Neutral Transition Metal Hydrides as Acids in Hydrogen Bonding and Proton Transfer: Media Polarity and Specific Solvation Effects

Vladislava A. Levina,[a] Oleg A. Filippov,[a] Evgenii I. Gutsul,[a] Natalia V. Belkova,[a] Lina M. Epstein,[a] Agusti Lledos,[b] Elena S. Shubina[a*]*

[a]*A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Vavilov Street 28, 119991 Moscow, Russia*

[b]*Departament de Química, Universitat Autonoma de Barcelona, 08193 Bellaterra, Spain*

Supporting Information

Table S1. Position of ν_{CO} bands of $CpM(CO)_3H$ in hexane at different temperatures

	1a		1b	
T (K)	ν^{s}_{CO}, cm^{-1}	ν^{as}_{CO}, cm^{-1}	ν^{s}_{CO}, cm^{-1}	ν^{as}_{CO}, cm^{-1}
290	2030	1946	2027	1939
190	2030	1944	2026	1936

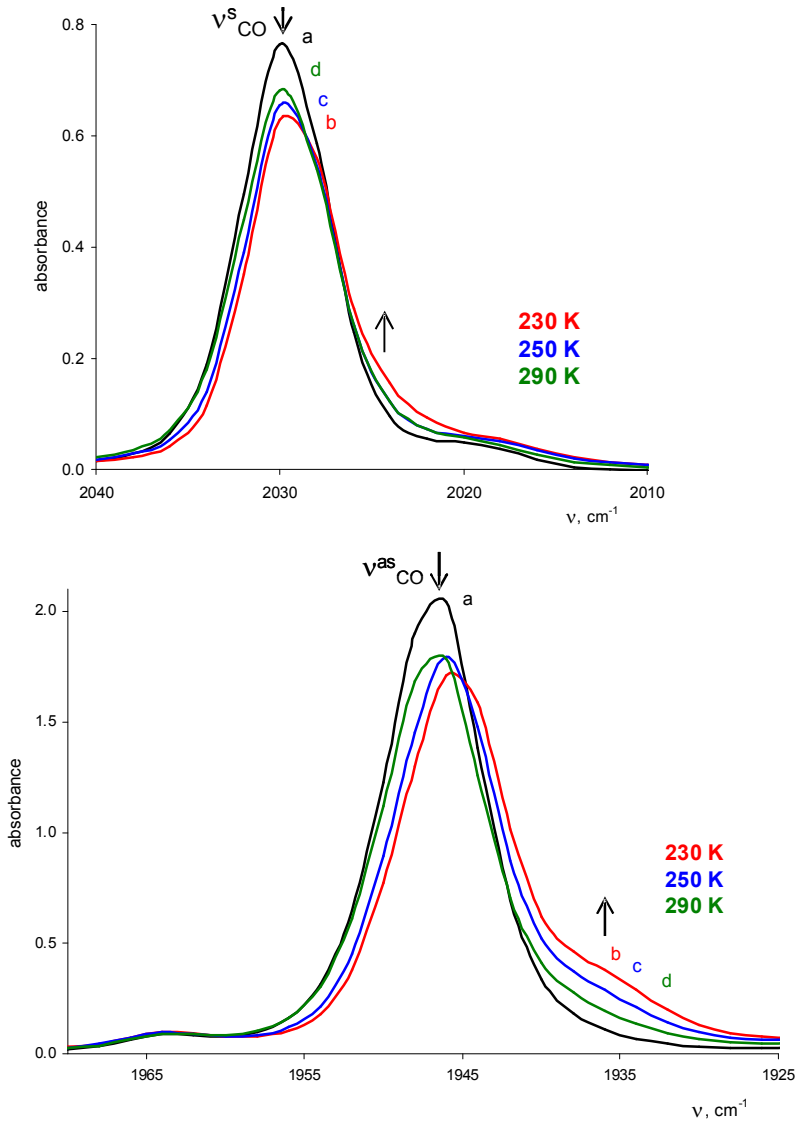


Figure S1. IR spectra (ν_{CO} range) of $CpMoH(CO)_3$ (0.001 M) in hexane at 290K – a, and with excess of HMPA (1:10) at different temperatures: 230 (b, red), 250 (c, blue), 290 K (d, green). l = 0.12 cm. Arrows indicate the band growth or decrease upon cooling.

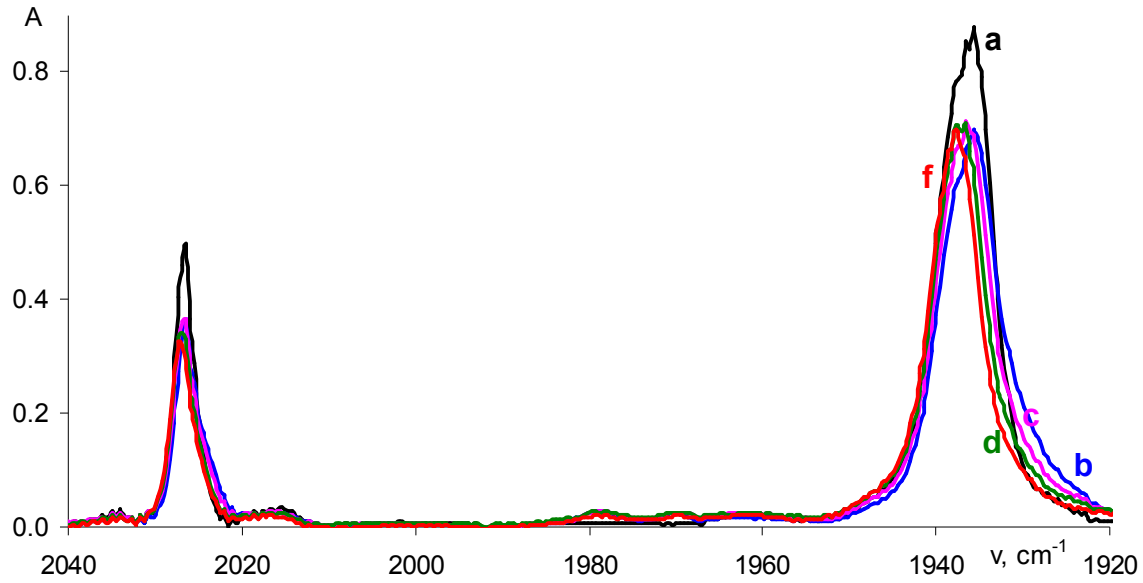


Figure S2. IR spectra in the range ν_{CO} of $CpW(CO)_3H$ (0.00075 M) in hexane – a, and with excess of Py (1:50) at the different temperatures: 190 K (b), 210 K (c), 230 K (d), 250 K (f). l = 0.12 cm.

