O	1.30211	0.94081	-2.46271
N	3.09562	0.60432	1.10950
C	0.99347	-0.83560	-0.56988
C	2.21341	-1.53555	-1.20037
C	3.51390	-0.76937	-0.94596
C	3.79361	-0.56567	0.54625
H	-2.54071	4.15964	1.19563
C	2.97533	0.47106	2.56125
C	3.79997	1.83956	0.77115
C	-1.58068	-1.29862	0.60572
C	-1.64312	-0.46414	1.72652
C	-2.86039	0.14267	2.03845
C	-3.99011	-0.10043	1.24914
C	-3.90784	-0.94753	0.13978
C	-2.69462	-1.55104	-0.19838
C	-0.67481	1.42947	-0.79375
C	0.02438	2.16331	0.17156
C	-0.66330	3.13785	0.89618
C	-2.01426	3.39117	0.63409
C	-2.68869	2.65901	-0.34730
C	-2.02056	1.67011	-1.07330
H	1.33429	-0.17945	0.24167
H	2.30416	-2.53815	-0.76657

Conformer **b** (-1847.21527)

N	-2.01020	2.78216	-0.13762
C	0.07354	0.61034	0.18543
C	-0.08119	2.82226	1.47406
C	0.81998	1.67925	0.99476
C	-0.82573	3.51834	0.33273
H	-0.77504	2.45535	2.23246
H	1.59388	2.10567	0.34620
H	-0.14361	3.61913	-0.52141
H	0.56207	3.56412	1.96443
H	1.34177	1.21253	1.83931
H	-1.11191	4.54305	0.63706
H	-0.78417	1.08068	-0.32145
C	-2.42062	3.28774	-1.44700
H	-3.30151	2.73590	-1.78716
H	-1.61187	3.12628	-2.16510
H	-2.67041	4.36312	-1.42608
C	-3.11104	2.89591	0.81866
H	-3.98851	2.38089	0.41709
H	-3.38591	3.94858	1.01021
H	-2.84267	2.41637	1.76138
S	-0.63866	-0.64091	1.28228
O	0.41900	-1.57488	1.70667
O	-1.40064	0.12154	2.28861
S	1.07383	-0.03908	-1.18292
O	0.49000	-1.31626	-1.61953
O	1.19046	1.10873	-2.10175
C	2.69571	-0.36192	-0.52836
C	5.24771	-0.86637	0.42919

H	2.04647	-1.68262	-2.27281	C	2.95946	-1.59302	0.08005
H	3.48738	0.18597	-1.47634	C	3.68733	0.61193	-0.68726
H	4.88061	-0.48291	0.72983	C	4.96997	0.34976	-0.20150
H	3.44443	-1.45004	1.09317	C	4.24685	-1.83419	0.56260
H	-3.73731	2.86061	-0.55319	H	2.17564	-2.33629	0.17015
H	-2.52358	1.08572	-1.83830	H	3.45933	1.53463	-1.21368
H	4.33525	-1.35170	-1.38206	H	5.75361	1.09387	-0.32141
H	2.39067	-0.42433	2.79010	H	4.46953	-2.78455	1.04120
H	3.95598	0.39567	3.06257	H	6.24789	-1.06537	0.80678
H	2.45272	1.34569	2.96101	C	-1.79977	-1.50930	0.26012
H	3.84847	1.96016	-0.31323	C	-3.66404	-2.87156	-1.26407
H	3.25534	2.69373	1.18472	C	-1.64342	-2.88261	0.07353
H	4.82779	1.85466	1.17516	C	-2.86960	-0.79917	-0.29242
H	-0.76582	-0.32054	2.35238	C	-3.79936	-1.49339	-1.06780
H	-2.93118	0.79474	2.90565	C	-2.59150	-3.56279	-0.69237
H	-4.93929	0.36447	1.50663	H	-0.79344	-3.39337	0.51626
H	-4.79134	-1.14204	-0.46379	H	-2.96148	0.27177	-0.12872
H	-2.60013	-2.21047	-1.05596	H	-4.63457	-0.95926	-1.51460
H	1.07588	1.96131	0.36439	H	-2.48791	-4.63339	-0.85057
H	-0.13868	3.71461	1.65478	H	-4.39382	-3.40676	-1.86688

Conformer **c** (-1847.21314)

