Supplementary material for the Physical Chemistry Chemical Physics

Substituent effect in benzene dication

by

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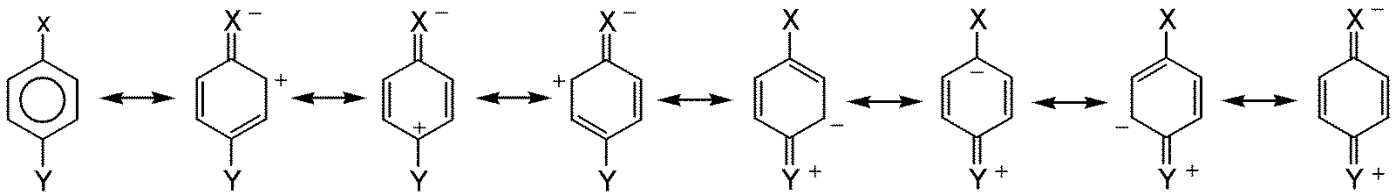
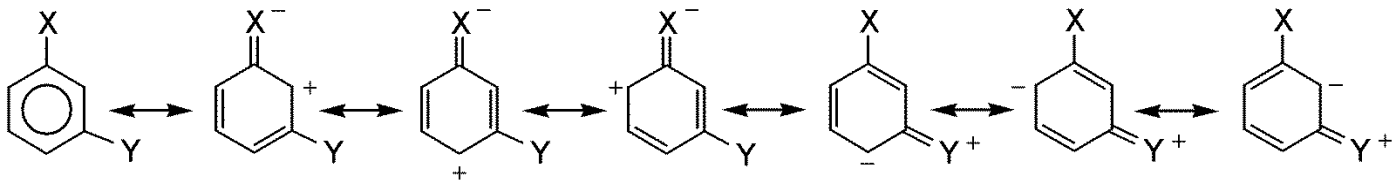
Scheme S1. Canonical forms with charge separation showing resonance effect between π-electron donating (Y) and π-electron accepting (X) substituents in *para*-disubstituted benzene derivative.



Scheme S2. Canonical forms with charge separation showing no resonance effect between π-electron donating (Y) and π-electron accepting (X) substituents in *meta*-disubstituted benzene derivative.



Scheme S3. Some of the canonical forms with double charge separation showing resonance effect between π-electron donating (Y) and π-electron accepting (X) substituents in *meta*-disubstituted benzene derivative.

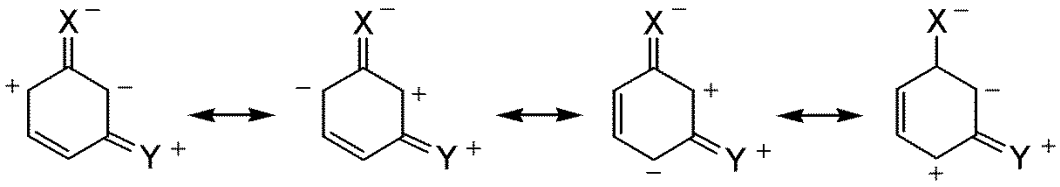


Table S1. The values of NICS indices estimated for mono- and disubstituted neutral benzene in the singlet state.

	NICS(0)	NICS(1)	$NICS(1)_{zz}$
benzene-0/1	-8.0451	-10.2141	-29.2472
$N(CH_3)2$-0/1	-8.0283	-9.0137	-24.8797
$NHCH_3$-0/1	-7.4880	-8.6355	-23.8094
NCH_2-0/1	-8.3335	-9.9712	-26.5767
NH_2-0/1	-7.8380	-9.1430	-24.9803
OCH_3-0/1	-8.9750	-9.9198	-27.1075
OH-0/1	-9.0782	-9.8512	-26.7642
Cl-0/1	-8.7980	-10.0098	-27.4001
CHO-0/1	-7.7210	-10.3411	-27.2274
NO_2-0/1	-9.0506	-10.3229	-27.5418
CN-0/1	-8.4657	-10.2032	-27.7768
p-CN-$N(CH_3)_2$-0/1	-8.1368	-9.1741	-22.5469
p-NO_2-$N(CH_3)_2$-0/1	-8.0275	-9.1117	-21.4430
p-Cl-CN-0/1	-8.9575	-9.8235	-25.6558
p-Cl-NO_2-0/1	-9.1732	-9.7997	-24.9367
m-CN-$N(CH_3)_2$-0/1	-8.3688	-9.2606	-23.5547
m-NO_2-$N(CH_3)_2$-0/1	-8.9218	-9.2710	-23.0800
m-Cl-CN-0/1	-9.1034	-9.9519	-25.9528
m-Cl-NO_2-0/1	-9.6158	-10.1195	-25.6960

Table S2. The values of NICS indices estimated for mono- and disubstituted singlet state dications.

	NICS(0)	NICS(1)	$NICS(1)_{zz}$
benzene-2/1	10.6796	7.3362	27.2099
$N(CH_3)_2$-2/1	10.7085	3.2220	14.8772
$NHCH_3$-2/1	10.9998	3.3131	14.7521
NCH_2-2/1	8.9939	2.4161	11.8279
NH_2-2/1	15.1307	6.5654	24.4471
OCH_3-2/1	20.8544	10.7934	36.5996
OH-2/1	27.2747	16.2139	52.7876
Cl-2/1	44.5590	29.6106	91.7551
CHO-2/1	13.8624	10.9421	40.5925
NO_2-2/1	9.6068	3.2722	14.6059
CN-2/1	37.6975	26.3293	80.8406
p-CN-$N(CH_3)_2$-2/1	7.4642	1.0089	7.9734
p-NO_2-$N(CH_3)_2$-2/1	5.2756	0.4298	5.3642
p-Cl-CN-2/1	26.8486	14.9624	46.5217
p-Cl-NO_2-2/1	7.0613	0.7922	6.4800
m-CN-$N(CH_3)_2$-2/1	9.0945	2.4717	13.4509
m-NO_2-$N(CH_3)_2$-2/1	6.2915	0.9371	9.3870
m-Cl-CN-2/1	31.8913	19.9049	62.7138
m-Cl-NO_2-2/1	10.2217	3.3587	13.2462

Table S3. The values of NICS indices estimated for mono- and disubstituted triplet state dications.

	NICS(0)	**NICS(1)**	**NICS(1)$_{zz}$**
benzene-2/3	-1.4169	-8.8151	-21.0941
$N(CH_3)_2$-2/3	32.8411	22.8338	73.3186
$NHCH_3$-2/3	4.7030	-1.7801	0.8278
NCH_2-2/3	4.1906	-2.0533	-1.3102
NH_2-2/3	2.4004	-3.9116	-6.1698
OCH_3-2/3	2.2037	-4.7030	-9.0533
OH-2/3	0.4311	-6.2626	-13.4014
Cl-2/3	2.5262	-4.9895	-10.6956
CHO-2/3	13.6496	5.9902	21.8668
NO_2-2/3	7.8100	0.6748	6.4953
CN-2/3	3.2359	-4.8417	-10.6981
p-CN-$N(CH_3)_2$-2/3	9.4919	3.2034	15.1680
p-NO_2-$N(CH_3)_2$-2/3	-3.2592	-5.6704	-10.6693
p-Cl-CN-2/3	3.0271	-4.2333	-8.3790
p-Cl-NO_2-2/3	8.4441	2.9786	12.6498
m-CN-$N(CH_3)_2$-2/3	3.4622	-2.1510	-1.8934
m-NO_2-$N(CH_3)_2$-2/3	-0.5151	-4.1945	-7.4972
m-Cl-CN-2/3	3.0047	-4.1860	-9.6259
m-Cl-NO_2-2/3	-2.4754	-3.0063	-5.4097

Table S4. Bond distances of benzene ring corresponding to optimized geometries at B3LYP/6-311++G(d,p) level of theory (atom numbering is consistent with the compound name).

benzene

	benzene-0/1	**benzene-2/1**	**benzene-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.39468	1.39183	1.42734
(2,3)	1.39464	1.39177	1.42734
(3,4)	1.39470	1.46172	1.42734
(4,5)	1.39463	1.39183	1.42734
(5,6)	1.39469	1.39177	1.42734
(6,1)	1.39464	1.46172	1.42734

N,N-dimethylaniline

	$N(CH_3)_2$-0/1	**$N(CH_3)_2$-2/1**	**$N(CH_3)_2$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.41232	1.47288	1.42195
(2,3)	1.39101	1.36087	1.44352
(3,4)	1.39325	1.42392	1.39214
(4,5)	1.39320	1.42380	1.39214
(5,6)	1.39105	1.36091	1.44358
(6,1)	1.41230	1.47301	1.42196