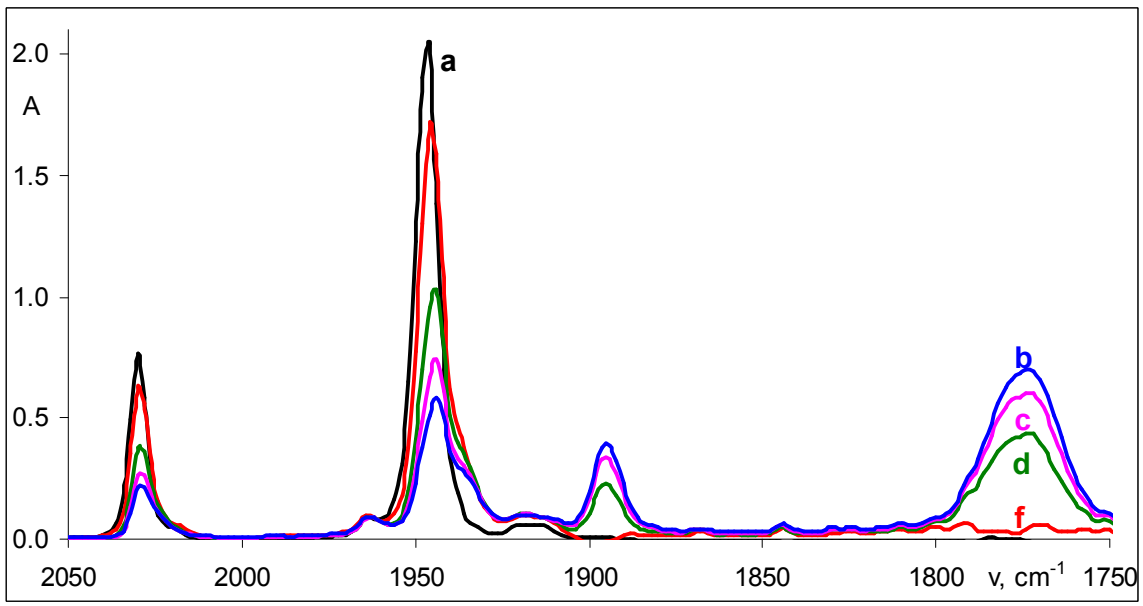


Figure S3. IR spectra (ν_{CO} range) of $CpMoH(CO)_3$ (0.001 M) in hexane – a, and with excess of HMPA (1:10) at different temperatures: 190 K (b), 200 K (c), 210 K (d), 230 K (f). l = 0.12 cm.

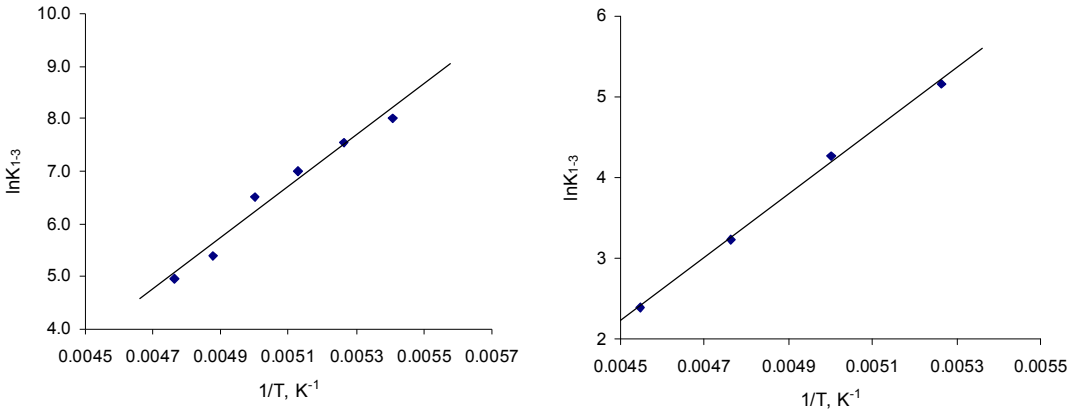


Figure S4. Van't Hoff plots for equilibrium constants of proton transfer, $K_{1\text{-}3}$, from $CpMoH(CO)_3$ (0.0005 M, left) or $CpWH(CO)_3$ (0.001 M, right) to HMPA (10 and 50 equiv., respectively).

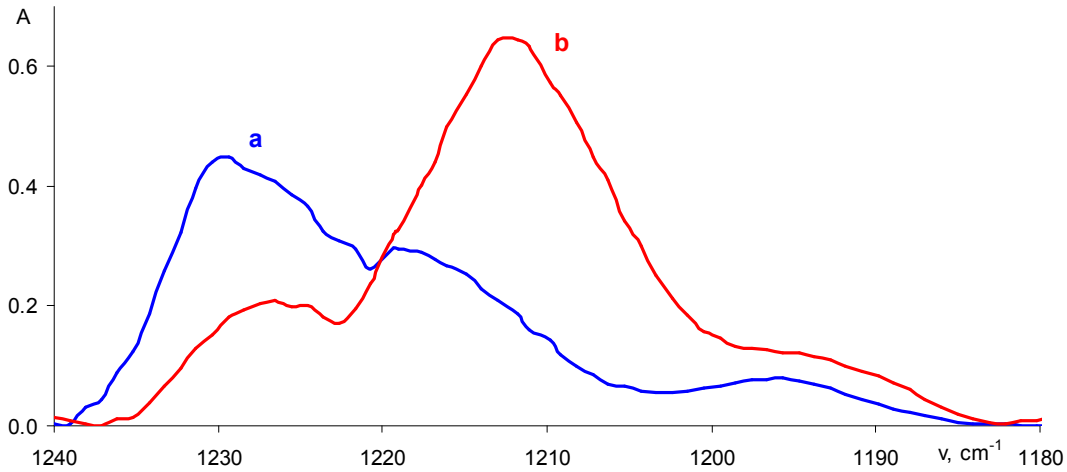


Figure S5. IR spectra in the range ν_{PO} of HMPA (0.01 M) in hexane – a, and with excess of DCM (1:5) at 190 K - b. l = 0.12 cm.