N	-0.84420	2.52295	0.78706
C	-0.03786	0.17861	-1.02787
C	-1.08542	2.42132	-1.72412
C	-0.87500	0.94200	-2.05979
C	-1.74927	2.65830	-0.36628
H	-0.14067	2.96156	-1.80162
H	-1.85718	0.45768	-2.11476
H	-2.55756	1.92568	-0.23484
H	-1.74826	2.83663	-2.49420
H	-0.42627	0.82185	-3.05285
H	-2.22262	3.65936	-0.35590
H	-0.20728	0.59722	-0.02614
C	-1.63309	2.50745	2.01860
H	-0.96223	2.40041	2.87619
H	-2.31653	1.65463	2.00333
H	-2.22185	3.43258	2.15236
C	0.11002	3.63398	0.83166
H	0.70800	3.55173	1.74396
H	-0.40017	4.61383	0.84200
H	0.78872	3.58562	-0.02024
S	1.73730	0.38584	-1.35342
O	2.12708	-0.48896	-2.46732
O	1.94774	1.84366	-1.43554
S	-0.51579	-1.57816	-0.96691
O	-0.94560	-2.01647	-2.30106
O	0.50800	-2.30554	-0.20159
C	-1.96661	-1.44021	0.06200
C	-4.20670	-1.16804	1.67232

Conformer **d** (-1847.21194)

N	0.82027	2.63297	0.44781
C	-0.00832	0.22717	-1.20191
C	1.75818	1.95960	-1.79259
C	0.68645	1.00600	-2.32765
C	1.19091	3.07229	-0.90779
H	2.53845	1.39914	-1.26522
H	-0.06163	1.59500	-2.87030
H	0.28224	3.45712	-1.38450
H	2.24986	2.43181	-2.65270
H	1.11480	0.29719	-3.04270
H	1.90977	3.91209	-0.84928
H	0.17958	0.73524	-0.24437
C	-0.06942	3.62504	1.05188
H	-0.31974	3.31474	2.07100
H	-0.98892	3.68549	0.46426
H	0.39266	4.62697	1.10323
C	2.00634	2.45294	1.28267
H	1.69688	2.12906	2.28004
H	2.59042	3.38600	1.37999
H	2.65195	1.67644	0.86723
S	0.61438	-1.48363	-1.03289
O	-0.47049	-2.32133	-0.49940
O	1.34806	-1.85913	-2.25107
S	-1.81354	0.33607	-1.39633
O	-2.07460	1.78858	-1.42157
O	-2.26059	-0.52670	-2.49687
C	-2.44401	-0.28609	0.14387
C	-3.45850	-1.22105	2.54306

C	-1.79612	-1.28907	1.44220	C	-3.24532	-1.42750	0.13673
C	-3.23286	-1.46501	-0.52758	C	-2.14199	0.40551	1.32088
C	-4.35737	-1.32944	0.29164	C	-2.65081	-0.07908	2.52823
C	-2.92989	-1.15754	2.24651	C	-3.75818	-1.88785	1.35032
H	-0.79681	-1.30460	1.87256	H	-3.43725	-1.94227	-0.80004
H	-3.32403	-1.62042	-1.59969	H	-1.52905	1.30290	1.28906
H	-5.35134	-1.35277	-0.14854	H	-2.42856	0.44347	3.45600
H	-2.81838	-1.05251	3.32323	H	-4.38466	-2.77620	1.36674
H	-5.08536	-1.06618	2.30484	H	-3.85680	-1.59050	3.48512
C	2.50629	-0.18488	0.14231	C	1.80891	-1.26641	0.27359
C	3.74911	-1.03457	2.46345	C	3.64883	-0.89650	2.31298
C	2.22359	0.47698	1.34104	C	1.35177	-1.19047	1.59327
C	3.39475	-1.25778	0.07588	C	3.16424	-1.16250	-0.04760
C	4.02251	-1.67503	1.25062	C	4.08640	-0.97990	0.98724
C	2.84894	0.03511	2.50858	C	2.28658	-1.00747	2.61425
H	1.52913	1.31366	1.35766	H	0.29158	-1.30006	1.81165
H	3.56749	-1.75456	-0.87441	H	3.48119	-1.25749	-1.08315
H	4.71887	-2.50935	1.22094	H	5.14711	-0.90918	0.75819
H	2.64190	0.53307	3.45312	H	1.95269	-0.95842	3.64817
H	4.23667	-1.37071	3.37551	H	4.37128	-0.75854	3.11400