N-methylaniline

	$NHCH_3$-0/1	**$NHCH_3$-2/1**	**$NHCH_3$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40498	1.47026	1.42798
(2,3)	1.39453	1.35885	1.44157
(3,4)	1.39168	1.43288	1.39454
(4,5)	1.39728	1.42648	1.39715
(5,6)	1.38747	1.35881	1.43921
(6,1)	1.40861	1.47849	1.42779

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N-methylideneaniline

	NCH_2-0/1	**NCH_2-2/1**	**NCH_2-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40179	1.47990	1.43324
(2,3)	1.39314	1.35838	1.43924
(3,4)	1.39365	1.42957	1.39681
(4,5)	1.39586	1.42960	1.39684
(5,6)	1.39053	1.35832	1.43924
(6,1)	1.40084	1.47984	1.43318

aniline

	NH_2-0/1	**NH_2-2/1**	**NH_2-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40294	1.48323	1.43617
(2,3)	1.39126	1.35557	1.43633
(3,4)	1.39459	1.43686	1.40100
(4,5)	1.39458	1.43686	1.40100
(5,6)	1.39126	1.35557	1.43633
(6,1)	1.40293	1.48322	1.43619

methoxybenzene

	OCH_3-0/1	**OCH_3-2/1**	**OCH_3-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.39736	1.47408	1.43711
(2,3)	1.39761	1.35404	1.43596
(3,4)	1.39012	1.45213	1.40046
(4,5)	1.39788	1.42642	1.40701
(5,6)	1.38778	1.35804	1.43398
(6,1)	1.40075	1.49871	1.43797

phenol (-0/1)

	OH-0/1	**OH-2/1**	**OH-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.39592	1.47454	1.44053
(2,3)	1.39421	1.35198	1.43140
(3,4)	1.39287	1.46139	1.40786
(4,5)	1.39590	1.43380	1.41259
(5,6)	1.39105	1.35616	1.43159
(6,1)	1.39586	1.50133	1.44195

chlorobenzene

	Cl-0/1	**Cl-2/1**	**Cl-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.39148	1.47917	1.43186
(2,3)	1.39397	1.35646	1.43531
(3,4)	1.39383	1.44799	1.40868
(4,5)	1.39383	1.44798	1.40869
(5,6)	1.39399	1.35646	1.43530
(6,1)	1.39151	1.47917	1.43185

benzaldehyde

	CHO-0/1	**CHO-2/1**	**CHO-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40167	1.43773	1.41896
(2,3)	1.38852	1.39773	1.44025
(3,4)	1.39830	1.38842	1.39094
(4,5)	1.39408	1.45041	1.39987
(5,6)	1.39251	1.40004	1.45020
(6,1)	1.39898	1.38551	1.39678

nitrobenzene

	NO_2-0/1	**NO_2-2/1**	**NO_2-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.39141	1.47650	1.39937
(2,3)	1.39145	1.35903	1.44722
(3,4)	1.39520	1.43358	1.40673
(4,5)	1.39524	1.43357	1.39852
(5,6)	1.39141	1.35901	1.43949
(6,1)	1.39136	1.47650	1.41314

benzonitrile

	CN-0/1	**CN-2/1**	**CN-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40259	1.50832	1.43470
(2,3)	1.39045	1.37200	1.43402
(3,4)	1.39474	1.40612	1.41072
(4,5)	1.39474	1.47655	1.41074
(5,6)	1.39045	1.37081	1.43402
(6,1)	1.40261	1.42188	1.43470

4-(N,N-dimethylamino)benzonitrile

	***p*-CN-N(CH$_3$)$_2$-0/1**	***p*-CN-N(CH$_3$)$_2$-2/1**	***p*-CN-N(CH$_3$)$_2$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40332	1.43541	1.41987
(2,3)	1.38362	1.35816	1.44931
(3,4)	1.41641	1.46747	1.40336
(4,5)	1.41646	1.46752	1.44215
(5,6)	1.38363	1.35818	1.40339
(6,1)	1.40325	1.43540	1.40155

4-nitro-N,N-dimethylaniline

	***p*-NO$_2$-N(CH$_3$)$_2$-0/1**	***p*-NO$_2$-N(CH$_3$)$_2$-2/1**	***p*-NO$_2$-N(CH$_3$)$_2$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.41903	1.46806	1.43507
(2,3)	1.38223	1.35967	1.37488
(3,4)	1.39453	1.42078	1.40960
(4,5)	1.39458	1.42074	1.40965
(5,6)	1.38228	1.35961	1.37481
(6,1)	1.41896	1.46808	1.43513

4-chlorobenzonitrile

	***p*-Cl-CN-0/1**	***p*-Cl-CN-2/1**	***p*-Cl-CN-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40215	1.45737	1.42294
(2,3)	1.38911	1.35624	1.43032
(3,4)	1.39306	1.46447	1.42424
(4,5)	1.39305	1.46447	1.42425
(5,6)	1.38908	1.35626	1.43031
(6,1)	1.40216	1.45741	1.42293

1-chloro-4-nitrobenzene

	***p*-Cl-NO$_2$-0/1**	***p*-Cl-NO$_2$-2/1**	***p*-Cl-NO$_2$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.39419	1.45091	1.44074
(2,3)	1.38948	1.35044	1.37692
(3,4)	1.39125	1.46981	1.41279
(4,5)	1.39122	1.46983	1.41268
(5,6)	1.38950	1.35043	1.37695
(6,1)	1.39421	1.45083	1.44079

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3-(N,N-dimethylamino)benzonitrile

	***m*-CN-N(CH$_3$)$_2$-0/1**	***m*-CN-N(CH$_3$)$_2$-2/1**	***m*-CN-N(CH$_3$)$_2$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40025	1.43952	1.41601
(2,3)	1.39050	1.41469	1.38420
(3,4)	1.38962	1.36437	1.41428
(4,5)	1.41444	1.47459	1.43186
(5,6)	1.41006	1.45735	1.40908
(6,1)	1.39869	1.37187	1.44972

3-nitro-N,N-dimethylaniline

	***m*-NO$_2$-N(CH$_3$)$_2$-0/1**	***m*-NO$_2$-N(CH$_3$)$_2$-2/1**	***m*-NO$_2$-N(CH$_3$)$_2$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.41020	1.46723	1.41650
(2,3)	1.38739	1.35498	1.41731
(3,4)	1.38947	1.41669	1.39853
(4,5)	1.39166	1.42050	1.38914
(5,6)	1.39008	1.36456	1.41005
(6,1)	1.41515	1.47124	1.42851

3-chlorobenzonitrile

	***m*-Cl-CN-0/1**	***m*-Cl-CN-2/1**	***m*-Cl-CN-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.40192	1.38108	1.43942
(2,3)	1.38872	1.40804	1.43265
(3,4)	1.39285	1.50362	1.42783
(4,5)	1.39349	1.37578	1.40606
(5,6)	1.39020	1.39750	1.40520
(6,1)	1.40159	1.49396	1.42682

1-chloro-3-nitrobenzene

	***m*-Cl-NO$_2$-0/1**	***m*-Cl-NO$_2$-2/1**	***m*-Cl-NO$_2$-2/3**
bond	d[Å]	d[Å]	d[Å]
(1,2)	1.39394	1.48617	1.42868
(2,3)	1.39353	1.36977	1.39607
(3,4)	1.39160	1.41470	1.40701
(4,5)	1.38993	1.46298	1.41292
(5,6)	1.39072	1.35611	1.39945
(6,1)	1.38926	1.43198	1.43867

Table S5. Atom coordinates corresponding to optimized geometries at B3LYP/6-311++G(d,p) level of theory.