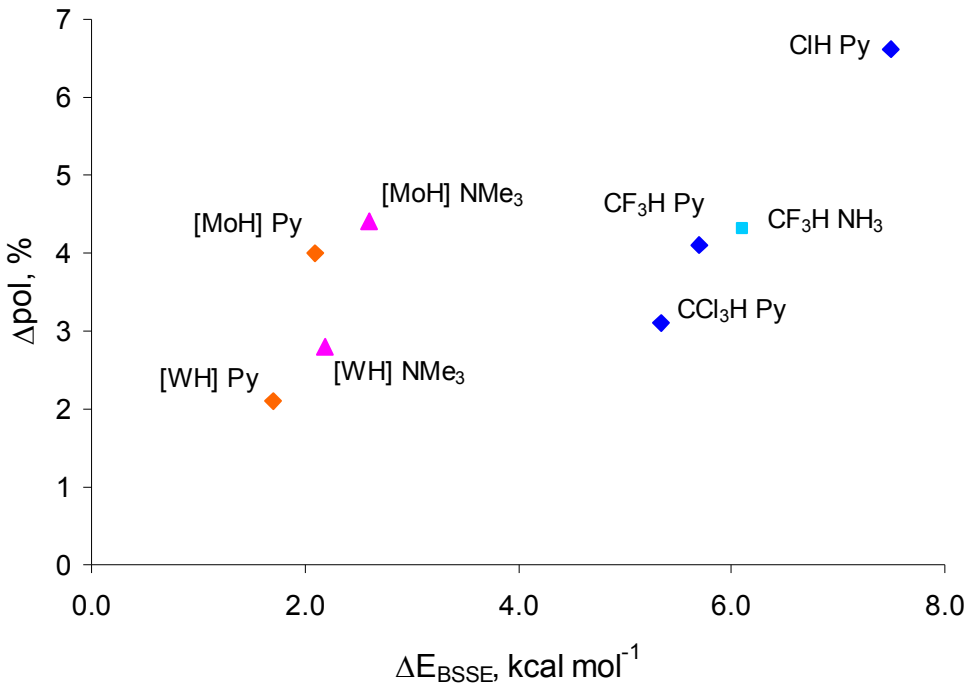


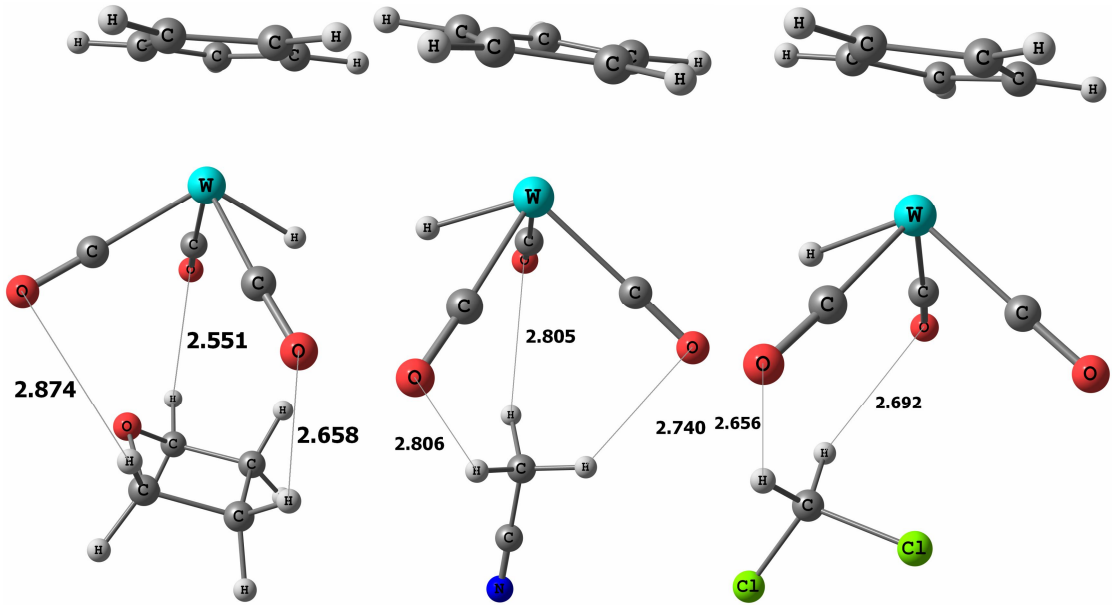
Figure S6. Dependence of the X-H (X = C, Mo, W) bond polarization change (Δpol, in % on H) on the hydrogen bond formation energy (ΔE_{BSSE}) for hydrides **1** or halomethanes (CF_3H,[56] CCl_3H[58]) interacting with nitrogen bases.

Complete Reference 30:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian, Inc.: Wallingford CT, 2004.

Table S2. AIM parameters of the hydrogen bonded complexes between hydrides **1** and bases

		H···X	CH···OC	CH···OC	CH···OC	CH···OC
1a/Py	r(H···X),[d] Å	2.476	2.668	2.691		
	ρ_c	0.013	0.006	0.006		
	$\nabla^2\rho_c$	-0.007	-0.006	-0.005		
	V(r)	-0.007	-0.004	-0.004		
	ε	0.010	0.090	0.102		
	E_{cont}, kcal·mol^{-1}	-2.1	-1.2	-1.1		
1b/Py	r(H···X),[d] Å	2.506	2.722	2.733		
	ρ_c	0.012	0.005	0.005		
	$\nabla^2\rho_c$	-0.007	-0.005	-0.005		
	V(r)	-0.007	-0.003	-0.003		
	ε	0.016	0.129	0.139		
	E_{cont}, kcal·mol^{-1}	-2.1	-1.0	-1.0		
1a/Me_3PO	r(H···X),[d] Å	2.139	2.662	2.756	2.794	
	ρ_c	0.020	0.006	0.005	0.005	
	$\nabla^2\rho_c$	-0.013	-0.005	-0.005	-0.005	
	V(r)	-0.012	-0.004	-0.003	-0.003	
	ε	0.072	0.096	0.108	0.036	
	E_{cont}, kcal·mol^{-1}	-3.8	-1.1	-0.9	-0.9	
1b/Me_3PO	r(H···X),[d] Å	2.156	2.651	2.739	2.787	
	ρ_c	0.019	0.006	0.005	0.005	
	$\nabla^2\rho_c$	-0.013	-0.005	-0.005	-0.005	
	V(r)	-0.012	-0.004	-0.003	-0.003	
	ε	0.067	0.083	0.118	0.103	
	E_{cont}, kcal·mol^{-1}	-3.7	-1.2	-1.0	-0.9	
1a/Me_3N	r(H···X),[d] Å	2.329	2.905	2.886	2.773	2.772
	ρ_c	0.018	0.004	0.004	0.005	0.005
	$\nabla^2\rho_c$	-0.009	-0.004	-0.004	-0.005	-0.005
	V(r)	-0.009	-0.002	-0.002	-0.003	-0.003
	ε	0.032	0.029	0.059	0.053	0.061
	E_{cont}, kcal·mol^{-1}	-2.9	-0.7	-0.7	-0.9	-0.9
1b/Me_3N	r(H···X),[d] Å	2.431	2.793	2.793	2.788	2.789
	ρ_c	0.015	0.005	0.005	0.005	0.005
	$\nabla^2\rho_c$	-0.008	-0.004	-0.004	-0.005	-0.005
	V(r)	-0.008	-0.003	-0.003	-0.003	-0.003
	ε	0.026	0.025	0.026	0.071	0.072
	E_{cont}, kcal·mol^{-1}	-2.5	-0.9	-0.9	-0.9	-0.9



ΔE_{BSSE}= -1.5 -2.3 -2.1 kcal·mol^{-1}

Figure S7. Calculated geometry and energy of complexes between $CpW(CO)_3H$ and (a) - THF, (b) – AN, (c) – DCM.

