Supporting Information for:

Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions

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Table S1: MGAE109/05 Database of Zero-Point-Exclusive Atomization Energies (kcal/mol)

Molecule	D_e	Molecule	D_e	Molecule	D_e
CH ($^2\Pi$)	84.00	S_2	101.67	H_2CCH	445.79
CH_2 ($^3B_1$)	190.72	Cl_2	57.98	$HCOOCH_3$	785.26
CH_2 ($^1A_1$)	181.37	SiO	192.08	HCOOH	500.98
CH_3 ($^2A''_2$)	307.44	SC	171.11	NF_3	204.53
CH_4	420.11	SO	125.22	PF_3	363.87
NH	83.67	ClO	64.49	SH	86.98
NH_2	181.90	ClF	61.48	$SiCl_4$	384.94
NH_3	297.90	Si_2H_6	534.66	SiF_4	574.35
OH	107.09	CH_3Cl	395.51	C_2H_5	603.75
OH_2	232.60	CH_3SH	473.84	C_4H_6 *d*	987.20
FH	141.18	HOCl	164.81	C_4H_6 *e*	1001.61
SiH_2 ($^1A_1$)	151.79	SO_2	258.62	HCOCOH	633.35
SiH_2 ($^3B_1$)	131.05	$AlCl_3$	306.26	CH_3CHO	677.03
SiH_3	227.58	AlF_3	426.50	C_2H_4O	650.70
SiH_4	322.40	BCl_3	322.90	C_2H_5O	698.64
PH_2	153.20	BF_3	470.04	H_3COCH_3	798.05
PH_3	241.56	C_2Cl_4	466.28	H_3CCH_2OH	810.36
SH_2	182.60	C_2F_4	589.36	C_3H_4 *f*	703.20
ClH	106.48	C_3H_4 *a*	704.79	C_3H_4 *g*	682.74
HCCH	405.36	C_4H_4O	993.74	H_3CCOOH	803.04
H_2CCH_2	563.51	C_4H_4S	962.73	H_3CCOCH_3	977.96
H_3CCH_3	712.80	C_4H_5N	1071.57	C_3H_6	853.41
CN	180.58	C_4H_6 *b*	1012.37	H_3CCHCH_2	860.61
HCN	313.05	C_4H_6 *c*	1004.13	C_3H_8	1006.87
CO	259.27	C_5H_5N	1237.69	$C_2H_5OCH_3$	1095.12
HCO	278.39	CCH	265.13	C_4H_{10} *h*	1303.04
H_2CO	373.82	CCl_4	312.74	C_4H_{10} *i*	1301.32
H_3COH	513.22	CF_3CN	639.85	C_4H_8 *j*	1149.01

N_2	228.42	CF_4	476.32	C_4H_8 [k]	1158.61
H_2NNH_2	438.60	CH_2OH	409.76	C_5H_8 [l]	1284.28
NO	152.05	CH_3CN	615.84	C_6H_6	1367.56
O_2	120.22	CH_3NH_2	582.56	CH_3CO	581.58
HOOH	268.57	CH_3NO_2	601.27	$(CH_3)_2CH$	900.75
F_2	38.20	$CHCl_3$	343.18	$(CH_3)_3C$	1199.34
CO_2	389.14	CHF_3	457.50	H_2CCO	532.32
Si_2	75.72	ClF_3	125.33		
P_2	117.09	H_2	109.48		

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[a] propyne

[b] *trans*-1,3-butadiene

[c] 2-butyne

[d] bicylobutane

[e] cyclobutene

[f] allene

[g] cyclopropene

[h] isobutane

[i] antiperiplanar butane

[j] cyclobutane

[k] isobutene

[l] spiropentane

Table S2: HTBH38/04 Database (kcal/mol)

Reaction	best estimate	
A + BC → AB + C	$V_f^{\neq}$	$V_r^{\neq}$
1. H + HCl → H_2 + Cl	5.7	8.7
2. OH + H_2 → H + H_2O	5.7	21.2
3. CH_3 + H_2 → H + CH_4	12.1	15.3
4. OH + CH_4 → CH_3 + H_2O	6.7	19.6
5. H + H_2 → H_2 + H	9.6	9.6
6. OH + NH_3 → H_2O + NH_2	3.2	12.7
7. HCl + CH_3 → Cl + CH_4	1.7	7.9
8. OH + C_2H_6 →H_2O + C_2H_5	3.4	19.9
9. F + H_2 → HF + H	1.8	33.4
10. O + CH_4 →OH + CH_3	13.7	8.1
11. H + PH_3→ PH_2 + H_2	3.1	23.2
12. H + HO → H_2 +O	10.7	13.1
13. H + H_2S → H_2 + HS	3.5	17.3
14. O + HCl → OH + Cl	9.8	10.4
15. NH_2 + CH_3→ CH_4 + NH	8.0	22.4
16. NH_2 + C_2H_5 → C_2H_6 + NH	7.5	18.3
17. C_2H_6 + NH_2 → NH_3 + C_2H_5	10.4	17.4
18. NH_2 + CH_4 → CH_3 + NH_3	14.5	17.8
19. *s-trans cis*-C_5H_8 → *s-trans cis*-C_5H_8	38.4	38.4

Table S3: Zero-Point-Exclusive Ionization Potentials (IP13/3) and Electron Affinities (EA13/3) Databases (kcal/mol)

	IP	EA
C	259.7	29.1
S	238.9	47.9
SH	238.9	53.3
Cl	299.1	83.4
Cl_2	265.3	55.6
OH	299.1	42.1
O	313.9	33.7
O_2	278.9	10.8
P	241.9	17.2
PH	234.1	23.2
PH_2	226.3	29.4
S_2	216.0	38.5
Si	187.9	31.9

Table S4: TMAE4/05 and MLBE4/05 Databases and Spin-Orbit Energies (ΔE_{SO}) (kcal/mol)

TMAE4/05			MLBE4/05		
Molecule	D_e	ΔE_{SO} [a]	Molecule	D_e	ΔE_{SO} [c]
Cr_2	36.0	0.0	$CrCH_3^+$	28.8	0.0
Cu_2	47.2	0.0	$NiCH_2^+$	76.3	-1.72
Zr_2	70.8	-3.3	$Fe(CO)_5$	148.7	-1.52
V_2	64.2	-1.83	VS	106.9	-1.47

[a] D_e does not include the spin-orbit energies.
[b] $\Delta E_{SO} = E_{SO}(A) + E_{SO}(B) - E_{SO}(AB)$, where $E_{SO}(A)$ and $E_{SO}(B)$ are the spin-orbit energies of atoms A and B and $E_{SO}(AB)$ is the spin orbit energy of the diatomic molecules AB.
[c] $\Delta E_{SO} \equiv nE_{SO}(L) + E_{SO}(M) - E_{SO}(ML_n)$, where n is the number of ligands, $E_{SO}(L)$ is the spin–orbit energy of the ligand, $E_{SO}(M)$ is the spin–orbit energy of the metal atom/ion, and $E_{SO}(ML_n)$ is the spin–orbit energy of the metal–ligand complex.