Conformer **e** (-1847.21092)

N	-2.24807	-1.19777	1.26061
C	0.05110	-0.68663	-0.70189
C	-1.42381	-2.80895	-0.45763
C	-0.99675	-1.61380	-1.32082
C	-1.57920	-2.47784	1.02564
H	-2.36733	-3.18883	-0.86741
H	-0.64266	-1.94808	-2.30252
H	-0.57917	-2.41295	1.46961
H	-0.69362	-3.61665	-0.54417
H	-1.87567	-0.98798	-1.50723
H	-2.09657	-3.31134	1.53977
H	-0.19926	-0.47439	0.34279
C	-2.15187	-0.82083	2.66587
H	-2.61022	0.16243	2.80599
H	-1.09762	-0.75541	2.95417
H	-2.65170	-1.54102	3.33858
C	-3.64752	-1.23155	0.85064
H	-4.08782	-0.24354	1.01040
H	-4.23347	-1.97905	1.41628
H	-3.72541	-1.46560	-0.21331
S	0.01045	0.93406	-1.54333
O	1.14081	1.73126	-1.04100
O	-0.21495	0.72526	-2.97887
S	1.71738	-1.42050	-0.72876
O	1.55066	-2.76362	-0.14390
O	2.29062	-1.23866	-2.06824
C	2.64821	-0.46163	0.44400
C	4.11474	0.99284	2.28763

Conformer **f** (-1847.21069)

N	2.44820	-0.40613	1.76026
C	0.74384	-0.22850	-0.83279
C	2.94233	0.97948	-0.26955
C	2.23269	-0.08029	-1.12086
C	2.59907	0.94635	1.22413
H	4.02060	0.84301	-0.41443
H	2.37547	0.14031	-2.18379
H	1.64701	1.46018	1.38698
H	2.71418	1.98195	-0.64908
H	2.67427	-1.06009	-0.92075
H	3.36224	1.52315	1.78406
H	0.58868	-0.28261	0.24948
C	1.90320	-0.34640	3.11322
H	1.75049	-1.36304	3.48755
H	0.93822	0.16952	3.09326
H	2.56766	0.18634	3.81768
C	3.71763	-1.12667	1.76885
H	3.55465	-2.13681	2.15390
H	4.47617	-0.62682	2.39848
H	4.11179	-1.21481	0.75486
S	0.15553	-1.85414	-1.44590
O	-0.13613	-1.77205	-2.88196
O	1.12766	-2.82841	-0.92249
S	-0.26308	1.15769	-1.47457
O	0.52181	1.88008	-2.48639
O	-1.61958	0.66322	-1.75396
C	-0.38117	2.18839	-0.02548
C	-0.52046	3.74357	2.26340

C	2.44868	-0.69791	1.80792	C	-1.12681	1.72549	1.06472
C	3.57153	0.47706	-0.01871	C	0.27412	3.42008	-0.00382
C	4.31032	1.20091	0.91834	C	0.19563	4.20080	1.15303
C	3.18905	0.04321	2.73111	C	-1.18604	2.51256	2.21630
H	1.76267	-1.47546	2.13552	H	-1.66017	0.77792	1.00538
H	3.69472	0.63164	-1.08590	H	0.82142	3.75227	-0.88236
H	5.03613	1.93513	0.57791	H	0.69616	5.16548	1.18771
H	3.05126	-0.12879	3.79595	H	-1.76116	2.17146	3.07404
H	4.69230	1.56438	3.01035	H	-0.57192	4.35235	3.16292
C	-1.48248	1.61856	-0.84663	C	-1.35208	-2.07954	-0.52991
C	-3.79426	2.69858	0.23632	C	-3.67630	-2.44419	0.92702
C	-1.44904	2.12598	0.45566	C	-1.25909	-2.29614	0.84944
C	-2.64512	1.64521	-1.61988	C	-2.57594	-2.04967	-1.19805
C	-3.80549	2.19558	-1.06821	C	-3.74266	-2.24221	-0.45564
C	-2.61685	2.66888	0.99357	C	-2.43796	-2.47178	1.57773
H	-0.51831	2.12468	1.01877	H	-0.28437	-2.35039	1.33111
H	-2.62078	1.27087	-2.64027	H	-2.59919	-1.86369	-2.26742
H	-4.71753	2.23425	-1.65908	H	-4.70728	-2.22421	-0.95670
H	-2.60656	3.08150	1.99984	H	-2.38916	-2.64434	2.65041
H	-4.69860	3.13098	0.65834	H	-4.59081	-2.58725	1.49787