Table S3. XYZ coordinates of all optimized geometries

a. free reactants

1a E=-601.338784141

6	2.032927000	-1.150357000	-0.151039000
6	2.187918000	0.000620000	-0.969958000
6	2.032983000	1.150605000	-0.149648000
6	1.778712000	0.714421000	1.179344000
6	1.778682000	-0.715768000	1.178494000
1	2.102235000	-2.177703000	-0.483201000
1	2.388876000	0.001257000	-2.032829000
1	2.102290000	2.178350000	-0.480573000
1	1.641600000	1.351882000	2.042422000
1	1.641585000	-1.354256000	2.040812000
42	-0.032066000	0.000073000	-0.118099000
1	-0.553200000	0.000429000	-1.749735000
6	-1.406481000	-0.000253000	1.336054000
6	-1.118270000	-1.547583000	-0.716858000
6	-1.118255000	1.547978000	-0.716366000
8	-2.203142000	-0.000564000	2.178489000
8	-1.710020000	-2.465602000	-1.109402000
8	-1.710079000	2.466038000	-1.108697000

1b E=-601.616781417

6	-1.611351000	-2.306083000	1.157976000
6	-2.248268000	-1.725874000	0.027334000
6	-1.660237000	-2.275224000	-1.144844000
6	-0.656865000	-3.203296000	-0.742741000
6	-0.626501000	-3.221781000	0.689104000
1	-1.840290000	-2.090890000	2.193042000
1	-3.034066000	-0.983272000	0.054030000
1	-1.934300000	-2.033932000	-2.163009000
1	-0.050459000	-3.808941000	-1.402205000
1	0.008206000	-3.842940000	1.306181000
74	0.037044000	-1.115622000	-0.016297000
1	-0.556119000	0.503789000	-0.000862000
6	1.990724000	-1.481045000	-0.045459000
6	0.604082000	-0.027758000	1.535903000
6	0.560991000	-0.015436000	-1.574409000
8	3.131463000	-1.703445000	-0.062771000
8	0.876122000	0.611775000	2.467579000
8	0.807737000	0.631188000	-2.508261000

Me_3N E=-174.336762836

7	0.000001000	-0.000069000	-0.362354000
6	0.001227000	1.382705000	0.059535000
1	0.885382000	1.891082000	-0.335458000
1	-0.882040000	1.892641000	-0.335431000
1	0.001352000	1.505957000	1.159147000
6	1.196821000	-0.692360000	0.059522000
1	2.080122000	-0.183096000	-0.336285000

1	1.194630000	-1.712626000	-0.334493000
1	1.304293000	-0.753274000	1.159154000
6	-1.198049000	-0.690235000	0.059522000
1	-1.305646000	-0.750922000	1.159153000
1	-1.197647000	-1.710515000	-0.334459000
1	-2.080442000	-0.179427000	-0.336321000

Me_3PO E=-536.219820266

1	5.037795000	-1.433584000	2.563570000
6	4.189270000	-1.355715000	1.879959000
1	4.005083000	-2.331022000	1.425149000
1	3.299160000	-1.071882000	2.444954000
1	5.720192000	1.271766000	2.144434000
6	4.886599000	1.405901000	1.451228000
1	4.009506000	1.743295000	2.007035000
1	5.145500000	2.179151000	0.725232000
15	4.472879000	-0.129709000	0.562446000
6	6.040561000	-0.645002000	-0.209652000
1	6.850819000	-0.735981000	0.517403000
1	5.894328000	-1.606779000	-0.705266000
1	6.321057000	0.087911000	-0.968741000
8	3.335146000	0.008155000	-0.399284000

Py E=-248.099298033

7	-0.483513000	3.006598000	-0.013883000
1	-0.483507000	3.130570000	2.042628000
6	-0.396815000	3.703660000	1.120403000
6	-0.206709000	5.083738000	1.173595000
1	-0.144474000	5.593594000	2.129429000
6	-0.100518000	5.780617000	-0.026285000
1	0.048056000	6.856394000	-0.031128000
1	-0.111444000	5.569689000	-2.180247000
6	-0.188394000	5.070505000	-1.219846000
6	-0.379410000	3.691045000	-1.154301000
1	-0.452035000	3.107794000	-2.071399000

THF E=-232.294350559

8	0.000098000	-1.239175000	-0.000420000
6	1.154360000	-0.429246000	0.131662000
6	-1.154423000	-0.429364000	-0.131133000
6	-0.727965000	0.988930000	0.226434000
6	0.727987000	0.988811000	-0.226646000
1	-1.940442000	-0.819399000	0.524873000
1	-1.526564000	-0.478498000	-1.165633000
1	1.941136000	-0.819376000	-0.523345000
1	1.525344000	-0.478060000	1.166626000
1	-0.788289000	1.145381000	1.308027000
1	-1.338922000	1.751891000	-0.260506000
1	0.788235000	1.144580000	-1.308343000
1	1.338967000	1.752093000	0.259763000

DCM E=-959.667173911

6	0.000000000	0.000000000	0.755518000
1	-0.897954000	0.000000000	1.369163000
1	0.897954000	0.000000000	1.369163000
17	0.000000000	1.482189000	-0.213866000
17	0.000000000	-1.482189000	-0.213866000

AN E=-132.661393062

1	-1.554876000	1.024050000	-0.037063000
6	-1.178480000	-0.000021000	-0.000006000
1	-1.554806000	-0.479982000	0.905390000
1	-1.554765000	-0.544157000	-0.868362000
6	0.275619000	0.000071000	0.000024000
7	1.440231000	-0.000030000	-0.000010000

b. Hydrogen bonded complexes of 1 with bases

1a/Me_3N E=-775.684334429

6	-1.800340000	-1.767189000	-1.143667000
6	-1.149796000	-2.266278000	0.017695000
6	-1.826177000	-1.750602000	1.155599000
6	-2.892926000	-0.928642000	0.702780000
6	-2.877373000	-0.939406000	-0.726695000
1	-1.524373000	-1.984605000	-2.167069000
1	-0.291876000	-2.925268000	0.032502000
1	-1.571565000	-1.950398000	2.188137000
1	-3.606857000	-0.410408000	1.328779000
1	-3.577647000	-0.430826000	-1.375582000
42	-0.897998000	0.103215000	-0.002439000
1	0.816216000	-0.082380000	-0.040203000
6	-1.533831000	1.991428000	-0.025599000
6	0.220649000	0.733328000	-1.487863000
6	0.185225000	0.762556000	1.505297000
8	-1.905986000	3.090911000	-0.041193000
8	0.922511000	1.044910000	-2.365383000
8	0.866371000	1.093065000	2.390367000
7	3.128319000	-0.358696000	0.000439000
6	3.680248000	0.981625000	0.010492000
1	3.352574000	1.520346000	-0.882474000
1	3.314525000	1.523131000	0.886976000
1	4.784795000	0.992306000	0.034565000
6	3.500623000	-1.091331000	-1.191730000
1	3.179424000	-0.539473000	-2.078533000
1	2.999129000	-2.063878000	-1.198725000
1	4.588582000	-1.268893000	-1.268209000
6	3.447895000	-1.088022000	1.209748000
1	4.531164000	-1.267726000	1.333050000
1	2.944136000	-2.059410000	1.198809000
1	3.091126000	-0.532558000	2.080692000