Table S5: Kinetics9 database (kcal/mol)[a]

Reaction	Best Estimates		
	$V_f^{\neq}$	$V_r^{\neq}$	ΔE
$OH + CH_4 \rightarrow CH_3 + H_2O$	6.7	19.6	–12.9
$H + OH \rightarrow O + H_2$	10.7	13.1	–2.4
$H + H_2S \rightarrow H_2 + HS$	3.5	17.3	–13.7

[a] from Lynch, B. J.; Truhlar, D. G. *J. Phys. Chem. A* **2003**, *107*, 8996; **2004**; *108*; 1460 (E).

Table S6: Noncovalent Databases (kcal/mol)

HB6/04		CT7/04		DI6/04		WI7/05		PPS5/05	
Complex	D_e	Complex	D_e	Complex	D_e	Complex	D_e	Complex	D_e
$(NH_3)_2$	3.15	$C_2H_4\cdots F_2$	1.06	$(H_2S)_2$	1.66	HeNe	0.04	$(C_2H_2)_2$	1.34
$(HF)_2$	4.57	$NH_3\cdots F_2$	1.81	$(HCl)_2$	2.01	HeAr	0.06	$(C_2H_4)_2$	1.42
$(H_2O)_2$	4.97	$C_2H_2\cdots ClF$	3.81	$HCl\cdots H_2S$	3.35	Ne_2	0.08	Sandwich $(C_6H_6)_2$	1.81
$NH_3\cdots H_2O$	6.41	$HCN\cdots ClF$	4.86	$CH_3Cl\cdots HCl$	3.55	NeAr	0.13	T-Shaped $(C_6H_6)_2$	2.74
$(HCONH_2)_2$	14.94	$NH_3\cdots Cl_2$	4.88	$HCN\cdots CH_3SH$	3.59	$CH_4\cdots Ne$	0.22	Parallel-Displaced $(C_6H_6)_2$	2.78
$(HCOOH)_2$	16.15	$H_2O\cdots ClF$	5.36	$CH_3SH\cdots HCl$	4.16	$C_6H_6\cdots Ne$	0.47		
		$NH_3\cdots ClF$	10.62			$(CH_4)_2$	0.51		
Average	8.37		4.63		3.07		0.22		0.22

Table S7: Bond Dissociation Energies (D_e, kcal/mol) for R-CH_3 and R-OCH_3 [a]

Method [b]	R-CH_3				R-OCH_3				MSE	MUE
	R=Me	R=Et	R=*i*-Pr	R=*t*-Bu	R=Me	R=Et	R=*i*-Pr	R=*t*-Bu		
Experiment	90.1	89.0	88.5	87.0	83.4	85.1	86.1	84.3		
M05-2X	90.1	88.5	87.5	87.0	84.2	85.6	85.5	84.6	-0.1	0.5
G3-RAD [c]	89.6	88.9	88.4	87.8	84.1	86.8	87.4	87.0	0.8	1.0
BMK [c]	90.7	88.7	86.9	84.6	82.4	83.5	82.6	80.7	-1.7	1.8
MPW1B95 [c]	91.6	88.8	86.3	83.4	82.4	82.8	81.2	78.7	-2.3	2.7
MPWB1K [c]	91.2	88.7	86.5	83.9	81.7	82.4	81.1	78.8	-2.4	2.7
M05	87.2	83.8	80.5	77.3	79.9	79.7	77.3	73.5	-6.8	6.8
B3LYP [c]	84.3	81.4	78.5	75.2	76.2	76.5	74.6	71.4	-9.4	9.4
TPSSh	83.2	80.4	77.6	75.0	75.7	76.0	74.2	71.1	-10.1	10.1
BLYP [c]	83.0	79.5	76.1	72.3	74.7	74.5	72.1	68.3	-11.6	11.6
Average										5.2