Conformer **g** (-1847.20950)

N	-4.13098	-2.15968	0.20265
C	-0.85950	-0.15997	-0.46592
C	-3.35619	-0.09627	-0.90995
C	-2.01605	-0.70108	-1.32840
C	-3.85923	-0.73488	0.38459
H	-3.26763	0.99050	-0.79829
H	-2.08868	-1.78733	-1.21117
H	-4.74676	-0.19349	0.76470
H	-4.08388	-0.26383	-1.71152
H	-1.79850	-0.50787	-2.38336
H	-3.08535	-0.64618	1.15731
H	-1.22729	0.26831	0.47316
C	-5.44818	-2.37885	-0.38011
H	-5.58318	-3.44617	-0.57614
H	-5.53522	-1.84848	-1.33141
H	-6.26621	-2.03879	0.28204
C	-3.99811	-2.89442	1.45615
H	-4.19089	-3.95480	1.26943
H	-4.70407	-2.54845	2.23356
H	-2.97448	-2.79041	1.82214
S	-0.02697	1.19517	-1.35180
O	1.01587	0.63739	-2.22489
O	-1.11555	2.02165	-1.89688
S	0.18670	-1.56397	0.04664
O	-0.55652	-2.15417	1.17554
O	0.52944	-2.35120	-1.14150
C	1.68244	-0.86886	0.70328
C	4.04438	0.10310	1.76886

Conformer **h** (-1847.20897)

N	0.71044	-3.80577	-0.40234
C	-0.52830	-0.20894	-0.57859
C	-0.45421	-2.31130	-2.01999
C	0.30347	-1.07311	-1.54300
C	-0.58579	-3.37308	-0.92981
H	-1.45282	-2.02308	-2.37236
H	1.22544	-1.39390	-1.05482
H	-1.16473	-4.23362	-1.31986
H	0.06228	-2.72472	-2.89317
H	0.59277	-0.46596	-2.40656
H	-1.14931	-2.96129	-0.08600
H	-1.52984	-0.63305	-0.42092
C	1.44844	-4.59951	-1.37959
H	2.39215	-4.92634	-0.93378
H	1.68509	-4.00081	-2.26198
H	0.88950	-5.49622	-1.70505
C	0.51328	-4.57974	0.82193
H	1.48737	-4.88605	1.21513
H	-0.09150	-5.48940	0.65447
H	0.02046	-3.94951	1.56414
S	-0.81516	1.43200	-1.33239
O	0.36937	2.27029	-1.08876
O	-1.26047	1.12984	-2.70346
S	0.12691	-0.13843	1.12752
O	-0.41767	1.06794	1.76993
O	-0.14739	-1.47489	1.68240
C	1.88767	0.04311	0.99363
C	4.63999	0.31200	0.89797

C	1.67609	-0.34994	2.00238
C	2.84319	-0.92006	-0.07232
C	4.03129	-0.43313	0.47745
C	2.86922	0.14816	2.52742
H	0.76587	-0.37010	2.59653
H	2.80333	-1.34272	-1.07197
H	4.95004	-0.47881	-0.10274
H	2.88635	0.55417	3.53596
H	4.97503	0.47557	2.19138
C	0.76209	2.13683	-0.06420
C	1.99479	3.69475	1.86969
C	-0.01815	2.71790	0.94186
C	2.13951	2.34662	-0.13988
C	2.75261	3.13264	0.83830
C	0.61172	3.48883	1.91975
H	-1.09940	2.59542	0.94743
H	2.70660	1.89907	-0.95032
H	3.82488	3.30699	0.79244
H	0.02047	3.94444	2.71045
H	2.47890	4.30402	2.62936