1a/Me_3PO E=-1137.57144182

6	-0.181860000	-3.434894000	-2.777772000

6	0.133273000	-2.116917000	-3.207435000
6	0.727755000	-2.206478000	-4.494549000
6	0.787793000	-3.578406000	-4.862505000
6	0.221790000	-4.341678000	-3.794517000
1	-0.647164000	-3.699017000	-1.837293000
1	-0.036134000	-1.207082000	-2.647091000
1	1.076976000	-1.372040000	-5.088313000
1	1.167166000	-3.971513000	-5.796154000
1	0.098246000	-5.416191000	-3.774782000
42	2.175402000	-3.313617000	-2.979616000
1	2.679942000	-2.122402000	-1.850810000
6	3.462938000	-4.800735000	-3.298359000
6	2.578662000	-3.707936000	-1.104383000
6	3.756546000	-2.205800000	-3.379212000
8	4.216417000	-5.666705000	-3.477529000
8	2.807428000	-3.882987000	0.028240000
8	4.664211000	-1.506435000	-3.584637000
1	4.676110000	-1.173250000	2.737805000
6	3.812194000	-1.144961000	2.069991000
1	3.405769000	-2.152446000	1.959915000
1	3.041617000	-0.505864000	2.505533000
1	5.818991000	1.078678000	1.403382000
6	4.984469000	1.119534000	0.699851000
1	4.219487000	1.794098000	1.089200000
1	5.337771000	1.517009000	-0.253594000
15	4.245629000	-0.519564000	0.418715000
6	5.621492000	-1.569145000	-0.140635000
1	6.480763000	-1.507203000	0.530766000
1	5.282649000	-2.606118000	-0.189270000
1	5.920154000	-1.257886000	-1.143925000
8	3.082907000	-0.485741000	-0.534524000

1a/Py E=-849.445788525

6	-1.632714000	-2.285113000	1.157346000
6	-2.232127000	-1.647834000	0.037762000
6	-1.690880000	-2.230025000	-1.140004000
6	-0.753382000	-3.226115000	-0.752496000
6	-0.717493000	-3.259374000	0.676015000
1	-1.839525000	-2.065478000	2.196529000
1	-2.970239000	-0.857784000	0.075333000
1	-1.951739000	-1.962734000	-2.155532000
1	-0.190555000	-3.864978000	-1.419668000
1	-0.120683000	-3.926505000	1.283401000
42	0.101574000	-1.164111000	-0.014571000
1	-0.216307000	0.521536000	0.001091000
6	2.042070000	-1.609645000	-0.034624000
6	0.639446000	-0.013970000	1.489250000
6	0.611732000	-0.008583000	-1.524117000
8	3.172392000	-1.874779000	-0.046358000
8	0.883259000	0.693766000	2.381491000
8	0.840397000	0.702130000	-2.417831000
7	-0.289859000	2.996227000	0.000800000

1	-0.276074000	3.100217000	2.057444000
6	-0.286316000	3.689174000	1.142519000
6	-0.283756000	5.081522000	1.198854000
1	-0.279721000	5.591011000	2.156739000
6	-0.282018000	5.791014000	0.001641000
1	-0.279107000	6.877000000	0.001967000
1	-0.272018000	5.592240000	-2.153550000
6	-0.279519000	5.082222000	-1.195961000
6	-0.282423000	3.689830000	-1.140552000
1	-0.269120000	3.101327000	-2.055706000

1b/Me_3N E=-775.961759812

6	1.779677000	-1.712019000	1.151108000
6	1.158725000	-2.267282000	-0.001157000
6	1.783263000	-1.710797000	-1.150876000
6	2.796069000	-0.810843000	-0.713761000
6	2.793946000	-0.811586000	0.718112000
1	1.525542000	-1.938499000	2.177914000
1	0.344339000	-2.979061000	-0.002804000
1	1.532205000	-1.935995000	-2.178724000
1	3.466092000	-0.249545000	-1.350579000
1	3.462215000	-0.251161000	1.357526000
74	0.759227000	0.066510000	-0.000167000
1	-0.932216000	-0.294551000	-0.001020000
6	1.261786000	1.983329000	-0.002068000
6	-0.353520000	0.651288000	1.509422000
6	-0.355519000	0.648162000	-1.509368000
8	1.566968000	3.106157000	-0.003225000
8	-1.046332000	0.929108000	2.405970000
8	-1.049764000	0.923735000	-2.405551000
7	-3.361449000	-0.390702000	0.000225000
6	-3.728733000	1.011606000	0.000125000
1	-3.312319000	1.501162000	0.884242000
1	-3.314679000	1.500387000	-0.885521000
1	-4.822593000	1.169256000	0.001526000
6	-3.805475000	-1.064049000	1.202591000
1	-3.382035000	-0.567716000	2.079549000
1	-3.454550000	-2.100263000	1.197618000
1	-4.905615000	-1.078868000	1.310310000
6	-3.808765000	-1.065042000	-1.200360000
1	-4.909196000	-1.079889000	-1.305079000
1	-3.457875000	-2.101266000	-1.195470000
1	-3.387635000	-0.569446000	-2.078836000

1b/Me_3PO E=-1137.84925769

6	-0.129921000	-3.369992000	-2.718272000
6	0.216714000	-2.070025000	-3.179201000
6	0.786291000	-2.200521000	-4.475315000
6	0.792632000	-3.581553000	-4.822267000
6	0.222865000	-4.309337000	-3.728802000
1	-0.582563000	-3.601438000	-1.763424000
1	0.098912000	-1.147440000	-2.626735000