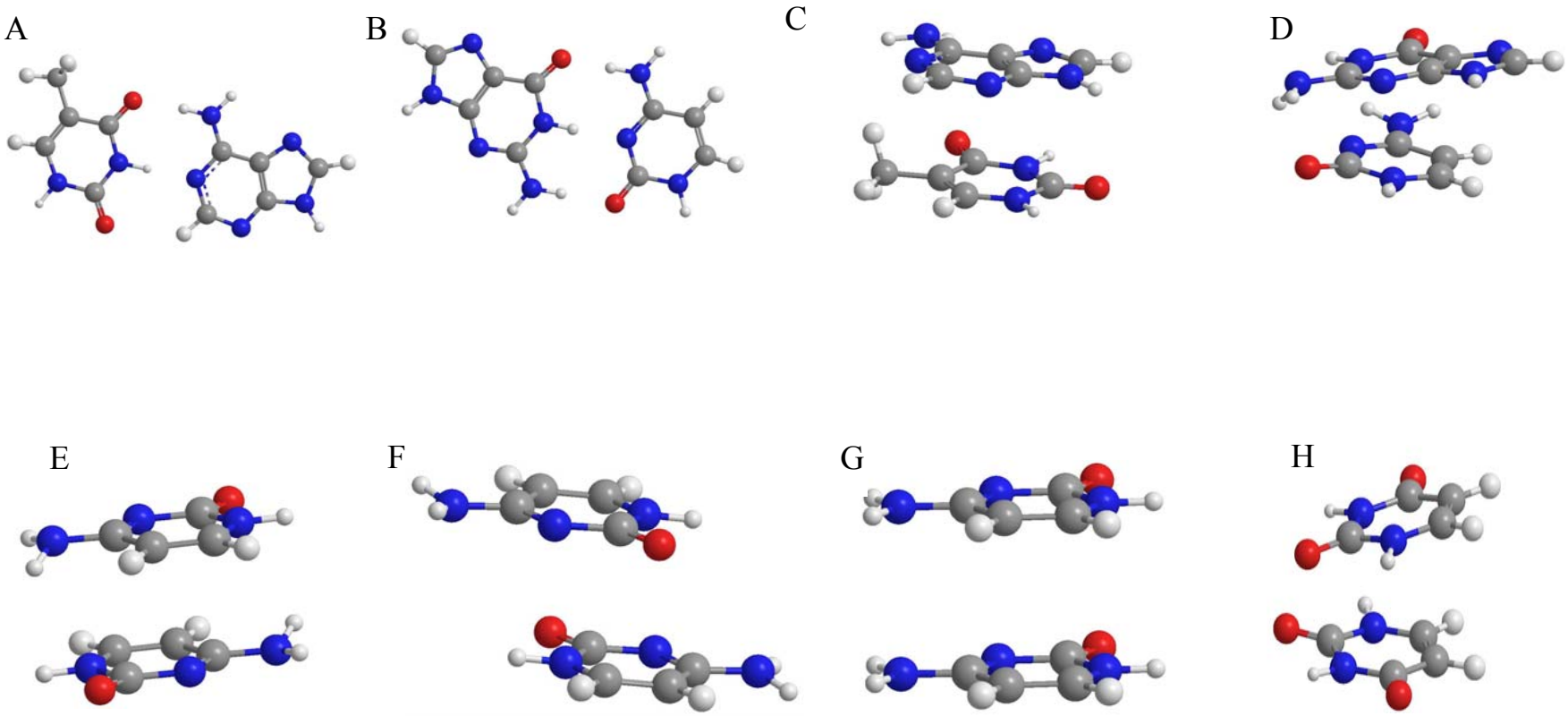
[a] The B3LYP/6-31G(d) geometries are used in the calculations in this table. Zero point energies were removed from the experimental data by using harmonic frequencies calculated with the B3LYP/6-31G(d) method with a scale factor of 0.9806. This scale factor was determined in a paper by Scott and Radom.[1]

[b] All DFT calculations in this table use the 6-311+G(3df,2p) basis set.

[c] Data for these methods are taken from a paper by Izgorodina et al.[2] Zero point energy was removed as in footnote a.

(1) Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502.
(2) Izgorodina, E. I.; Coote, M. L.; Radom, L. *J. Phys. Chem. A* **2005**, *109*, 7558.

Figure S-1: Structures of the nucleobase pairs. (A) A···T WC, (B) G···C WC, (C) A···T stacking, (D) G···C stacking, (E) C···C antiparallel, (F) C···C displaced, (G) C···C parallel, (H) U···U stacking.



Geometries (Å) for the nucleobase pairs

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#METHOD scf=tight IOps

A

0 1

N	-1.92524600	0.51912600	0.00038900
C	-1.21564400	-0.60374000	-0.00057200
C	0.17938900	-0.51355400	-0.00053000
C	0.70171600	0.76540000	-0.00018400
N	0.01932900	1.90243100	-0.00001200
C	-1.28125000	1.68201400	0.00036200
N	1.17021600	-1.45913900	0.00004600
C	2.26317100	-0.76519300	0.00030300
N	2.05070500	0.58137000	0.00032800
N	-1.85479100	-1.77973200	-0.00396300
H	-1.91096700	2.55748700	0.00090600
H	3.25444700	-1.17673000	0.00084600
H	2.74164600	1.30385400	-0.00108500
H	-2.85231300	-1.78920300	0.01274900
H	-1.33859500	-2.63335300	0.01279600

****

#METHOD scf=tight IOps

C geometry

0 1

C	1.17233400	-0.52022500	0.00012800
N	1.26892900	0.87981700	0.00210700
C	0.20187500	1.69339600	-0.00012300
C	-1.04036900	1.17683600	-0.00138900
C	-1.12037500	-0.25132600	0.00000500
N	-0.08041300	-1.03897200	0.00100900
O	2.19640100	-1.16243400	-0.00161200
N	-2.33053200	-0.83385300	-0.00047900
H	2.20339300	1.23980700	0.00106500
H	0.39724700	2.75192100	-0.00051100
H	-1.91273100	1.80262900	-0.00346300
H	-3.17381400	-0.30385500	0.00306400

H	-2.37198400	-1.83206600	0.00256200

****

#METHOD scf=tight IOps

G

0 1

O	-0.20447000	2.65696600	-0.00318800
C	-0.21802300	1.45140800	0.00284100
N	-1.45983600	0.77712300	-0.00402500
C	-1.65187400	-0.56527000	-0.00283500
N	-0.68481300	-1.42717700	0.00626700
C	0.52779000	-0.84078900	-0.00064900
C	0.84706500	0.49951800	0.00782300
N	2.20124200	0.67919300	0.00800200
C	2.68697400	-0.51718900	0.00100400
N	1.71818800	-1.48285800	-0.00419500
N	-2.93851400	-0.99860900	-0.05914900
H	-2.24783100	1.39478900	-0.07205600
H	3.73050900	-0.76636100	-0.00094400
H	1.84580600	-2.47438700	-0.01085200
H	-3.04290900	-1.98211600	0.09210700
H	-3.65527800	-0.42741900	0.33985000

****

#METHOD scf=tight IOps

T

0 1

N	-1.11294200	-1.22801900	-0.00048000
C	0.23353200	-1.46841900	-0.00009700
C	1.14396100	-0.48848500	-0.00023800
C	0.66139400	0.88537000	-0.00106500
N	-0.71797100	1.02041700	-0.00075800
C	-1.65843400	0.02703700	-0.00068900
C	2.61375800	-0.70583700	0.00051300
O	1.37202800	1.86258000	0.00061500
O	-2.84733000	0.22971000	0.00118300

H	-1.77305000	-1.97962900	0.00089500
H	0.51218200	-2.50829300	0.00043900
H	-1.07507300	1.95898400	0.00035100
H	3.06940600	-0.24559600	-0.87078900
H	3.06872400	-0.24465300	0.87167300
H	2.85135500	-1.76391400	0.00117900