C	2.44052	1.32646	1.01774
C	2.67726	-1.11135	0.93280
C	4.06477	-0.96238	0.87905
C	3.83006	1.45015	0.96589
H	1.79561	2.19656	1.07475
H	2.20535	-2.09130	0.90593
H	4.69784	-1.84507	0.82904
H	4.28128	2.43904	0.98393
H	5.72155	0.41905	0.85941
C	-2.20896	2.11631	-0.47191
C	-4.40772	3.20458	0.81017
C	-3.48407	1.63780	-0.78896
C	-2.00966	3.13519	0.46077
C	-3.12479	3.68116	1.09780
C	-4.58665	2.18779	-0.13272
H	-3.61074	0.87822	-1.55651
H	-1.00457	3.48243	0.67529
H	-2.99064	4.47614	1.82698
H	-5.58616	1.82897	-0.36547
H	-5.27031	3.63161	1.31605

Conformer **i** (-1847.20583)

N	-4.55722	0.33155	-0.40260
C	-0.95294	-0.43872	0.44057
C	-3.20653	-1.67052	0.24296
C	-2.20461	-0.96252	1.15787
C	-3.78329	-0.82084	-0.88782
H	-2.76337	-2.57533	-0.18566
H	-2.69560	-0.11171	1.63766
H	-4.45261	-1.46947	-1.46470
H	-4.04246	-1.98946	0.87606
H	-1.87749	-1.64458	1.95005
H	-2.99294	-0.51104	-1.59355
H	-1.20664	0.16352	-0.43731
C	-5.79151	0.49946	-1.16386
H	-6.36651	1.32760	-0.73961
H	-6.39511	-0.40847	-1.08606
H	-5.61663	0.71318	-2.23412
C	-3.79222	1.57294	-0.43493
H	-4.42288	2.39173	-0.07656
H	-3.44333	1.82988	-1.45449
H	-2.93031	1.51761	0.23203
S	-0.01411	-1.86552	-0.22185
O	-0.00056	-2.91141	0.80847
O	-0.60692	-2.09867	-1.55174
S	-0.05217	0.66451	1.57887
O	-1.06961	1.59789	2.09149
O	0.76547	-0.15062	2.48977
C	1.03418	1.60207	0.52652
C	2.73133	3.17265	-1.00223

Conformer **j** (-1847.20574)

N	3.80386	-2.17516	0.07786
C	-0.16918	-0.58181	0.15845
C	1.38781	-2.51703	-0.41919
C	1.19293	-1.00338	-0.39942
C	2.83170	-2.87726	-0.75958
H	1.11624	-2.93052	0.55968
H	1.98248	-0.57311	0.22131
H	3.03179	-2.59263	-1.80005
H	0.71988	-2.97412	-1.15525
H	1.33113	-0.58512	-1.40401
H	2.96122	-3.97634	-0.69504
H	-0.56224	-1.33739	0.85309
C	5.15527	-2.42662	-0.40775
H	5.86964	-1.85700	0.19338
H	5.23613	-2.09441	-1.44654
H	5.43596	-3.49471	-0.36115
C	3.68961	-2.56436	1.47955
H	4.48563	-2.07632	2.04856
H	3.77798	-3.65679	1.62613
H	2.73524	-2.22967	1.89351
S	-1.39530	-0.43707	-1.18083
O	-1.26843	0.89661	-1.78966
O	-1.21571	-1.65444	-1.99003
S	-0.02336	0.88394	1.23909
O	-1.36294	1.46635	1.41236
O	0.75162	0.38645	2.38888
C	0.99512	2.05388	0.37247
C	2.59491	3.91920	-0.90829

C	2.39402	1.63201	0.83858	C	2.37514	2.03968	0.60417
C	0.49854	2.36866	-0.51491	C	0.39537	2.99668	-0.46788
C	1.36242	3.14344	-1.29007	C	1.21108	3.92930	-1.11031
C	3.24206	2.42550	0.06313	C	3.17335	2.98090	-0.04875
H	2.76770	1.04023	1.66869	H	2.80360	1.32539	1.30154
H	-0.57228	2.38006	-0.70756	H	-0.67901	2.99474	-0.61068
H	0.96371	3.74041	-2.10679	H	0.76257	4.66866	-1.76905
H	4.30402	2.46065	0.29405	H	4.24732	2.98377	0.12002
H	3.39766	3.78659	-1.60370	H	3.22163	4.65013	-1.41379
C	1.66113	-1.33833	-0.48697	C	-2.97385	-0.56284	-0.37870
C	4.29790	-0.66233	-0.98231	C	-5.44311	-0.79898	0.85038
C	1.97705	-0.67477	-1.67715	C	-3.72478	0.59079	-0.14657
C	2.63318	-1.68265	0.45561	C	-3.43363	-1.83379	-0.01925
C	3.96142	-1.33928	0.19424	C	-4.67818	-1.94310	0.60346
C	3.30797	-0.32790	-1.91311	C	-4.97069	0.46070	0.46882
H	1.20193	-0.46743	-2.41022	H	-3.33639	1.55904	-0.44364
H	2.34551	-2.21380	1.35790	H	-2.84443	-2.71662	-0.25468
H	4.73646	-1.61084	0.90719	H	-5.05371	-2.92270	0.88861
H	3.57567	0.18586	-2.83325	H	-5.57110	1.34700	0.65754
H	5.33605	-0.40520	-1.18115	H	-6.41264	-0.89007	1.33415