Neutral singlet state species

Benzene-0/1

C	-1.87329400	0.10766100	0.00005600
C	-0.47861300	0.10759200	0.00050400
C	0.21881000	1.31533000	-0.00005100
C	-0.47851800	2.52318400	-0.00104100
C	-1.87314800	2.52325200	-0.00148400
C	-2.57059600	1.31547000	-0.00093900
H	-2.41550900	-0.83147900	0.00048600
H	0.06350500	-0.83160400	0.00128300
H	1.30322800	1.31531600	0.00029200
H	0.06376200	3.46228600	-0.00147100
H	-2.41532900	3.46241200	-0.00226200
H	-3.65501500	1.31555800	-0.00128300

E= -232.3113044au

$N(CH_3)_2$-0/1

C	-1.83297900	0.04221200	-0.03836300
C	-0.69396900	0.22111900	0.74371500
C	0.00613500	1.42309200	0.73248500
C	-0.41037100	2.49900500	-0.08208700
C	-1.57547100	2.31066600	-0.85778400
C	-2.26320700	1.10179000	-0.83419700
H	-2.37528000	-0.89546900	-0.02222700
H	-0.34155400	-0.58331000	1.38068500
H	0.88025100	1.51938800	1.36118000
H	-1.94985400	3.10738800	-1.48528600
H	-3.15252000	0.99403000	-1.44618800
N	0.30632000	3.69172800	-0.12928300
C	-0.29741800	4.85517300	-0.75869000
H	-0.52103700	4.65973800	-1.81081300
H	-1.22751400	5.17429900	-0.26424600
H	0.40975500	5.68343800	-0.72488300
C	1.34082100	3.93563600	0.86268700
H	2.11719100	3.16756400	0.81484600
H	1.81669700	4.89265700	0.65063900
H	0.94991200	3.96412100	1.89129000

E= -366.3141467au

$NHCH_3$-0/1

C	-1.90051400	0.02383400	-0.01777100
C	-0.50419700	0.07521000	-0.02429200
C	0.16126100	1.29096800	0.04039400
C	-0.55442700	2.50207200	0.11250100

C	-1.95829100	2.44608500	0.11192600
C	-2.61389800	1.21677100	0.05121300
H	-2.41730800	-0.92697500	-0.06782900
H	0.07221600	-0.84202800	-0.07996200
H	1.24698400	1.31530100	0.04299900
H	-2.54110000	3.35696500	0.16164700
H	-3.69857200	1.19943200	0.05407400
N	0.13786500	3.70277200	0.21500000
C	-0.50723200	4.98647900	0.01498300
H	-1.02342500	5.06491400	-0.95288900
H	-1.23649400	5.18185600	0.80666000
H	0.25018500	5.76949600	0.06735400
H	1.10118900	3.65668300	-0.07713300

E= - 327.0020257au

NCH_2-0/1

C	-1.92049100	0.05067100	0.18398100
C	-0.52850000	0.14427700	0.13896900
C	0.08561500	1.36555100	-0.11584100
C	-0.68751900	2.52044100	-0.29144800
C	-2.08548200	2.42171000	-0.26032800
C	-2.69415200	1.19068700	-0.02595800
H	-2.39729500	-0.90564600	0.36550200
H	0.07974600	-0.74060900	0.28955200
H	1.16447800	1.44831100	-0.17371300
H	-2.69005700	3.30102300	-0.45175400
H	-3.77637800	1.12204700	-0.01581700
N	-0.01435100	3.73422500	-0.55440500
C	-0.39636400	4.80359600	0.01010700
H	-1.20922500	4.84550600	0.74553000
H	0.10932200	5.73687400	-0.23210000

E= -325.7708734au

NH_2-0/1

C	-0.07389500	-0.47674000	0.02238200
C	1.31697500	-0.47534200	0.05546900
C	2.02774200	0.73420100	0.05013900
C	1.30632800	1.93671000	0.00805400
C	-0.08449100	1.92461100	-0.02481900
C	-0.78797700	0.72047900	-0.01785800
H	-0.60277500	-1.42368400	0.02888000
H	1.86031300	-1.41485900	0.08113900
H	1.84142900	2.88123900	-0.00354300
H	-0.62167900	2.86638300	-0.05566400
H	-1.87102100	0.71520000	-0.04260400
N	3.42570900	0.73994900	0.02645400
H	3.86461000	1.58642200	0.35747100
H	3.87218000	-0.08828000	0.39172300

E= -287.6877297au

Supplementary material for the Physical Chemistry Chemical Physics

OCH_3-0/1

C	-0.04234300	-0.47354500	0.00230700
C	1.34527600	-0.45551000	0.01355700
C	2.02992500	0.76651800	0.00947900
C	1.31216400	1.96535200	-0.00593600
C	-0.08495700	1.93012600	-0.01710100
C	-0.76947700	0.72023000	-0.01310000
H	-0.56176000	-1.42547300	0.00563400
H	1.92234400	-1.37237700	0.02562700
H	1.82047600	2.92016900	-0.00945100
H	-0.63446900	2.86502800	-0.02908200
H	-1.85278000	0.70250800	-0.02177200
O	3.39331300	0.68173800	0.02134600
C	4.14965000	1.88417300	0.01816300
H	5.19463400	1.57843400	0.02924500
H	3.95557400	2.47709400	-0.88240100
H	3.94073400	2.49115500	0.90595400

E= -346.8676283au

OH-0/1

C	-0.06192600	-0.48039200	-0.00472500
C	1.32893900	-0.49030100	0.01555700
C	2.02619300	0.71885000	0.03047400
C	1.33091900	1.92928900	0.02511400
C	-0.06314200	1.92594100	0.00469000
C	-0.76721500	0.72421200	-0.01028400
H	-0.59878400	-1.42243700	-0.01629200
H	1.88722800	-1.41863200	0.02004500
H	1.87552400	2.86912200	0.03683800
H	-0.59638500	2.87003400	0.00063200
H	-1.85046100	0.72485100	-0.02602100
H	3.76149300	1.54519300	0.05887800
O	3.39467000	0.65508200	0.05020800

E= -307.5587318au

Cl-0/1

C	-1.87460300	0.10537200	0.00003000
C	-0.48077700	0.10837800	0.00049000
C	0.22332200	1.31148200	-0.00000300
C	-0.48725300	2.50788600	-0.00098900
C	-1.87862800	2.52516200	-0.00146000
C	-2.56878800	1.31403400	-0.00093300
H	-2.41650700	-0.83307600	0.00043200
H	0.06654300	-0.82736400	0.00125300
H	1.30572900	1.32317200	0.00035600
H	-2.40959400	3.46846900	-0.00221600
H	-3.65281300	1.32045200	-0.00129200
Cl	0.39302800	4.03273900	-0.00161300

E= -691.9342954au

Supplementary material for the Physical Chemistry Chemical Physics

CHO-0/1

C	-0.07413500	-0.48351100	-0.14483000
C	1.31834900	-0.47654200	-0.14963200
C	2.01715300	0.72684400	-0.00578700
C	1.31238100	1.92918300	0.14370300
C	-0.07611300	1.92109700	0.14815300
C	-0.76962200	0.71549100	0.00396400
H	-0.61497100	-1.41613200	-0.25651000
H	1.86965900	-1.40474200	-0.26529100
H	1.87154900	2.85087900	0.25411800
H	-0.62421800	2.84923800	0.26353500
H	-1.85396500	0.71335300	0.00786800
C	3.49781200	0.71369900	-0.01399500
O	4.20212800	1.69181300	0.10255200
H	3.94905000	-0.29361100	-0.13962200

E= -345.6691786au

NO_2-0/1

C	-1.87055600	0.11233500	-0.00010100
C	-0.48577500	0.11447000	0.17041400
C	0.21722900	1.31522600	0.17138100
C	-0.49210200	2.49978400	-0.00056000
C	-1.87270100	2.52180900	-0.17224500
C	-2.56111000	1.31258600	-0.17073300
H	-2.41251200	-0.82639400	0.00004500
H	0.04824200	-0.81885300	0.30279600
H	1.29006500	1.34843700	0.30096300
H	-2.38038900	3.46742700	-0.30255400
H	-3.63643600	1.30835900	-0.30283000
N	0.24877400	3.78214100	-0.00145400
O	1.46295000	3.73717800	0.15093100
O	-0.39640000	4.81156700	-0.15460300

E= -436.8747227au

CN-0/1

C	-1.86462800	0.12268100	-0.00001500
C	-0.46989200	0.12083100	0.00048600
C	0.23103800	1.32168400	0.00005100
C	-0.47089900	2.53601200	-0.00089200
C	-1.87348800	2.53701200	-0.00139600
C	-2.56336200	1.32977300	-0.00095400
H	-2.40669000	-0.81598600	0.00032900
H	0.07295800	-0.81706100	0.00121900
H	1.31398100	1.32968200	0.00043200
H	-2.40783100	3.47899300	-0.00212900
H	-3.64701700	1.33126300	-0.00134200
C	0.24508500	3.77594200	-0.00134900
N	0.82275100	4.77681500	-0.00171700