****

#METHOD scf=tight IOps

U

0 1

O	-2.28857200	-0.99706000	-0.00074100
C	-1.27340400	-0.34525300	0.00006300
N	-0.03443300	-0.97674100	0.00075400
C	1.20423500	-0.39883500	-0.00007700
N	1.16521200	0.97448000	-0.00128900
C	0.00646300	1.69144600	0.00012800
C	-1.19224800	1.10068900	0.00080300
O	2.23629900	-1.02037400	0.00028500
H	-0.04487400	-1.98090600	-0.00014400
H	2.05825000	1.42544100	0.00064700
H	0.12518400	2.76067100	0.00017100
H	-2.10610700	1.66181600	0.00121700

****

#METHOD scf=tight IOps

A...T Stacking

0 1

N	-2.00016100	0.79470600	1.22794900
C	-0.95473000	1.66989400	1.33741500
C	-0.22191400	2.05613100	0.28618000
C	-0.55000900	1.48737900	-1.01078500
N	-1.65354200	0.64916700	-1.02115900
C	-2.37745200	0.21409800	0.05135400
C	0.91186400	3.01288100	0.36096500
O	0.06255300	1.70092900	-2.03264300

O	-3.26396700	-0.60633700	-0.02738800
H	-2.48736400	0.47559500	2.04132500
H	-0.76082200	2.02801600	2.33352500
H	-1.85362400	0.20008100	-1.89726300
H	1.83996300	2.53215400	0.06905100
H	0.75186800	3.84594100	-0.31662000
H	1.02916300	3.39733100	1.36796500
N	2.49171800	-0.09572300	0.89753800
C	2.09138200	-0.42662100	-0.32666800
C	0.97929400	-1.26583400	-0.46001700
C	0.35733600	-1.64113800	0.71794000
N	0.72117500	-1.30360700	1.94939200
C	1.80088700	-0.54448800	1.93989900
N	0.33022700	-1.77848800	-1.55077600
C	-0.65703000	-2.44595000	-1.04138700
N	-0.69330000	-2.40727600	0.31960800
N	2.76397300	0.03807400	-1.38871800
H	2.17366800	-0.23932500	2.90531900
H	-1.39631100	-2.98416700	-1.60333500
H	-1.40693900	-2.79077900	0.90643600
H	3.43105500	0.76345900	-1.22053800
H	2.29224300	0.03888400	-2.27182000

****

#METHOD scf=tight IOps

G...C stacking

0 1

C	-1.84020300	1.09432700	0.77482800
N	-1.06392800	0.38088500	1.68266700
C	-1.05740300	-0.96567700	1.74058100
C	-1.84137600	-1.67662200	0.91469300
C	-2.62222700	-0.92330900	-0.01323600
N	-2.63105400	0.38670400	-0.05519700
O	-1.72168800	2.30917500	0.74737700
N	-3.41164600	-1.57364400	-0.88197700
H	-0.45250100	0.93147100	2.25456800
H	-0.39447500	-1.41742700	2.45738400
H	-1.83612000	-2.74969600	0.91711800
H	-3.20271500	-2.52657900	-1.09687200
H	-3.78658700	-1.01913200	-1.62599900
O	-0.30384100	-1.13603900	-1.94807400

C	0.46944000	-0.46650900	-1.30113400
N	0.32096000	0.92896600	-1.26050000
C	1.07317500	1.80710300	-0.54871800
N	2.10019000	1.44716700	0.16528600
C	2.31381800	0.12148700	0.13142900
C	1.58741600	-0.86176300	-0.50522500
N	2.11342000	-2.09885000	-0.25441600
C	3.13226400	-1.86998700	0.50632700
N	3.30365800	-0.54032600	0.77783600
N	0.72815000	3.11471800	-0.65046800
H	-0.46500600	1.27605100	-1.78304800
H	3.79503000	-2.61543100	0.90195600
H	4.02949800	-0.11676800	1.31968000
H	1.26986300	3.69031100	-0.03438300
H	-0.26042400	3.28847100	-0.56471300

****

#METHOD scf=tight IOps

C...C antiparallel stacking

0 1

C	0.75510800	-1.01600600	-1.54663100
N	-0.50372900	-1.58201600	-1.75077000
C	-1.63336500	-0.85752000	-1.85134000
C	-1.57583000	0.48261600	-1.81114600
C	-0.27561400	1.04464100	-1.64776500
N	0.81849000	0.33690000	-1.52805300
O	1.69971200	-1.76235100	-1.37744300
N	-0.15325000	2.38615700	-1.62220100
H	-0.52088600	-2.58232700	-1.77885200
H	-2.55332400	-1.40478600	-1.95838700
H	-2.45822700	1.09087800	-1.85781800
H	-0.94665900	2.93510800	-1.36067000
H	0.75097300	2.74099400	-1.38490300
C	-0.75510800	1.01600600	1.54663100
N	0.50372900	1.58201600	1.75077000
C	1.63336500	0.85752000	1.85134000
C	1.57583000	-0.48261600	1.81114600
C	0.27561400	-1.04464100	1.64776500
N	-0.81849000	-0.33690000	1.52805300
O	-1.69971200	1.76235100	1.37744300
N	0.15325000	-2.38615700	1.62220100

H	0.52088600	2.58232700	1.77885200
H	2.55332400	1.40478600	1.95838700
H	2.45822700	-1.09087800	1.85781800
H	0.94665900	-2.93510800	1.36067000
H	-0.75097300	-2.74099400	1.38490300

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#METHOD scf=tight IOps

C...C displaced stacking

0 1

C	-0.85376800	-1.68068900	-0.80480900
N	-0.82815900	-1.43714400	0.57191300
C	0.28886600	-1.50185200	1.31461600
C	1.45920600	-1.83812500	0.74162300
C	1.41948500	-2.05727200	-0.66626200
N	0.33352600	-1.97412500	-1.38969700
O	-1.91292200	-1.59288600	-1.38772300
N	2.56801500	-2.32120800	-1.31995300
H	-1.70786000	-1.18560000	0.97997200
H	0.19683700	-1.24761100	2.35625500
H	2.37376000	-1.85565400	1.30284200
H	3.39702900	-2.55467300	-0.81703600
H	2.49469600	-2.60023400	-2.27718700
C	0.85376800	1.68068900	0.80480900
N	0.82815900	1.43714400	-0.57191300
C	-0.28886600	1.50185200	-1.31461600
C	-1.45920600	1.83812500	-0.74162300
C	-1.41948500	2.05727200	0.66626200
N	-0.33352600	1.97412500	1.38969700
O	1.91292200	1.59288600	1.38772300
N	-2.56801500	2.32120800	1.31995300
H	1.70786000	1.18560000	-0.97997200
H	-0.19683700	1.24761100	-2.35625500
H	-2.37376000	1.85565400	-1.30284200
H	-3.39702900	2.55467300	0.81703600
H	-2.49469600	2.60023400	2.27718700