1	1.153733000	-1.388095000	-5.087826000
1	1.140680000	-4.001551000	-5.756099000
1	0.061756000	-5.377971000	-3.688496000
74	2.202371000	-3.332936000	-2.980312000
1	2.699474000	-2.102194000	-1.881626000
6	3.448665000	-4.837458000	-3.320903000
6	2.615470000	-3.767528000	-1.117325000
6	3.799549000	-2.272398000	-3.414347000
8	4.177934000	-5.722940000	-3.520291000
8	2.841858000	-3.955948000	0.014962000
8	4.714145000	-1.586582000	-3.645728000
1	4.652977000	-1.215364000	2.704810000
6	3.783763000	-1.176652000	2.044407000
1	3.385456000	-2.184679000	1.911168000
1	3.011651000	-0.555152000	2.502081000
1	5.774384000	1.072773000	1.422591000
6	4.935959000	1.128120000	0.724711000
1	4.171064000	1.790678000	1.134312000
1	5.283440000	1.549907000	-0.220426000
15	4.200740000	-0.506308000	0.406440000
6	5.577437000	-1.534649000	-0.188542000
1	6.443182000	-1.478693000	0.475067000
1	5.246047000	-2.573066000	-0.253541000
1	5.863085000	-1.203353000	-1.189206000
8	3.029639000	-0.451349000	-0.535370000

1b/Py E=-849.723091489

6	-1.605730000	-2.319388000	1.158220000
6	-2.232801000	-1.721180000	0.031434000
6	-1.658528000	-2.281729000	-1.142314000
6	-0.675251000	-3.232579000	-0.745188000
6	-0.642608000	-3.255006000	0.685958000
1	-1.825046000	-2.100088000	2.194610000
1	-3.000983000	-0.960331000	0.061547000
1	-1.927339000	-2.030966000	-2.159677000
1	-0.082026000	-3.848627000	-1.407008000
1	-0.018314000	-3.889503000	1.300118000
74	0.064767000	-1.148259000	-0.017026000
1	-0.411766000	0.507828000	-0.010119000
6	2.014088000	-1.500311000	-0.040509000
6	0.572170000	-0.000451000	1.496078000
6	0.537788000	0.003629000	-1.537171000
8	3.157081000	-1.718775000	-0.054785000
8	0.793326000	0.700169000	2.401408000
8	0.739086000	0.706780000	-2.445285000
7	-0.489442000	3.012289000	-0.001888000
1	-0.453357000	3.107688000	2.055212000
6	-0.389527000	3.695158000	1.141496000
6	-0.200742000	5.074533000	1.202227000
1	-0.125555000	5.575331000	2.161786000
6	-0.107454000	5.781564000	0.007266000
1	0.040890000	6.857374000	0.010835000

1	-0.127978000	5.589893000	-2.148558000
6	-0.202121000	5.082616000	-1.192334000
6	-0.391030000	3.702884000	-1.140778000
1	-0.456302000	3.121647000	-2.058342000

c. Transition states of proton transfer form **1** to bases

1a/Me_3N E=-775.676828800

6	-1.488556000	-1.835844000	-1.150348000
6	-0.774000000	-2.272363000	-0.000069000
6	-1.488433000	-1.835903000	1.150308000
6	-2.641286000	-1.132967000	0.714419000
6	-2.641361000	-1.132930000	-0.714300000
1	-1.207054000	-2.016594000	-2.179508000
1	0.127538000	-2.870767000	-0.000134000
1	-1.206821000	-2.016708000	2.179428000
1	-3.395537000	-0.690963000	1.351500000
1	-3.395676000	-0.690889000	-1.351279000
42	-0.767048000	0.120393000	-0.000003000
1	1.217481000	-0.010296000	-0.000022000
6	-1.624692000	1.905458000	-0.000025000
6	0.267909000	0.893105000	-1.463147000
6	0.267869000	0.893126000	1.463163000
8	-2.142330000	2.947835000	-0.000038000
8	0.906248000	1.311433000	-2.355472000
8	0.906184000	1.311466000	2.355497000
7	2.682286000	-0.338150000	0.000002000
6	3.401337000	0.938472000	0.000010000
1	3.121174000	1.508411000	-0.886381000
1	3.121146000	1.508416000	0.886390000
1	4.488007000	0.781949000	0.000028000
6	2.953990000	-1.115290000	-1.208336000
1	2.717718000	-0.515455000	-2.086990000
1	2.321240000	-2.005293000	-1.215544000
1	4.005389000	-1.426943000	-1.254071000
6	2.953954000	-1.115284000	1.208352000
1	4.005358000	-1.426912000	1.254134000
1	2.321225000	-2.005303000	1.215533000
1	2.717631000	-0.515454000	2.086995000

1a/Py E=-849.431659643

6	-1.713536000	-1.302876000	0.985909000
6	-1.989867000	-0.711744000	-0.278308000
6	-1.530868000	-1.606433000	-1.287362000
6	-0.969881000	-2.739495000	-0.648704000
6	-1.084913000	-2.557845000	0.762267000
1	-1.955742000	-0.879035000	1.951709000
1	-2.494711000	0.231135000	-0.444642000
1	-1.597205000	-1.448357000	-2.355826000
1	-0.536971000	-3.597730000	-1.145306000
1	-0.767178000	-3.257307000	1.523528000
42	0.376976000	-0.875646000	-0.047522000
1	0.308896000	1.222734000	0.021006000

6	2.111430000	-1.829177000	-0.078907000
6	1.189657000	0.073621000	1.444450000
6	1.193465000	0.208968000	-1.445939000
8	3.123721000	-2.405659000	-0.095563000
8	1.628502000	0.659146000	2.367514000
8	1.622040000	0.886030000	-2.308119000
7	-0.030039000	2.492281000	0.052976000
1	0.313476000	2.624850000	2.078436000
6	-0.051434000	3.162925000	1.210203000
6	-0.506671000	4.473369000	1.273761000
1	-0.512589000	4.998118000	2.222029000
6	-0.943555000	5.086221000	0.102198000
1	-1.302096000	6.110300000	0.121276000
1	-1.240415000	4.822636000	-2.026819000
6	-0.913735000	4.375254000	-1.095296000
6	-0.447052000	3.068270000	-1.078954000
1	-0.384048000	2.457408000	-1.973447000

1b/Me_3N E=-775.951825108

6	1.329605000	-1.848927000	1.151551000
6	0.611554000	-2.281700000	-0.000052000
6	1.329707000	-1.848889000	-1.151577000
6	2.491423000	-1.156363000	-0.715375000
6	2.491362000	-1.156386000	0.715475000
1	1.044881000	-2.024987000	2.180335000
1	-0.295438000	-2.871089000	-0.000103000
1	1.045072000	-2.024907000	-2.180393000
1	3.248629000	-0.720362000	-1.352569000
1	3.248517000	-0.720413000	1.352748000
74	0.638636000	0.089626000	-0.000003000
1	-1.407771000	-0.054233000	-0.000020000
6	1.506054000	1.857449000	-0.000012000
6	-0.389855000	0.855712000	1.462240000
6	-0.389874000	0.855699000	-1.462242000
8	2.045338000	2.892386000	-0.000016000
8	-1.032377000	1.262520000	2.362443000
8	-1.032409000	1.262502000	-2.362436000
7	-2.809474000	-0.321516000	0.000001000
6	-3.483818000	0.982411000	0.000001000
1	-3.181720000	1.539743000	0.886626000
1	-3.181752000	1.539727000	-0.886645000
1	-4.573944000	0.859644000	0.000021000
6	-3.108680000	-1.089648000	1.210329000
1	-2.850307000	-0.497142000	2.087192000
1	-2.507723000	-2.001210000	1.215918000
1	-4.170041000	-1.362726000	1.252115000
6	-3.108712000	-1.089668000	-1.210306000
1	-4.170082000	-1.362717000	-1.252079000
1	-2.507780000	-2.001247000	-1.215875000
1	-2.850325000	-0.497192000	-2.087186000