E= -324.5778391au

Supplementary material for the Physical Chemistry Chemical Physics

***m*-CN-N(CH_3)$_2$-0/1**

C	-1.88574100	0.06243300	0.02661300
C	-0.49852500	0.09560900	-0.06297800
C	0.20018100	1.29672400	-0.04963600
C	-0.47429400	2.53461000	0.06594600
C	-1.88197200	2.49962400	0.14002700
C	-2.56837900	1.28103400	0.12515000
H	0.05475900	-0.83268200	-0.14943600
H	1.27774800	1.26996600	-0.12851500
H	-2.45732400	3.41062000	0.21007400
N	0.21631900	3.73263400	0.11322000
C	-0.51679200	4.98756700	0.03970300
H	-1.06047400	5.10552100	-0.90846700
H	-1.23580800	5.07090100	0.85955300
H	0.18542700	5.81416000	0.13584700
C	1.64131400	3.75236600	-0.18014200
H	2.01229900	4.76943600	-0.06369300
H	2.19646500	3.11897000	0.51774800
H	1.86713900	3.41835000	-1.20291900
H	-2.43100800	-0.87176900	0.01408000
C	-3.99902800	1.29097000	0.20701500
N	-5.15291900	1.29878100	0.27312500

E= -458.5825426au

***m*-NO_2-N(CH_3)$_2$-0/1**

C	-1.87822800	0.06038800	0.03569100
C	-0.48913100	0.09464500	-0.04149400
C	0.20963800	1.29631600	-0.03582400
C	-0.46432900	2.53700200	0.05964200
C	-1.87280500	2.50440300	0.12134300
C	-2.53233500	1.28382700	0.11301200
H	0.06429300	-0.83463400	-0.11216200
H	1.28784800	1.26788600	-0.10485300
H	-2.46606800	3.40298500	0.17531100
N	0.22396900	3.73538700	0.09940800
C	-0.51212100	4.98783100	0.00386600
H	-1.04094800	5.09564100	-0.95363600
H	-1.24466500	5.07415700	0.81094900
H	0.18613000	5.81718600	0.10499700
C	1.65119300	3.75398900	-0.18311800
H	2.01988200	4.77265800	-0.07399000
H	2.20163500	3.12850600	0.52556400
H	1.88527700	3.41024400	-1.20079000
H	-2.43807900	-0.86285200	0.03026600
N	-4.01359800	1.29608100	0.18395100
O	-4.57725500	2.38288300	0.24612100
O	-4.59242100	0.21688800	0.17716700

E= -570.8 800511au

Supplementary material for the Physical Chemistry Chemical Physics

_m_-Cl-CN-0/1

C	-1.86247100	0.11917600	0.00000800
C	-0.46899800	0.12535300	0.00047500
C	0.23471600	1.32429200	0.00003100
C	-0.46915400	2.53632300	-0.00089200
C	-1.87104800	2.54432600	-0.00136800
C	-2.54788200	1.33170900	-0.00090800
H	0.06860400	-0.81526500	0.00119300
H	1.31707400	1.33188700	0.00039000
H	-2.41444800	3.47960700	-0.00208300
C	0.24340200	3.77842700	-0.00136400
N	0.82132100	4.77872000	-0.00174400
H	-2.41317100	-0.81271300	0.00035300
Cl	-4.30153100	1.33155000	-0.00148900

E= -784.1982789au

_m_-Cl-NO_2-0/1

C	-1.86886600	0.10900300	0.00349200
C	-0.47595800	0.11248700	0.04508100
C	0.23133100	1.31093900	0.04370100
C	-0.48899400	2.49884400	-0.00014200
C	-1.87862600	2.53422800	-0.04238600
C	-2.55577000	1.32117400	-0.03969800
H	0.05982700	-0.82832500	0.07884700
H	1.31125400	1.33822400	0.07526700
H	-2.40035400	3.47974500	-0.07602800
N	0.24804000	3.78620000	-0.00267400
O	1.46996600	3.73678600	0.03412300
O	-0.41057200	4.81643800	-0.04132500
H	-2.42020500	-0.82254500	0.00450900
Cl	-4.30739000	1.31863100	-0.09143800

E= -896.4946378au

_p_-CN-N(CH_3)$_2$-0/1

C	-1.88100700	0.06116000	0.06228400
C	-0.48426200	0.09002300	-0.07024800
C	0.20615000	1.28901000	-0.08291800
C	-0.47233700	2.52595400	0.04294200
C	-1.88276300	2.48476100	0.16683200
C	-2.56485100	1.28099300	0.17841300
H	0.06129500	-0.84102700	-0.16709400
H	1.28093400	1.26390600	-0.19182800
H	-2.45098600	3.39978800	0.25345200
H	-3.64396400	1.27996100	0.27527900
N	0.21203000	3.71995500	0.04794900
C	-0.51737600	4.97929200	0.06694300
H	-1.14363400	5.11102200	-0.82524400
H	-1.15912200	5.05320600	0.95054300
H	0.19460400	5.80170200	0.10624700
C	1.64621800	3.74046100	-0.20005600
H	2.00399800	4.76612900	-0.13115800

H	2.18744700	3.14880300	0.54518400
H	1.90075400	3.35531900	-1.19616900
C	-2.58841900	-1.17679500	0.07249900
N	-3.16241400	-2.18166900	0.08095800

E= -458.5854448au

p-NO_2-N(CH_3)$_2$-0/1

C	-1.86630300	0.09437000	0.04497700
C	-0.48082100	0.09786000	-0.11400100
C	0.20696800	1.29659700	-0.13984500
C	-0.47359500	2.53468900	-0.00786400
C	-1.88274700	2.49546700	0.15460700
C	-2.56507300	1.29365000	0.17969800
H	0.04296900	-0.84282900	-0.21629700
H	1.27997500	1.27352500	-0.26370500
H	-2.44611500	3.41111700	0.26134200
H	-3.63931700	1.26976500	0.30264500
N	0.20538300	3.72580200	-0.03742400
C	-0.51237700	4.98530700	0.10353400
H	-1.25108600	5.12097200	-0.69445800
H	-1.03026100	5.05178400	1.06723800
H	0.19791700	5.80766200	0.04665100
C	1.65271400	3.74420200	-0.20020400
H	1.99686500	4.77646000	-0.20492200
H	2.16003500	3.22220900	0.61926900
H	1.95881800	3.28145300	-1.14519200
N	-2.58912000	-1.17100200	0.06993100
O	-1.94069300	-2.20923300	-0.05189300
O	-3.81060400	-1.13553100	0.21126400

E= -570.8843152au

p-Cl-CN-0/1

C	-1.85755900	0.13492800	-0.00000400
C	-0.46460400	0.11888500	0.00050100
C	0.22875400	1.32254100	0.00005100
C	-0.46960500	2.53841200	-0.00089600
C	-1.87174900	2.53546400	-0.00139100
C	-2.56780400	1.33332900	-0.00094700
H	0.06803600	-0.82306900	0.00123600
H	1.31156100	1.32424000	0.00043300
H	-2.41148100	3.47418200	-0.00212800
H	-3.64987700	1.32381800	-0.00132400
C	0.24585700	3.77722500	-0.00136200
N	0.82372900	4.77789800	-0.00173700
Cl	-2.73341800	-1.38214200	0.00055900

E= -784.1992938au

p-Cl-NO_2-0/1

C	-1.86354900	0.12455100	-0.00008500
C	-0.47025600	0.10710700	0.04683300
C	0.22503600	1.31011400	0.04647700
C	-0.49041000	2.50238200	-0.00064800
C	-1.88064100	2.52599400	-0.04760600
C	-2.57518900	1.32253200	-0.04723400
H	0.06058100	-0.83495600	0.08310000
H	1.30541500	1.33356200	0.08182600
H	-2.40022900	3.47349700	-0.08377200
H	-3.65647000	1.31139800	-0.08301700
N	0.24856200	3.78200800	-0.00133700
O	1.47133300	3.73092500	0.03938700
O	-0.40671400	4.81563300	-0.04256100
Cl	-2.73836100	-1.39060200	0.00035500

E= -896.4959589au

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Benzene-2/1

C	-1.78184300	0.12216800	0.02237300
C	-0.42600800	0.01603500	-0.27365600
C	0.16050400	1.24331800	0.02098500
C	-0.56993600	2.50866600	-0.02337300
C	-1.92577100	2.61480000	0.27265200
C	-2.51229400	1.38751500	-0.02195200
H	-2.31040800	-0.75010800	0.43189800
H	0.11696200	-0.92475700	-0.26736400
H	1.18062700	1.26495800	0.42947000
H	-0.04136700	3.38092800	-0.43292500
H	-2.46874200	3.55559200	0.26634800
H	-3.53244200	1.36586300	-0.43036800