****

#METHOD scf=tight IOps

C...C parallel stacking

0 1

C	0.918196	-0.921509	0.000000
N	-0.369369	-1.514131	0.000000
C	-1.525251	-0.808201	0.000000
C	-1.485860	0.556831	0.000000
C	-0.172365	1.145560	0.000000
N	0.952696	0.454027	0.000000
O	1.902046	-1.650842	0.000000
N	-0.059643	2.501884	0.000000
H	-0.369376	-2.530931	0.000000
H	-2.453346	-1.381336	0.000000
H	-2.397789	1.150603	0.000000
H	-0.868459	3.105290	0.000000
H	0.869663	2.904066	0.000000
C	0.918196	-0.921509	3.400000
N	-0.369369	-1.514131	3.400000
C	-1.525251	-0.808201	3.400000
C	-1.485860	0.556831	3.400000
C	-0.172365	1.145560	3.400000
N	0.952696	0.454027	3.400000
O	1.902046	-1.650842	3.400000
N	-0.059643	2.501884	3.400000
H	-0.369376	-2.530931	3.400000
H	-2.453346	-1.381336	3.400000
H	-2.397789	1.150603	3.400000
H	-0.868459	3.105290	3.400000
H	0.869663	2.904066	3.400000

****

#METHOD scf=tight IOps

C...C (MP2/6-31G**) face to face stacking for vertical separation profile

0 1

C	0.918196	-0.921509	0.000000
N	-0.369369	-1.514131	0.000000
C	-1.525251	-0.808201	0.000000
C	-1.485860	0.556831	0.000000
C	-0.172365	1.145560	0.000000

N	0.952696	0.454027	0.000000
O	1.902046	-1.650842	0.000000
N	-0.059643	2.501884	0.000000
H	-0.369376	-2.530931	0.000000
H	-2.453346	-1.381336	0.000000
H	-2.397789	1.150603	0.000000
H	-0.868459	3.105290	0.000000
H	0.869663	2.904066	0.000000
C	-0.918196	-0.921509	3.300000
N	0.369369	-1.514131	3.300000
C	1.525251	-0.808201	3.300000
C	1.485860	0.556831	3.300000
C	0.172365	1.145560	3.300000
N	-0.952696	0.454027	3.300000
O	-1.902046	-1.650842	3.300000
N	0.059643	2.501884	3.300000
H	0.369376	-2.530931	3.300000
H	2.453346	-1.381336	3.300000
H	2.397789	1.150603	3.300000
H	0.868459	3.105290	3.300000
H	-0.869663	2.904066	3.300000

****

#METHOD scf=tight IOps

U...U Stacking

0 1

O	2.37179300	0.24679400	-1.90357700
C	2.05879700	0.15364200	-0.74247100
N	2.05401000	1.23141400	0.10781100
C	1.57449100	1.17446700	1.37837800
C	1.13252400	0.03140100	1.91583100
C	1.12674400	-1.17428200	1.11754600
N	1.66238500	-1.01412300	-0.15292100
O	0.69067200	-2.24797000	1.46633600
H	2.27443300	2.11048500	-0.31841900
H	1.57092500	2.10786000	1.91273400
H	0.75358100	-0.01734600	2.91785100
H	1.58247800	-1.80138800	-0.77463500
O	-1.01620300	2.61848800	-0.27981700
C	-1.42747100	1.48351600	-0.19143800
N	-1.00321900	0.51512400	-1.09258200

C	-1.30217000	-0.82153100	-1.08737000
N	-2.16129900	-1.18656900	-0.08382900
C	-2.64570900	-0.31335800	0.83902100
C	-2.34098400	0.98937000	0.81348600
O	-0.84643600	-1.60940500	-1.87730700
H	-0.37039200	0.81119400	-1.81793700
H	-2.31211900	-2.17262200	0.00551400
H	-3.29114600	-0.74195800	1.58524000
H	-2.72682800	1.68023600	1.53731800

****

Geometries (Å) for the DM6/05 database. (We are grateful to Benoit Champagne for supplying the MP2/6-31G(d) geometry for N6.)

****

```
%mem=1000mb
#METHOD/gen  scf=tight
IOPS

BF

0 1
     5          0       0.000000    0.000000   -0.819386
     9          0       0.000000    0.000000    0.455214
```

****

```
%mem=1000mb
#METHOD/gen  scf=tight
IOPS

CuH

0 1
    29          0       0.000000    0.000000    0.000
     1          0       0.000000    0.000000   -1.509
```

****

```
#METHOD/gen  scf=tight
IOPS

H2O

0 1
0  1
     8          0       0.000000    0.000000    0.678243
     6          0       0.000000   -0.000000   -0.533274
     1          0      -0.000000    0.938317   -1.113147
     1          0      -0.000000   -0.938317   -1.113147
```

****

```
%mem=1000mb
#METHOD/gen  scf=tight
IOPS

N6

0 1
 c     -.534222        .000000      -.044695
 c      .621847        .000000       .691997
 h     -.481694        .000000     -1.136271
 h      .562309        .000000      1.786220
 c     1.939959        .000000       .081135
 c     3.131291        .000000       .766199
 h     1.974846        .000000     -1.016781
 h     3.112165        .000000      1.862994
 c     4.432734        .000000       .123147
 c     5.636091        .000000       .788568
 h     4.443607        .000000      -.974826
 h     5.633927        .000000      1.885678
 c     6.926970        .000000       .125441
 c     8.137891        .000000       .775522
 h     6.921942        .000000      -.972188
 h     8.151412        .000000      1.872324
 c     9.419271        .000000       .091721
 c    10.636738        .000000       .723484
 h     9.397699        .000000     -1.005193
 h    10.671786        .000000      1.818771
 c    11.901090        .000000       .000859
 c    13.110031        .000000       .610063
 h    11.872793        .000000     -1.092104
 h    13.293226        .000000      1.681867
 n    14.356328        .000000      -.164772
 o    14.309782        .000000     -1.448157
 o    15.447921        .000000       .519097
 n    -1.826636        .000000       .464180
 h    -1.995112        .000000      1.459502
 h    -2.627604        .000000      -.145700

**********************************************************
```

```
%mem=1000mb
#METHOD/gen  scf=tight
IOPS

H2O

0 1
     8          0       0.000000    0.000000    0.118196
     1          0      -0.000000    0.758055   -0.472784
     1          0      -0.000000   -0.758055   -0.472784

**********************************************************


%mem=1000mb
#METHOD/gen  scf=tight
IOPS

LiCl

0 1
     3          0       0.000000    0.000000   -1.740928
    17          0       0.000000    0.000000    0.307223

**********************************************************
```