1b/Py E=-849.705667568

6	-1.439567000	-1.957497000	1.308380000
6	-1.957130000	-0.928778000	0.465556000
6	-1.767517000	-1.335585000	-0.887105000
6	-1.138388000	-2.615651000	-0.882951000
6	-0.927574000	-2.986591000	0.478218000
1	-1.428555000	-1.949052000	2.389950000
1	-2.444646000	-0.021406000	0.796548000
1	-2.078028000	-0.786087000	-1.765676000
1	-0.876473000	-3.202300000	-1.752516000
1	-0.459704000	-3.900146000	0.820272000
74	0.354680000	-1.051169000	0.047071000
1	0.264294000	1.117343000	-0.041357000
6	2.091848000	-1.979550000	0.084861000
6	1.132231000	0.054699000	1.441507000
6	1.140270000	-0.099069000	-1.447765000
8	3.107483000	-2.556150000	0.105231000
8	1.527553000	0.754378000	2.307608000
8	1.554546000	0.495703000	-2.382179000
7	-0.034408000	2.342663000	-0.080712000
1	-0.381634000	2.331464000	1.947003000
6	-0.427146000	2.939417000	1.050145000
6	-0.841832000	4.263286000	1.055539000
1	-1.149435000	4.730136000	1.983868000
6	-0.844089000	4.966024000	-0.147342000
1	-1.162136000	6.003222000	-0.173197000
1	-0.416306000	4.848355000	-2.266472000
6	-0.431334000	4.329583000	-1.315142000
6	-0.026973000	3.003431000	-1.244871000
1	0.321450000	2.442600000	-2.105141000

d. hydrogen bonded ion pairs

3a/$^{+}$HMe$_3$N(A) E=-775.686629734

6	1.638767000	-1.788249000	1.150951000
6	0.930958000	-2.248980000	0.003356000
6	1.632593000	-1.791371000	-1.149216000
6	2.764405000	-1.056047000	-0.717388000
6	2.768116000	-1.054092000	0.711024000
1	1.367677000	-1.974160000	2.182093000
1	0.061590000	-2.894342000	0.006604000
1	1.356118000	-1.980249000	-2.178393000
1	3.501537000	-0.588596000	-1.356322000
1	3.508484000	-0.584703000	1.344789000
42	0.837813000	0.145070000	0.000120000
1	-1.747108000	-0.167778000	0.000102000
6	1.596367000	1.962944000	0.000344000
6	-0.329047000	0.808189000	1.398626000
6	-0.328791000	0.808838000	-1.398239000
8	2.071307000	3.030043000	0.000285000
8	-1.058043000	1.167029000	2.264624000
8	-1.057628000	1.168056000	-2.264217000
7	-2.792614000	-0.366620000	-0.000107000

6	-3.466449000	0.959566000	-0.000068000
1	-3.150034000	1.499957000	0.890282000
1	-3.149711000	1.500177000	-0.890170000
1	-4.547193000	0.809417000	-0.000281000
6	-3.076612000	-1.142608000	1.232032000
1	-2.782441000	-0.541896000	2.090445000
1	-2.484158000	-2.056744000	1.209353000
1	-4.139895000	-1.383306000	1.267990000
6	-3.076148000	-1.142295000	-1.232550000
1	-4.139428000	-1.382932000	-1.268999000
1	-2.483755000	-2.056473000	-1.209852000
1	-2.781612000	-0.541378000	-2.090695000

3a/$^{+}$HMe$_3$N(C) E=-775.693254991

6	2.921894000	-0.144280000	1.195958000
6	2.923025000	-1.189022000	0.232122000
6	2.919875000	-0.583732000	-1.060331000
6	2.918492000	0.822708000	-0.889960000
6	2.920924000	1.099726000	0.510887000
1	2.924120000	-0.274857000	2.270200000
1	2.942508000	-2.250139000	0.439820000
1	2.924299000	-1.109078000	-2.006146000
1	2.923339000	1.559242000	-1.682370000
1	2.937469000	2.080192000	0.966980000
42	0.869908000	-0.001112000	0.000850000
1	-1.866826000	0.001304000	-0.001062000
6	-0.231326000	1.499342000	-0.568810000
6	-0.235974000	-0.253852000	1.583323000
6	-0.234350000	-1.250338000	-1.003742000
8	-0.888561000	2.421096000	-0.918239000
8	-0.897630000	-0.409226000	2.553618000
8	-0.895099000	-2.017114000	-1.619634000
7	-2.913561000	0.002230000	-0.003342000
6	-3.331830000	0.228507000	-1.413245000
1	-2.932101000	1.187522000	-1.738035000
1	-2.915336000	-0.570396000	-2.024178000
1	-4.421509000	0.225655000	-1.461415000
6	-3.337257000	1.109426000	0.896150000
1	-2.928127000	2.040028000	0.506948000
1	-2.933547000	0.915840000	1.888410000
1	-4.427160000	1.144787000	0.920585000
6	-3.337975000	-1.330917000	0.503769000
1	-4.427886000	-1.370836000	0.517782000
1	-2.932868000	-1.458938000	1.505948000
1	-2.930248000	-2.092669000	-0.158478000

3a/$^{+}$HPy(A) E=-849.436667420

6	-1.623908000	-1.781713000	1.157779000
6	-2.099234000	-1.036986000	0.040304000
6	-1.674363000	-1.712140000	-1.139180000
6	-0.944503000	-2.865585000	-0.754641000
6	-0.912997000	-2.907642000	0.672361000