$CH_4{\cdots}NH_3$ complex (-96.68547)

H	-0.00081	0.28799	0.00397
C	0.00168	1.37876	0.00181
N	-0.00150	-2.48348	0.00232
H	-0.93955	-2.87229	-0.05289
H	0.42596	-2.86977	0.84030
H	0.51668	-2.85742	-0.78875
H	1.02828	1.74552	-0.04328
H	-0.54881	1.74745	-0.86508
H	-0.47196	1.75076	0.91161

$CH_3F{\cdots}NH_3$ complex (-195.68849)

H	0.07626	0.18403	0.04142
C	0.00777	1.27271	0.04537
N	0.23596	-2.35439	0.03223
F	-1.28064	1.65585	-0.34401
H	-0.73479	-2.39958	-0.26879
H	0.29764	-2.89353	0.89275
H	0.77909	-2.85739	-0.66560
H	0.72683	1.70091	-0.65713
H	0.20053	1.66184	1.04804

$CH_2F_2{\cdots}NH_3$ complex (-294.71623)

H	0.02277	0.12414	0.02089
C	0.00406	1.21312	0.01319
N	0.06172	-2.28614	0.03861
F	-0.17248	1.65212	-1.27543
F	-1.05527	1.65141	0.76827
H	-0.76226	-2.56304	0.56733
H	0.83036	-2.85988	0.37823
H	-0.10603	-2.56712	-0.92476
H	0.91503	1.66790	0.40682

$CHF_3{\cdots}NH_3$ complex (-393.75940)

H	0.00092	0.06891	-0.00082
C	0.00128	1.15737	-0.00005
N	0.00076	-2.21586	-0.00223
F	1.16685	1.64292	0.48115
F	-0.16482	1.64455	-1.24942
F	-0.99774	1.64340	0.76912
H	-0.74538	-2.60288	0.57141
H	0.87115	-2.60206	0.35669
H	-0.12302	-2.60134	-0.93585

$CH_3CN{\cdots}NH_3$ complex (-188.69159)

H	0.79379	0.29719	0.04698
C	0.70830	1.38673	0.12602
N	0.97784	-2.04853	-0.12320
H	0.01334	-2.36434	-0.04831
H	1.49288	-2.51457	0.62030
H	1.33579	-2.41912	-1.00058

$CH_2(CN)_2{\cdots}NH_3$ complex (-280.68627)

H	0.12940	0.06679	0.06190
C	0.01114	1.16582	0.05093
N	0.00121	-2.07381	0.02234
H	-0.66264	-2.38470	0.72890
H	0.85459	-2.60793	0.17254
H	-0.37296	-2.37312	-0.87598

H	1.10413	1.84743	-0.78227	H	0.99175	1.62250	0.22608
C	-0.69350	1.76706	0.30334	C	-0.90622	1.55673	1.12809
N	-1.82830	2.06109	0.44623	N	-1.63006	1.84071	2.01755
H	1.29645	1.73485	0.97858	C	-0.48844	1.57795	-1.26633
				N	-0.86915	1.87946	-2.34331

$CH(CN)_3 \cdots NH_3$ complex (-372.67255)

H	0.00085	0.00617	0.00000
C	0.00089	1.12725	-0.00002
N	0.00073	-1.97224	0.00005
H	-0.57259	-2.35752	0.74851
H	0.93552	-2.35764	0.12233
H	-0.36082	-2.35759	-0.87064
C	1.39148	1.57667	0.17939
N	2.52203	1.89099	0.32525
C	-0.53900	1.57670	-1.29402
N	-0.97793	1.89104	-2.34603
C	-0.84977	1.57676	1.11453
N	-1.54135	1.89115	2.02066