Geometries (Å) for the ABDE4/05 database

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

c2h6

0,1
C,-0.7652714924,0.,0.
C,0.7652714924,0.,0.
H,1.1643473724,1.0209355355,0.0000019949
H,1.1643473724,-0.5104694954,0.8841551119
H,1.1643473724,-0.5104660401,-0.8841571069
H,-1.1643473724,-1.0209355355,-0.0000019949
H,-1.1643473724,0.5104660401,0.8841571069
H,-1.1643473724,0.5104694954,-0.8841551119

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

c2h6o

0,1
O
C,1,B1
C,1,B1,2,A1
H,2,B2,1,A2,3,-180.,0
H,3,B2,1,A2,2,-180.,0
H,2,B3,1,A3,4,D1,0
H,3,B3,1,A3,5,-D1,0
H,2,B3,1,A3,4,-D1,0
H,3,B3,1,A3,5,D1,0

```
B1=1.40986
B2=1.09336
B3=1.1029
A1=112.3117
A2=107.2509
A3=111.8183
D1=-119.2954

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

c4h10

0,1
C
H,1,B1
C,1,B2,2,A1
C,1,B2,2,A1,3,120.,0
C,1,B2,2,A1,3,-120.,0
H,3,B3,1,A2,2,180.,0
H,4,B3,1,A2,2,180.,0
H,5,B3,1,A2,2,-180.,0
H,3,B4,1,A3,6,D1,0
H,3,B4,1,A3,6,-D1,0
H,4,B4,1,A3,7,D1,0
H,4,B4,1,A3,7,-D1,0
H,5,B4,1,A3,8,D1,0
H,5,B4,1,A3,8,-D1,0

B1=1.10055806
B2=1.53533785
B3=1.09809054
B4=1.09665434
A1=107.76891525
A2=110.85328092
A3=111.37203544
D1=119.7978593

EXTBASIS
```

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

PrOCH3-c1-6dub3

0,1
O,0.2581838741,0.937874606,0.0407424579
C,1.6365622261,1.0422982793,0.3233044075
H,1.8990698734,2.1004086002,0.2355469898
H,2.2623399434,0.4702401473,-0.3784687165
C,-0.2958120265,-0.3650962082,0.2296077208
H,0.0737268667,-0.770233074,1.1884225371
C,0.0999562654,-1.3221886514,-0.8997878285
C,-1.8070752191,-0.1766021952,0.3188323899
H,-2.3094122994,-1.1343594496,0.4933835016
H,-2.0591701944,0.5065049853,1.1358104054
H,-2.1901489088,0.2507080646,-0.6147505549
H,-0.3461659892,-2.3107435182,-0.7410685375
H,-0.2515839876,-0.9340770207,-1.8625311037
H,1.1853093402,-1.4555173912,-0.960633128
H,1.868776887,0.7036044613,1.346608805

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

ch3

0,2
C,0.,0.,0.
H,0.,-1.082752,0.
H,-0.937690738,0.541376,0.
H,0.937690738,0.541376,0.

```
EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

ch3o

0,2
O,-0.0717954037,0.7904851464,0.
C,0.070527331,-0.5706524031,0.
H,-0.9643070065,-0.9734523539,0.
H,0.557753125,-0.9632571993,0.9088020881
H,0.557753125,-0.9632571993,-0.9088020881

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

iPr

0,2
H,-1.5741282257,0.3384466025,0.
C,-0.4949973207,0.2014373026,0.
C,0.1885698354,-0.059540887,-1.3011394423
C,0.1885698354,-0.059540887,1.3011394423
H,-0.3378996345,0.4075090427,-2.1413392395
H,-0.3378996345,0.4075090427,2.1413392395
H,1.2217611291,0.3159557584,-1.2963791248
H,1.2217611291,0.3159557584,1.2963791248
H,0.256775568,-1.1397546885,-1.5289592366
H,0.256775568,-1.1397546885,1.5289592366

EXTBASIS

************************************************************
```

Geometries (Å) for the noncovalent interaction database

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

Ar

0 1
Ar

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

C2H2-C2H2

0 1

6	0	-0.412546	1.678175	-0.000000
6	0	0.412546	2.561627	-0.000000
1	0	-1.132026	0.890809	-0.000000
1	0	1.134651	3.345770	-0.000000
6	0	0.412546	-1.678175	-0.000000
6	0	-0.412546	-2.561627	-0.000000
1	0	1.132026	-0.890809	-0.000000
1	0	-1.134651	-3.345770	-0.000000

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

C2H2-ClF

0 1
1 0 0.000000 1.671891 -2.212555
6 0 -0.000000 0.605293 -2.199559
6 0 -0.000000 -0.605293 -2.199559
1 0 -0.000000 -1.671891 -2.212555
17 0 0.000000 -0.000000 0.611880
9 0 0.000000 -0.000000 2.268651

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

C2H2

0 1
6 0 0.000004 -0.604204 0.000000
6 0 0.000004 0.604198 0.000000
1 0 0.006795 -1.670128 0.000000
1 0 -0.006839 1.670163 -0.000000