E= -231.4099497au

$N(CH_3)_2$-2/1

C	-1.92662500	0.11677100	0.03870600
C	-0.79926800	0.25766800	0.89684900
C	-0.07909200	1.41235000	0.88514600
C	-0.48245100	2.52118600	0.00336500
C	-1.66328900	2.33835600	-0.85778200
C	-2.34377900	1.16004600	-0.83599600
H	-2.48641900	-0.81591600	0.05204900
H	-0.52545500	-0.55529900	1.56000500
H	0.75805200	1.52795500	1.55962900
H	-1.96370100	3.11753500	-1.54464400
H	-3.19884400	1.00582400	-1.48463200
N	0.19711500	3.64865500	-0.01634200
C	-0.22997500	4.85839400	-0.75786200
H	0.31098800	4.87939100	-1.71282400
H	-1.30214000	4.88693000	-0.91496400

Supplementary material for the Physical Chemistry Chemical Physics

H	0.08222500	5.72612700	-0.17366000
C	1.47845300	3.85635400	0.69639600
H	2.10027600	4.49656500	0.06688100
H	1.26496100	4.40028600	1.62567000
H	1.99487200	2.92508400	0.89749000

E= -365.5841153au

$NHCH_3$-2/1

C	-1.85576900	0.02966100	-0.07484900
C	-0.43634500	0.07633900	0.05897000
C	0.18173400	1.28462100	0.12537700
C	-0.62667000	2.52072200	0.05843600
C	-2.08812200	2.43638200	-0.07834200
C	-2.66718600	1.20874600	-0.14202400
H	-2.34476200	-0.94147100	-0.12808600
H	0.13130300	-0.84665800	0.10562600
H	1.26105100	1.36489000	0.22666000
H	-2.68785400	3.33648800	-0.12765300
H	-3.74233900	1.10732800	-0.24338000
N	0.00776600	3.65710500	0.12401900
C	-0.47773600	5.03453400	0.08819500
H	-1.55658400	5.09221300	-0.00449400
H	-0.13227400	5.52807900	1.00721300
H	0.01944400	5.53615000	-0.75386100
H	1.02858600	3.59470600	0.21706800

E= -326.2513491au

NCH_2-2/1

C	-1.86496200	-0.04108000	0.00885500
C	-0.45698500	0.19095000	0.09552400
C	0.01734800	1.46362800	0.07703800
C	-0.95668900	2.57216300	-0.03396300
C	-2.40937500	2.30387800	-0.12245600
C	-2.82646000	1.01132400	-0.09907000
H	-2.22238700	-1.06911500	0.02595800
H	0.22006700	-0.65293900	0.17555200
H	1.07457800	1.69988600	0.13988200
H	-3.09281900	3.14290900	-0.20287400
H	-3.88169500	0.76727000	-0.16140500
N	-0.53872700	3.77264700	-0.05344800
C	-0.12832500	4.94677600	-0.07326100
H	-0.01191400	5.50387300	0.86670100
H	0.11769000	5.42649200	-1.03075700

E= -325.00083au

NH_2-2/1

C	-0.04891900	-0.53997200	0.02074600
C	1.30434600	-0.55714200	0.09786300
C	2.03139100	0.73555100	0.11490300

Supplementary material for the Physical Chemistry Chemical Physics

C	1.29300400	2.02020000	0.04841800
C	-0.06005100	1.98816100	-0.02771300
C	-0.73611100	0.72036100	-0.04163800
H	-0.62267500	-1.46102400	0.00562600
H	1.86969200	-1.48418500	0.14752600
H	1.85019100	2.95339900	0.06225400
H	-0.64188300	2.90286700	-0.07810700
H	-1.82411000	0.71440100	-0.10251300
N	3.32047100	0.74257400	0.18893300
H	3.86530400	1.61255300	0.20383000
H	3.87279500	-0.12145500	0.23709600

E= -286.9064466au

OCH_3-2/1

C	-0.02347200	-0.54273900	-0.07048600
C	1.33138800	-0.46734100	-0.12465500
C	1.99374400	0.87402000	-0.03422100
C	1.19533700	2.10455700	0.11147700
C	-0.15178600	1.97699300	0.16047300
C	-0.76851600	0.66538400	0.07097900
H	-0.54102200	-1.49456500	-0.13249100
H	1.98162400	-1.33178600	-0.23133500
H	1.67746200	3.07281800	0.17655300
H	-0.79228400	2.84690300	0.26692400
H	-1.85598800	0.60902800	0.11469800
O	3.24443200	0.81600400	-0.09508700
C	4.27541200	1.89215100	-0.04453600
H	4.90452300	1.60206500	0.80130400
H	4.82651800	1.76040400	-0.97955000
H	3.82093200	2.87172300	0.06242400

E= -346.0584382au

OH-2/1

C	-0.04766700	-0.55467000	-0.00480500
C	1.30830800	-0.56288400	0.01618700
C	2.03188700	0.75248400	0.03146200
C	1.31219500	2.03944800	0.02468300
C	-0.03893700	1.99658900	0.00362300
C	-0.72754100	0.70768100	-0.01049600
H	-0.62171600	-1.47643500	-0.01660800
H	1.91588000	-1.46558600	0.02271300
H	1.87196400	2.97219200	0.03623500
H	-0.63397000	2.90544000	-0.00270200
H	-1.81847400	0.71426000	-0.02599300
H	3.82940400	1.47399100	0.06083100
O	3.28572100	0.64830300	0.04998300

E= -306.7152843au

Supplementary material for the Physical Chemistry Chemical Physics

Cl-2/1

C	-1.85591100	0.13644800	0.00107100
C	-0.40865500	0.09660600	-0.02156300
C	0.28597100	1.26117500	0.01391000
C	-0.47575100	2.52913600	0.01191600
C	-1.95471300	2.55368100	0.01054500
C	-2.61494700	1.36927400	-0.02488100
H	-2.40045400	-0.80742400	0.05679700
H	0.09693100	-0.86461100	-0.03587100
H	1.37170900	1.30181000	0.02840000
H	-2.46316800	3.51389800	0.02265500
H	-3.70011000	1.32565200	-0.04157300
Cl	0.33875800	3.94106300	-0.02735200

E= -691.0580188au

CHO-2/1

C	-0.00582200	-0.47530700	0.03010800
C	1.36046100	-0.56571900	-0.26178000
C	1.95413100	0.67008900	-0.06184100
C	1.26197100	1.92821300	-0.13325500
C	-0.10909000	1.99335200	0.13057600
C	-0.75369500	0.76741800	0.03425100
H	-0.49228700	-1.37133200	0.43192600
H	1.89288500	-1.51118500	-0.24429200
H	1.78698800	2.82739600	-0.46247800
H	-0.64328200	2.93784600	0.12840700
H	-1.83550500	0.71952400	-0.11339400
C	3.51480500	0.69002600	0.18105000
O	4.16156700	0.31485700	1.07323900
H	3.93192900	1.11187800	-0.78429100

E= -344.7659967au

NO_2-2/1

C	-1.82199000	0.18035700	0.06579100
C	-0.39073800	0.14113300	-0.00567200
C	0.30726700	1.29598000	-0.16701100
C	-0.46479800	2.55453300	-0.16721500
C	-1.94106300	2.58099200	-0.16983400
C	-2.58209300	1.39357500	-0.00834900
H	-2.36119700	-0.76278700	0.14914700
H	0.12196900	-0.81545400	0.02825000
H	1.38951400	1.33224800	-0.27008700
H	-2.45891700	3.53175700	-0.27514100
H	-3.66660700	1.34992100	0.02340300
N	0.21316500	3.74172100	0.40420600
O	0.58562400	4.39541100	1.27483300
O	0.22914300	3.76668700	-0.89087300

E= -435.9658005au

Supplementary material for the Physical Chemistry Chemical Physics

CN-2/1

C	-1.88328300	0.17972200	0.01144400
C	-0.40775200	0.14374700	0.05285800
C	0.32180800	1.28804600	-0.14064800
C	-0.41662900	2.50221500	-0.09322400
C	-1.92421900	2.51646100	-0.04863200
C	-2.62714400	1.36083900	0.18119400
H	-2.40254600	-0.74367000	-0.26544000
H	0.08028100	-0.81232000	0.24888400
H	1.40766000	1.29138400	-0.15213100
H	-2.43240200	3.45889200	-0.25663600
H	-3.71280200	1.35154800	0.21614900
C	0.22576200	3.72334800	0.06625600
N	0.75327300	4.76742900	0.17265000