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

C2H2-C2H2

0 1
6 0 1.857768 0.472803 0.472425
6 0 1.857768 -0.472803 -0.472425
1 0 0.933772 0.874688 0.874063
1 0 2.783818 0.871709 0.871556

```
    1          0       2.783818   -0.871709   -0.871556
    1          0       0.933772   -0.874688   -0.874063
    6          0      -1.857768    0.472803   -0.472425
    6          0      -1.857768   -0.472803    0.472425
    1          0      -2.783818    0.871709   -0.871556
    1          0      -0.933772    0.874688   -0.874063
    1          0      -0.933772   -0.874688    0.874063
    1          0      -2.783818   -0.871709    0.871556

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

C2H4-F2

0  1
    6          0       0.000000   -2.192850   -0.668395
    6          0      -0.000000   -2.192860    0.668395
    1          0      -0.925187   -2.192316   -1.233982
    1          0       0.925187   -2.192325   -1.233983
    1          0      -0.925187   -2.192320    1.233982
    1          0       0.925187   -2.192311    1.233982
    9          0       0.000000    0.785688    0.000000
    9          0       0.000000    2.205648    0.000001

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

C2H4

0  1
    6          0      -0.000000    0.000000    0.668078
    6          0       0.000000    0.000000   -0.668078
```

```
     1          0      -0.000000    0.924533    1.234919
     1          0      -0.000000   -0.924533    1.234919
     1          0       0.000000    0.924533   -1.234919
     1          0      -0.000000   -0.924533   -1.234919

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

benzene

0  1
     6          0       0.000000    1.395671   -0.617158
     6          0      -1.208686    0.697835   -0.617158
     6          0      -1.208686   -0.697835   -0.617158
     6          0      -0.000000   -1.395671   -0.617158
     6          0       1.208686   -0.697835   -0.617158
     6          0       1.208686    0.697835   -0.617158
     1          0       0.000000    2.479876   -0.616998
     1          0      -2.147636    1.239938   -0.616998
     1          0      -2.147636   -1.239938   -0.616998
     1          0      -0.000000   -2.479876   -0.616998
     1          0       2.147636   -1.239938   -0.616998
     1          0       2.147636    1.239938   -0.616998

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

benzene

0  1
    10          0       0.000000    0.000000    2.600194
     6          0       0.000000    1.395663   -0.619351
```

```
 6          0      -1.208680    0.697831   -0.619351
 6          0      -1.208680   -0.697831   -0.619351
 6          0      -0.000000   -1.395663   -0.619351
 6          0       1.208680   -0.697831   -0.619351
 6          0       1.208680    0.697831   -0.619351
 1          0       0.000000    2.480037   -0.617549
 1          0      -2.147775    1.240018   -0.617549
 1          0      -2.147775   -1.240018   -0.617549
 1          0      -0.000000   -2.480037   -0.617549
 1          0       2.147775   -1.240018   -0.617549
 1          0       2.147775    1.240018   -0.617549

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

CH3Cl

0  1
    6         -0.000000   -0.000000   -1.126268
   17          -0.000000   -0.000000    0.658206
    1         -0.000000    1.030970   -1.470596
    1          0.892846   -0.515485   -1.470596
    1         -0.892846   -0.515485   -1.470596

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

CH3Cl-HCl

0   1
    6          0      -1.495128    1.125799   -0.000002
   17          0       -1.402476   -0.662544    0.000139
```

```
     1          0      -0.481069    1.518361   -0.001216
     1          0      -2.027181    1.435163    0.895312
     1          0      -2.029240    1.434923   -0.894172
    17          0       2.139608    0.037298   -0.000138
     1          0       0.977002   -0.514054    0.000072

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

CH3SH

0  1
     6         -0.047882    1.151506    0.000000
    16          -0.047882   -0.664959    0.000000
     1          1.284337   -0.821047    0.000000
     1         -1.094713    1.456621    0.000000
     1          0.431885    1.547369    0.893710
     1          0.431885    1.547369   -0.893710

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

CH3SH-HCl

0   1
     6         -1.447648    1.155649    0.018513
    16          -1.414595   -0.659846   -0.083544
     1         -1.466284    1.516816   -1.009880
     1         -0.552971    1.535265    0.510012
     1         -2.344239    1.497733    0.531863
     1         -1.377361   -0.890921    1.238214
    17          2.125766    0.024081    0.003156
```

```
     1          0.922238   -0.444635   -0.098247

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

CH4-CH4

0  1
     6          0      -0.000000    0.000000    1.807279
     1          0      -0.000000    1.026643    1.442400
     1          0      -0.889099   -0.513322    1.442400
     1          0      -0.000000    0.000000    2.896843
     1          0       0.889099   -0.513322    1.442400
     6          0      -0.000000   -0.000000   -1.807279
     1          0       0.889099    0.513322   -1.442400
     1          0      -0.000000   -0.000000   -2.896843
     1          0      -0.889099    0.513322   -1.442400
     1          0      -0.000000   -1.026643   -1.442400

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

CH4

0  1
C
H,1,RCH
H,1,RCH,2,109.471221
H,1,RCH,2,109.471221,3,109.471221,1
H,1,RCH,2,109.471221,3,109.471221,-1

RCH=1.08947061
```

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

CH4-Ne

0 1

10	0.000705	-0.035049	-1.742602
6	-0.000705	0.035048	1.742577
1	-0.001157	0.057524	2.831863
1	-0.021214	1.054308	1.358368
1	-0.879607	-0.503714	1.390162
1	0.899157	-0.467924	1.390162

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

Cl2

0 1

17	0	0.000000	0.000000	1.005661
17	0	0.000000	0.000000	-1.005661

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

ClF

0 1
9 0 0.000000 0.000000 -1.073995
17 0 0.000000 0.000000 0.568585

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

F2

0 1
9 0.000000 0.000000 1.41423
9 0.000000 0.000000 0.0

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

H2O-ClF

0 1
8 0 2.239819 0.000027 -0.088231
1 0 2.600887 0.761963 0.377055
1 0 2.601087 -0.761727 0.377194
17 0 -0.315868 -0.000066 -0.016914
9 0 -1.972308 0.000074 0.026570

EXTBASIS

****

```
%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

H2O

0  1
 O
 H,1,OH
 H,1,OH,2,HOH
     Variables:
 OH=0.96183119
 HOH=103.92150313

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

H2O-H2O

0   1
     8          0       1.531750    .005922    -.120880
     1          0        .575968   -.005249     .024966
     1          0       1.906249   -.037561     .763218
     8          0      -1.396226   -.004990     .106766
     1          0      -1.789372   -.742283    -.371009
     1          0      -1.777037    .777638    -.304264

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS
```

HCL

0 1
16 0.000000 -0.000000 0.103894
1 -0.000000 0.961162 -0.831153
1 -0.000000 -0.961162 -0.831153

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

H2S-H2S

0 1
16 -2.030996 0.103233 -0.000782
1 -1.934020 -0.818462 0.969676
1 -1.940450 -0.836616 -0.954299
16 2.079838 -0.085112 0.000181
1 2.339154 1.231019 -0.002214
1 0.753848 0.134121 -0.003537