E= -323.6556857au

***m*-CN-N(CH_3)$_2$-2/1**

C	-1.89169900	0.09346900	0.02712400
C	-0.48023500	0.06744100	-0.06472600
C	0.21912700	1.23846600	-0.09801100
C	-0.49179800	2.52761800	-0.01375700
C	-1.94512600	2.52060700	0.09424600
C	-2.62581400	1.32953700	0.10078700
H	0.03581800	-0.88564600	-0.10280500
H	1.29961500	1.21147400	-0.13789200
H	-2.50279800	3.44635400	0.12205800
N	0.17968400	3.66618400	-0.02805900
C	-0.45008300	4.98475900	0.21293500
H	-0.72286100	5.41598000	-0.76019500
H	-1.31740600	4.90866400	0.86055600
H	0.30066600	5.63125300	0.66962300
C	1.62936400	3.77663500	-0.29469800
H	1.77806400	4.66862800	-0.90932000
H	2.13910600	3.94249700	0.66379700
H	2.02835000	2.90904600	-0.80646300
H	-2.44715200	-0.84239600	0.04374500
C	-4.04619900	1.27815800	0.17231900
N	-5.19923700	1.21709500	0.23105300

E= -457.8180881au

***m*-NO_2-N(CH_3)$_2$-2/1**

C	-1.88362900	0.08326900	-0.00911600
C	-0.46461800	0.06628400	-0.07199200
C	0.23370400	1.23861300	-0.06909000
C	-0.47409800	2.52676200	-0.00410800
C	-1.94000000	2.51498000	0.05721000
C	-2.57541700	1.31826000	0.04783100
H	0.05593100	-0.88471800	-0.10143500
H	1.31517400	1.21321800	-0.06265000
H	-2.53384000	3.42106600	0.03396900
N	0.18385600	3.66986500	-0.03138800

C	-0.45120000	4.98655300	0.19934600
H	-0.64557900	5.44692700	-0.77898400
H	-1.36171600	4.90680000	0.78292000
H	0.27475100	5.61162200	0.72434600
C	1.63427500	3.78002900	-0.30076200
H	1.78984400	4.69060500	-0.88438400
H	2.14850500	3.90643000	0.66171200
H	2.01975300	2.92384100	-0.84241200
H	-2.45766300	-0.84145000	0.00050900
N	-4.07695900	1.29280800	0.16807500
O	-4.65700700	2.32136900	-0.08375000
O	-4.52618500	0.22828300	0.54557400

E= -570.1099432au

***m*-Cl-CN-2/1**

C	-1.82792700	0.08120900	0.00004000
C	-0.45215800	0.07606500	0.00049300
C	0.21033800	1.30656000	0.00005600
C	-0.53588500	2.60080000	-0.00094600
C	-1.91682100	2.62079500	-0.00141900
C	-2.58405100	1.38088400	-0.00094700
H	0.10743800	-0.85457600	0.00120800
H	1.29962100	1.34952400	0.00044800
H	-2.47384400	3.55241500	-0.00214400
C	0.23737300	3.77168000	-0.00137900
N	0.91112300	4.72652200	-0.00172500
H	-2.40531800	-0.84196600	0.00038500
Cl	-4.23347400	1.28347900	-0.00147000

E= -783.3008818au

***m*-Cl-NO_2-2/1**

C	-1.80374900	0.09018200	0.11410500
C	-0.43499800	0.12338700	0.07292100
C	0.19296500	1.36511400	-0.18234800
C	-0.60408200	2.59191300	-0.18095800
C	-1.95710800	2.62277500	-0.09499100
C	-2.59396200	1.34404600	0.00416000
H	0.15269200	-0.78841000	0.12036600
H	1.24635100	1.41283000	-0.45526000
H	-2.52934600	3.54648800	-0.08038600
N	0.24167800	3.76718600	0.03611800
O	1.10570800	3.41880800	0.86915900
O	0.08315700	4.83948800	-0.44871600
H	-2.34876600	-0.84758200	0.19574700
Cl	-4.23685600	1.22560500	0.02141200

E= -895.5914535au

Supplementary material for the Physical Chemistry Chemical Physics

p-CN-N$(CH_3)_2$-2/1

C	-1.88491900	0.06771300	0.05277200
C	-0.45492800	0.05871900	-0.07145900
C	0.22647700	1.23287500	-0.11205600
C	-0.48589100	2.51135200	-0.00480900
C	-1.94661500	2.48279900	0.13335300
C	-2.61443200	1.30023200	0.14806700
H	0.06832200	-0.88941200	-0.12597200
H	1.30541100	1.21113400	-0.17811900
H	-2.51058300	3.40415600	0.17846400
H	-3.69565800	1.27373100	0.22525800
N	0.16929600	3.65564300	-0.03171400
C	-0.45909800	4.97197400	0.22297000
H	-0.67978500	5.43886300	-0.74552000
H	-1.35426400	4.88957900	0.82902700
H	0.27779200	5.59194900	0.73700400
C	1.61703600	3.77085300	-0.31972900
H	1.76718200	4.69949600	-0.87364000
H	2.15009700	3.85510700	0.63599300
H	1.98851300	2.93446800	-0.90092700
C	-2.58174200	-1.14946000	0.08122200
N	-3.15991600	-2.15982000	0.10462500

E= -457.8301864au

p-NO_2-N$(CH_3)_2$-2/1

C	-1.86866700	0.10060500	0.04716400
C	-0.44988800	0.05792600	-0.01403500
C	0.23266500	1.23320500	-0.05123200
C	-0.48581400	2.51271400	-0.00758200
C	-1.95181200	2.48835900	0.06635600
C	-2.62137900	1.30509400	0.08236400
H	0.06747500	-0.89583600	-0.02819500
H	1.31341300	1.21182100	-0.07277900
H	-2.51638300	3.41048400	0.06817500
H	-3.70534500	1.27048100	0.11884400
N	0.17055500	3.65716100	-0.03410200
C	-0.46833000	4.97903200	0.15733300
H	-0.64836500	5.41879200	-0.83213000
H	-1.38834000	4.91233600	0.72724600
H	0.24594700	5.61396700	0.68474200
C	1.63004800	3.76592100	-0.25869900
H	1.80634600	4.68271100	-0.82440100
H	2.11994100	3.86951500	0.71810100
H	2.02639400	2.91751800	-0.80523800
N	-2.59436900	-1.16500700	0.07490800
O	-2.70816800	-1.71558500	-0.99655600
O	-2.99238800	-1.50692100	1.16506400

E= -570.1161722au

_p_-Cl-CN-2/1

C	-1.86338300	0.12474700	0.00000400
C	-0.39910900	0.10083100	0.00054000
C	0.27534300	1.27750000	0.00008600
C	-0.47684200	2.52580700	-0.00089300
C	-1.93394800	2.55334300	-0.00142900
C	-2.61595000	1.38105300	-0.00098200
H	0.11403100	-0.85647000	0.00128200
H	1.36070700	1.31104600	0.00044100
H	-2.44743700	3.51014800	-0.00217200
H	-3.70152000	1.34697200	-0.00133800
C	0.21876900	3.73040400	-0.00134200
N	0.80499600	4.74601000	-0.00172000
Cl	-2.68381900	-1.29568400	0.00051500

E= -783.3129935au

_p_-Cl-NO_2-2/1

C	-1.84394600	0.15026800	0.02111200
C	-0.40348200	0.13243000	-0.15173100
C	0.27792700	1.29545500	-0.23386300
C	-0.47478700	2.55083900	-0.10059600
C	-1.93997700	2.57293700	0.01402200
C	-2.59057200	1.39217800	0.09267200
H	0.10769900	-0.82195300	-0.23098400
H	1.35376000	1.33029000	-0.38343100
H	-2.45980300	3.52686200	0.04278700
H	-3.67093900	1.35454800	0.19129600
N	0.26003900	3.73651300	0.36332500
O	0.73024400	4.39282100	1.18819400
O	0.14280800	3.78301000	-0.92597700
Cl	-2.65986200	-1.28205300	0.10489400

E= -895.608089au

Triplet state dications

Benzene-2/3

C	-1.88860000	0.08106400	-0.03788000
C	-0.46330600	0.08104100	0.03847500
C	0.24943700	1.31532000	-0.03798800
C	-0.46318600	2.54976600	0.03689500
C	-1.88848000	2.54978800	-0.03946000
C	-2.60122400	1.31551000	0.03700300
H	-2.43088800	-0.85822200	-0.14629200
H	0.07888300	-0.85816200	0.14809000
H	1.33401900	1.31519500	-0.14648300
H	0.07910200	3.48905200	0.14530700
H	-2.43067000	3.48899200	-0.14907500
H	-3.68580500	1.31563500	0.14549800

E= -231.4136408au

Supplementary material for the Physical Chemistry Chemical Physics

$N(CH_3)_2$-2/3

C	-1.97610700	0.05282200	-0.07219800
C	-0.78028800	0.18323100	-0.77295300
C	-0.02353000	1.41234400	-0.75040700
C	-0.47245300	2.53524200	-0.00238400
C	-1.69398600	2.38294800	0.70938300
C	-2.43235400	1.14342400	0.66297400
H	-2.53759100	-0.87434600	-0.09833900
H	-0.38640600	-0.64566000	-1.35433500
H	0.91027900	1.43773400	-1.29935600
H	-2.11796500	3.19936800	1.28170100
H	-3.36358500	1.08514800	1.21941500
N	0.23676800	3.70681200	0.03055300
C	1.36099500	3.97271200	-0.88078500
H	2.29619300	3.66097300	-0.39624100
H	1.23587000	3.46110700	-1.83212400
H	1.41055800	5.04858400	-1.05197700
C	-0.07227900	4.78768500	0.98035600
H	0.85258700	5.32412500	1.19478900
H	-0.77253100	5.48994400	0.50812300
H	-0.48827100	4.40006700	1.90728600

E= -365.5559087au

$NHCH_3$-2/3

C	-1.89937500	-0.04525500	0.10499100
C	-0.51175100	0.04381000	-0.03138600
C	0.15108900	1.32008700	-0.08689800
C	-0.59528500	2.53454300	-0.00558300
C	-2.01236800	2.42722700	0.13396400
C	-2.64271600	1.13184000	0.18650800
H	-2.38908000	-1.01227500	0.14613900
H	0.09620900	-0.85458200	-0.09842600
H	1.23317500	1.34236300	-0.19203200
H	-2.64188000	3.30703300	0.20396900
H	-3.72360800	1.09474500	0.29235800
N	0.05446800	3.71375700	-0.06133700
C	-0.46922500	5.07449200	-0.00274200
H	-0.14935500	5.60148100	-0.91059700
H	-1.55064200	5.09676800	0.08485300
H	-0.00637400	5.58145600	0.85384000
H	1.07096100	3.66234500	-0.15874500

E= -326.2232899au

NCH_2-2/3

C	-1.88931400	-0.12483600	0.01590100
C	-0.52335900	0.15396600	0.10305300
C	-0.02865500	1.50531400	0.07978500
C	-0.94822500	2.59853400	-0.03545200
C	-2.34779400	2.30273100	-0.12429000
C	-2.79295000	0.93434500	-0.09657500

H	-2.24347800	-1.14985500	0.03530800
H	0.19947000	-0.65303400	0.19102300
H	1.03871900	1.69339100	0.14947900
H	-3.07220000	3.10711800	-0.21231700
H	-3.86069700	0.74321800	-0.16612400
N	-0.51999400	3.83713000	-0.05877900
C	-0.11246200	5.01241200	-0.08249100
H	0.00146100	5.58195300	0.85054000
H	0.13882400	5.49627600	-1.03678400

E= -324.9687666au

NH_2-2/3

C	-0.10160400	-0.48464000	0.01747100
C	1.33230600	-0.49844700	0.09963200
C	2.06630000	0.73588900	0.11699000
C	1.32114700	1.96185000	0.05095200
C	-0.11257200	1.93187000	-0.03023000
C	-0.81471100	0.71961700	-0.04620300
H	-0.62669800	-1.43675700	0.00592700
H	1.85370600	-1.45181400	0.14856200
H	1.83385700	2.92110200	0.06177600
H	-0.64625700	2.87799200	-0.07937300
H	-1.89847000	0.71346500	-0.10745900
N	3.39276900	0.74336000	0.19244900
H	3.93299000	1.61060600	0.20615800
H	3.94068500	-0.11780400	0.24057300

E= -286.8834158au

OCH_3-2/3

C	-0.06835900	-0.49128800	0.05224700
C	1.36205900	-0.42369200	0.12722700
C	2.03016100	0.84716200	0.04767700
C	1.23069700	2.03338800	-0.09023600
C	-0.19909400	1.92029000	-0.16010500
C	-0.83976600	0.67709400	-0.08739200
H	-0.54819600	-1.46590700	0.10521900
H	1.96060900	-1.32453900	0.24381000
H	1.68293700	3.01896100	-0.13540800
H	-0.78261000	2.83103300	-0.27095500
H	-1.92240700	0.61475100	-0.14087100
O	3.31537700	0.79478500	0.11921600
C	4.29376500	1.89861400	0.06225400
H	5.05270300	1.54350000	-0.63701500
H	3.83409500	2.83087500	-0.25335600
H	4.71633500	1.95058700	1.07015800

E= -346.0404749au

Supplementary material for the Physical Chemistry Chemical Physics

OH-2/3

C	-0.07957100	-0.49649100	-0.00495500
C	1.35181400	-0.50667800	0.01728100
C	2.07388500	0.74136400	0.03210800
C	1.33520100	1.97806600	0.02497300
C	-0.09559300	1.94301400	0.00255800
C	-0.79521700	0.72137600	-0.01186900
H	-0.61055300	-1.44646000	-0.01644800
H	1.91254400	-1.44031000	0.02326100
H	1.85432500	2.93551900	0.03642100
H	-0.63935800	2.88554900	-0.00306200
H	-1.88184000	0.71515300	-0.02849300
H	3.88369800	1.47498200	0.06199600
O	3.35772000	0.64572900	0.05134100

E= -306.7036685au

Cl-2/3

C	-1.88655900	0.08468900	0.00002500
C	-0.47787400	0.08792000	0.00051100
C	0.25448400	1.32232100	-0.00000300
C	-0.45307100	2.56713700	-0.00099200
C	-1.88490200	2.55763200	-0.00149500
C	-2.58798500	1.30631600	-0.00091900
H	-2.43005800	-0.85662600	0.00040900
H	0.07593000	-0.84874600	0.00128900
H	1.34281300	1.31208000	0.00035600
H	-2.43790500	3.49509200	-0.00231700
H	-3.67605400	1.31776100	-0.00123200
Cl	0.38084000	4.01113000	-0.00157700

E= -691.0570904au

CHO-2/3

C	-0.09898200	-0.47867400	-0.13184900
C	1.35113300	-0.48146300	-0.14706200
C	2.04331900	0.72417900	-0.01182900
C	1.31929800	1.93523800	0.13840800
C	-0.12074700	1.91395100	0.15038400
C	-0.81409200	0.71563200	0.01613500
H	-0.61714100	-1.42828400	-0.23865300
H	1.86659900	-1.43150700	-0.26470400
H	1.82933400	2.88987500	0.24604000
H	-0.64936900	2.85630000	0.26690500
H	-1.89945700	0.70282900	0.02555500
C	3.50938600	0.70734300	-0.02906200
O	4.24320200	1.67047700	0.07735300
H	4.06257400	-0.25883800	-0.14939700

E= -344.7934689au

NO_2-2/1

C	-1.87788300	0.08184200	-0.02768300
C	-0.48167000	0.08313800	0.05252500
C	0.25178300	1.32174900	0.05772100
C	-0.47569500	2.53302500	0.03447000
C	-1.87193700	2.56404900	-0.05378600
C	-2.57862700	1.30112800	-0.06204700
H	-2.42357500	-0.85732600	-0.05239100
H	0.07464800	-0.84919500	0.11642700
H	1.34040400	1.31490400	0.08736100
H	-2.42479200	3.49992300	-0.10700200
H	-3.66596600	1.31597600	-0.09237700
N	0.26832000	3.79971000	0.08093600
O	1.00447600	4.13399800	0.94118500
O	0.01979400	4.44315100	-0.98389100