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

H2S-HCl

0 1
16 0 1.842529 0.000013 -0.101543
1 0 1.822779 -0.961810 0.834650
1 0 1.821877 0.961860 0.834622
17 0 -1.911636 -0.000011 0.003498
1 0 -0.627317 -0.000058 -0.104051

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCL

0 1
Cl
H,1,R
Variables:
R=1.27907275

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCl-HCl

0 1
17 1.860824 -0.065411 -0.000068
1 1.753941 1.210981 0.000341
17 -1.925266 0.005571 -0.000097
1 -0.658427 -0.193703 0.002476

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCN-CH3SH

0 1
6 1.996443 0.057185 -0.006483
7 2.980218 0.658345 0.109450
1 1.072341 -0.485189 -0.106416
16 -1.514399 -0.799994 -0.116979
6 -1.570144 1.012974 0.011607
1 -1.554579 -1.052600 1.200492
1 -1.545560 1.392381 -1.010196
1 -0.708661 1.402553 0.553097
1 -2.493145 1.339923 0.486654

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCN-ClF

0 1
9 0 -0.000000 0.000000 2.425920
17 0 -0.000000 0.000000 0.769574
7 0 0.000000 0.000000 -1.839519
6 0 0.000000 0.000000 -2.995731
1 0 0.000000 0.000000 -4.065026

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCN

0 1
6 0 -0.000000 -0.000000 -0.501032

```
    7          0      -0.000000   -0.000000    0.657069
    1          0      -0.000000   -0.000000   -1.570053

EXTBASIS

****************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCONH2

0  1
     6          0       -.160685    .388399   -.000538
     8          0      -1.195705   -.246392    .000189
     7          0       1.083300   -.158419   -.000291
     1          0       -.139918   1.490350    .001393
     1          0       1.182258  -1.160415    .001116
     1          0       1.904316    .419735    .001245

EXTBASIS

****************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCONH2-HCONH2

0   1
     8         -1.141087   1.445212    .000000
     6          -.061754   2.030947    .000000
     1          -.013687   3.130169    .000000
     7          1.141087   1.435877    .000000
     1          1.217686    .416527    .000000
     1          1.971446   2.002095    .000000
     8          1.141087  -1.445212    .000000
     6           .061754  -2.030947    .000000
     1           .013687  -3.130169    .000000
     7         -1.141087  -1.435877    .000000
```

```
     1         -1.217686    -.416527     .000000
     1         -1.971446   -2.002095     .000000

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCOOH

0  1
     6          0       -.134702     .401251    -.000249
     8          0      -1.134262    -.264582     .000069
     8          0       1.118680    -.091075     .000056
     1          0       -.107617    1.495465     .000513
     1          0       1.040484   -1.057714    -.000020

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HCOOH-HCOOH

0   1
     6          -.120234    1.914070     .000000
     1          -.167295    3.007018     .000000
     8         -1.121857    1.220982     .000000
     8          1.121857    1.480489     .000000
     1          1.127582     .489024     .000000
     8          1.121857   -1.220982     .000000
     6           .120234   -1.914070     .000000
     8         -1.121857   -1.480489     .000000
     1         -1.127582    -.489024     .000000
     1           .167295   -3.007018     .000000
```

```
EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HeAr

0  1
He
Ar, 1, MRe

MRe=3.480

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

He

0  1
He

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HeNe

0  1
```

```
He
Ne, 1, MRe

MRe=3.031

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HF

0  1
 F
 H,1,B1
     Variables:
 B1=0.92073754

EXTBASIS

************************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

HF-HF

0   1
     9          0       1.323736    -.090226    -.000007
     1          0       1.740437     .733390     .000013
     9          0      -1.457195     .019257    -.000011
     1          0       -.539310    -.094664     .000145

EXTBASIS

************************************************************
```

```
%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NeNe

0  1
Ne
Ne, 1, MRe

MRe=3.091

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NeAr

0  1
Ne
Ar, 1, MRe

MRe=3.489

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

Ne

0  1
Ne
```

```
EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NH3-Cl2

0  1
     7          0       0.000000    0.000000   -2.838451
     1          0       0.000000    0.942687   -3.215383
     1          0       0.816391   -0.471343   -3.215383
     1          0      -0.816391   -0.471343   -3.215383
    17          0       0.000000    0.000000   -0.150044
    17          0       0.000000    0.000000    1.886239

EXTBASIS

**********************************************************


%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NH3-ClF

0  1
     7          0       0.000000    0.000000   -2.057899
     1          0       0.000000    0.949605   -2.414488
     1          0       0.822382   -0.474803   -2.414488
     1          0      -0.822382   -0.474803   -2.414488
    17          0       0.000000    0.000000    0.243855
     9          0       0.000000    0.000000    1.944803

EXTBASIS

**********************************************************


%mem=1500mb
```

#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NH3-F2

0 1
7 0 0.000000 0.000000 -2.149985
1 0 0.000000 0.939652 -2.534401
1 0 0.813762 -0.469826 -2.534401
1 0 -0.813762 -0.469826 -2.534401
9 0 0.000000 0.000000 0.545771
9 0 0.000000 0.000000 1.971240

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NH3

0 1
7 0 0.000000 0.000000 0.115013
1 0 0.000000 0.939752 -0.268364
1 0 0.813850 -0.469876 -0.268364
1 0 -0.813850 -0.469876 -0.268364

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NH3-H2O

0 1
7 0 -1.395591 -0.021564 0.000037
1 0 -1.629811 0.961096 -0.106224

1	0	-1.862767	-0.512544	-0.755974
1	0	-1.833547	-0.330770	0.862307
8	0	1.568501	0.105892	0.000005
1	0	0.606736	-0.033962	-0.000628
1	0	1.940519	-0.780005	0.000222

EXTBASIS

****

%mem=1500mb
#METHOD
scf=(xqc,maxcycle=400,tight)
IOPS

NH3-NH3

0 1

7	0	1.575225	0.000085	-0.042607
1	0	2.131108	0.813949	-0.286614
1	0	1.496450	-0.002936	0.970257
1	0	2.131721	-0.811892	-0.291453
7	0	-1.688245	0.000083	0.104848
1	0	-2.126403	-0.812680	-0.317310
1	0	-2.127442	0.811842	-0.318158
1	0	-0.714297	0.000543	-0.192407

EXTBASIS

****