E= -435.9580023au

CN-2/3

C	-1.88038100	0.09544100	-0.00002300
C	-0.46963800	0.09525800	0.00049700
C	0.26127600	1.32902900	0.00006200
C	-0.44753200	2.57640800	-0.00090600
C	-1.88220500	2.56684600	-0.00144300
C	-2.58565300	1.31721400	-0.00092400
H	-2.42423100	-0.84636300	0.00030200
H	0.08148200	-0.84320000	0.00124300
H	1.34999500	1.31861700	0.00045700
H	-2.43533900	3.50465200	-0.00225500
H	-3.67393300	1.32560200	-0.00124500
C	0.24947000	3.78354000	-0.00134000
N	0.83869600	4.80459500	-0.00170300

E= -323.6660212au

***m*-CN-N(CH_3)$_2$-2/3**

C	-1.89668200	0.01366400	0.05971900
C	-0.51384600	0.05345500	0.01305000
C	0.18512000	1.28245100	-0.02170800
C	-0.50199900	2.53846400	0.00094800
C	-1.90985800	2.51069200	0.05272000
C	-2.60577200	1.23919300	0.07863200
H	0.05638400	-0.86968400	0.00787700
H	1.26780400	1.25043300	-0.04015300
H	-2.50646200	3.41430800	0.04342100
N	0.18588800	3.72806500	-0.03975900
C	-0.44910500	5.02381500	0.23999200
H	-0.73152100	5.49547200	-0.71095300
H	-1.31480200	4.91872900	0.88825400
H	0.29013300	5.66326300	0.72577900
C	1.61825000	3.78312600	-0.36896500
H	1.84069300	4.77415300	-0.76331500
H	2.20481600	3.64000200	0.54930200
H	1.88290100	3.02754400	-1.10662600

H	-2.43560300	-0.92710400	0.08495400
C	-4.00321400	1.25946500	0.12511400
N	-5.17373900	1.28631900	0.16403600

E= -457.8040656au

***m*-NO_2-$N(CH_3)_2$-2/3**

C	-1.88744300	0.01413300	0.02415300
C	-0.50021600	0.05718900	-0.03454100
C	0.19307200	1.28473800	-0.06143400
C	-0.49607200	2.53441700	0.00196300
C	-1.91011800	2.50485000	0.07982600
C	-2.55290800	1.24184700	0.10000400
H	0.06807200	-0.86691500	-0.04790900
H	1.27460800	1.25663600	-0.10389200
H	-2.51205800	3.40384600	0.10088700
N	0.18621200	3.72565000	-0.02188100
C	-0.45193200	5.01152500	0.29381800
H	-0.77437100	5.48980000	-0.64075900
H	-1.29295000	4.88816500	0.97112500
H	0.29552300	5.65436900	0.76115300
C	1.61396300	3.79750800	-0.36925700
H	1.81928700	4.79274700	-0.76257700
H	2.21301200	3.65797800	0.54098500
H	1.87779800	3.04935700	-1.11389600
H	-2.43282300	-0.92365900	0.04076600
N	-4.01537700	1.25308300	0.13308000
O	-4.43192800	1.93497000	-0.83238000
O	-4.67547100	0.65918000	0.92218600

E= -570.0942972au

***m*-Cl-CN-2/3**

C	-1.87116200	0.09801400	0.00001600
C	-0.46514300	0.10901800	0.00048900
C	0.25246400	1.31716300	0.00004700
C	-0.44986300	2.55916000	-0.00089900
C	-1.88919200	2.57520100	-0.00139900
C	-2.59524500	1.32861900	-0.00091900
H	0.07432400	-0.83448300	0.00120900
H	1.33939100	1.31308000	0.00041800
H	-2.43155500	3.51836900	-0.00213300
C	0.23816400	3.77408900	-0.00136400
N	0.81406500	4.79958500	-0.00175800
H	-2.41428100	-0.84405100	0.00036200
Cl	-4.26555400	1.33962800	-0.00146600

E= -783.306822au

Supplementary material for the Physical Chemistry Chemical Physics

_m_-Cl-NO_2-2/3

C	-1.87418400	0.09323400	-0.02602500
C	-0.47844800	0.09236700	-0.05658700
C	0.24412700	1.29954400	-0.03997300
C	-0.47696000	2.51186000	0.04161000
C	-1.87451300	2.58013500	0.06720400
C	-2.58613700	1.33006600	0.04109900
H	0.06057700	-0.85010400	-0.08555200
H	1.33118100	1.30032700	-0.06837700
H	-2.40964300	3.52475700	0.11727600
N	0.26788800	3.77606500	0.05886500
O	1.13929100	4.04975000	0.80875000
O	-0.14482000	4.49507500	-0.90060600
H	-2.42939600	-0.84045100	-0.05108100
Cl	-4.25527900	1.34920500	0.08472400

E= -895.599272au

_p_-CN-$N(CH_3)_2$-2/3

C	-1.94609900	0.03415900	0.05058900
C	-0.52807200	0.03965800	-0.02156500
C	0.21766200	1.28205600	-0.05012500
C	-0.45821900	2.51158700	-0.02101000
C	-1.89805900	2.47359900	0.05125400
C	-2.61325400	1.26642200	0.07824400
H	0.02054900	-0.89827000	-0.06195300
H	1.29853500	1.21338500	-0.05974300
H	-2.46745500	3.39506100	0.06554100
H	-3.69748000	1.29698700	0.11195500
N	0.22258600	3.70462200	-0.02972300
C	-0.45023500	4.97243500	0.28771500
H	-0.95939300	5.34828000	-0.61147600
H	-1.17060100	4.84193900	1.09540000
H	0.30476900	5.69996100	0.58156800
C	1.65095000	3.80962900	-0.35714400
H	1.79483500	4.72297100	-0.93945400
H	2.22280600	3.91194600	0.57501700
H	2.00186900	2.95890400	-0.93349200
C	-2.62903700	-1.20375100	0.07612700
N	-3.17436000	-2.22962900	0.09708200

E= -457.7912147au

_p_-NO_2-$N(CH_3)_2$-2/3

C	-1.85904200	0.10638500	0.04853500
C	-0.45296400	0.07175400	-0.04562600
C	0.22438300	1.26755100	-0.08261200
C	-0.48979200	2.51008200	-0.00732800
C	-1.92097500	2.49398800	0.09704600
C	-2.60422900	1.30104200	0.11532000
H	0.08664100	-0.86875000	-0.08212100
H	1.30410900	1.24857100	-0.12942100
H	-2.48770400	3.41403500	0.12204000

H	-3.68752100	1.28720200	0.17297200
N	0.18552600	3.69315500	-0.03569200
C	-0.44850500	4.98055600	0.28790700
H	-0.79161900	5.45024500	-0.64407100
H	-1.27553800	4.85916400	0.98117000
H	0.31033000	5.62735900	0.73044200
C	1.61016900	3.78629900	-0.39261600
H	1.78159400	4.76386500	-0.84441800
H	2.21038300	3.72661100	0.52556600
H	1.90011100	3.00482200	-1.08923800
N	-2.55629600	-1.11672300	0.07640600
O	-2.03132100	-2.24586500	0.02108300
O	-3.79420500	-1.23705300	0.16000500

E= -570.0913479au

***p*-Cl-CN-2/3**

C	-1.89034000	0.07813200	0.00000600
C	-0.46615000	0.09146500	0.00052000
C	0.24738700	1.33108500	0.00005100
C	-0.45060000	2.57106000	-0.00090500
C	-1.87345700	2.55584400	-0.00141600
C	-2.59062700	1.31831800	-0.00093100
H	0.08978700	-0.84405600	0.00128000
H	1.33566400	1.31563500	0.00043000
H	-2.43073400	3.49075000	-0.00219200
H	-3.67874600	1.33221700	-0.00128000
C	0.25115800	3.78648100	-0.00135900
N	0.83519000	4.79869100	-0.00173400
Cl	-2.72669300	-1.36991400	0.00052200

E= -783.2989066au

***p*-Cl-NO_2-2/3**

C	-1.87185200	0.10987500	-0.00082500
C	-0.43211800	0.08698200	0.04775500
C	0.25297800	1.28136200	0.04785500
C	-0.50958100	2.46970800	-0.00024700
C	-1.91987100	2.53594000	-0.04877900
C	-2.61156700	1.34533300	-0.04908500
H	0.09308700	-0.86191100	0.08332700
H	1.33864800	1.29962400	0.08339700
H	-2.44702200	3.48521100	-0.08456900
H	-3.69588500	1.32559000	-0.08478300
N	0.21108800	3.71718300	-0.00032100
O	1.44416000	3.81696600	0.04141500
O	-0.31761100	4.83548300	-0.04234300
Cl	-2.70534600	-1.33320000	-0.00107800

E= -895.5911048au