1	-1.783424000	-1.534831000	2.199365000
1	-2.716273000	-0.148946000	0.080924000
1	-1.880498000	-1.404109000	-2.156034000
1	-0.500680000	-3.591297000	-1.422819000
1	-0.439002000	-3.670065000	1.275928000
42	0.293634000	-0.973345000	-0.012149000
1	0.151293000	1.628047000	-0.008319000
6	2.106130000	-1.744909000	-0.023576000
6	0.948332000	0.168161000	1.411571000
6	0.935240000	0.171965000	-1.438534000
8	3.168470000	-2.231107000	-0.030714000
8	1.278372000	0.862639000	2.316579000
8	1.257690000	0.868744000	-2.344513000
7	-0.076159000	2.668249000	-0.005674000
1	-0.035187000	2.675288000	2.050666000
6	-0.217123000	3.288676000	1.175642000
6	-0.543741000	4.633863000	1.206702000
1	-0.654290000	5.135767000	2.159962000
6	-0.715477000	5.312786000	0.001641000
1	-0.969634000	6.367553000	0.004551000
1	-0.670535000	5.143805000	-2.157708000
6	-0.552773000	4.638362000	-1.207188000
6	-0.225865000	3.293087000	-1.183584000
1	-0.050558000	2.683026000	-2.062298000

3a/$^{+}$HPy(B) E=-849.437410539

6	4.197604000	-4.610586000	1.672871000
6	3.188391000	-4.074756000	0.823992000
6	3.816588000	-3.512141000	-0.316453000
6	5.225299000	-3.699610000	-0.176116000
6	5.455112000	-4.373700000	1.048360000
1	4.037259000	-5.121975000	2.612318000
1	2.123658000	-4.095221000	1.015861000
1	3.317747000	-3.040006000	-1.152201000
1	5.981997000	-3.387178000	-0.883384000
1	6.421542000	-4.658119000	1.443775000
42	4.505324000	-2.236259000	1.585421000
1	3.725543000	0.677324000	3.553449000
6	5.746462000	-1.736212000	2.996028000
6	3.242344000	-1.280728000	2.654608000
6	4.834009000	-0.495754000	0.785625000
8	6.460004000	-1.412014000	3.881924000
8	2.552983000	-0.575051000	3.342979000
8	4.993515000	0.582261000	0.325460000
7	4.513557000	1.350009000	3.599189000
1	3.848312000	2.271914000	1.874867000
6	4.604386000	2.293530000	2.647793000
6	5.651022000	3.195670000	2.679976000
1	5.729149000	3.949633000	1.907259000
6	6.595643000	3.093111000	3.699875000
1	7.428150000	3.787441000	3.738687000
1	7.214239000	1.971237000	5.448257000

6	6.481560000	2.089221000	4.660247000
6	5.416452000	1.211648000	4.583863000
1	5.268346000	0.379759000	5.258888000

3a/$^{+}$HPy(C) E=-849.439729391

6	-0.954196000	-2.823248000	1.241725000
6	-1.782986000	-1.922388000	0.513561000
6	-1.612085000	-2.176689000	-0.871021000
6	-0.668336000	-3.241159000	-1.006962000
6	-0.265442000	-3.634615000	0.293976000
1	-0.877757000	-2.893416000	2.318171000
1	-2.434883000	-1.173711000	0.944251000
1	-2.115404000	-1.665339000	-1.680450000
1	-0.330604000	-3.676447000	-1.937846000
1	0.441302000	-4.419818000	0.528215000
42	0.471659000	-1.397796000	-0.023668000
1	2.426394000	0.361133000	-0.210282000
6	2.265705000	-1.724793000	0.678076000
6	0.438625000	0.334631000	0.877629000
6	1.162448000	-0.627269000	-1.670922000
8	3.337020000	-1.927617000	1.130705000
8	0.415067000	1.366292000	1.452073000
8	1.556749000	-0.181181000	-2.696447000
7	3.223035000	1.045838000	-0.151839000
1	3.158758000	0.894115000	1.899161000
6	3.669355000	1.366940000	1.070002000
6	4.720394000	2.257035000	1.200761000
1	5.082289000	2.518037000	2.187263000
6	5.288867000	2.797370000	0.048482000
1	6.114139000	3.497017000	0.128603000
1	5.222221000	2.845563000	-2.116443000
6	4.798212000	2.439923000	-1.206362000
6	3.744684000	1.545104000	-1.281978000
1	3.286450000	1.199315000	-2.201527000

3b/$^{+}$HMe$_3$N(A) E=-775.959304204

6	1.513192000	-1.788737000	1.150229000
6	0.821423000	-2.264087000	-0.003104000
6	1.518051000	-1.785640000	-1.152240000
6	2.635779000	-1.028469000	-0.712981000
6	2.632885000	-1.030447000	0.717765000
1	1.239369000	-1.981123000	2.179076000
1	-0.039308000	-2.919706000	-0.005826000
1	1.248453000	-1.975069000	-2.182747000
1	3.365996000	-0.544903000	-1.347300000
1	3.360574000	-0.548771000	1.356401000
74	0.697478000	0.104957000	0.000055000
1	-1.899879000	-0.194580000	-0.000111000
6	1.432013000	1.922426000	-0.000004000
6	-0.471720000	0.740525000	1.403154000
6	-0.471691000	0.740626000	-1.403023000
8	1.907509000	2.992240000	-0.000300000

8	-1.205197000	1.079786000	2.277640000
8	-1.205299000	1.079826000	-2.277431000
7	-2.954159000	-0.356028000	-0.000067000
6	-3.576623000	0.995015000	0.000074000
1	-3.238815000	1.521981000	0.890534000
1	-3.238898000	1.522119000	-0.890336000
1	-4.662487000	0.886637000	0.000118000
6	-3.269187000	-1.120417000	1.231235000
1	-2.949599000	-0.532830000	2.089571000
1	-2.715644000	-2.058743000	1.207296000
1	-4.341349000	-1.318504000	1.267286000
6	-3.269372000	-1.120226000	-1.231441000
1	-4.341551000	-1.318237000	-1.267394000
1	-2.715896000	-2.058595000	-1.207703000
1	-2.949835000	-0.532538000	-2.089725000

3b/$^{+}$HMe$_3$N(C) E=-775.967555626

6	-2.744645000	0.807793000	-0.906447000
6	-2.739602000	-0.604447000	-1.050479000
6	-2.743587000	-1.193059000	0.249256000
6	-2.745225000	-0.127762000	1.199191000
6	-2.748077000	1.104225000	0.494384000
1	-2.754507000	1.531018000	-1.710168000
1	-2.738482000	-1.144331000	-1.987958000
1	-2.755855000	-2.250535000	0.472908000
1	-2.750075000	-0.241411000	2.274971000
1	-2.760712000	2.090949000	0.936427000
74	-0.722801000	0.002246000	0.001582000
1	1.998908000	-0.000498000	-0.001957000
6	0.376815000	-1.054643000	-1.196321000
6	0.378905000	-0.513993000	1.512112000
6	0.376968000	1.568201000	-0.310256000
8	1.035802000	-1.707181000	-1.938247000
8	1.042103000	-0.832230000	2.444635000
8	1.042115000	2.533566000	-0.502309000
7	3.047373000	-0.000615000	-0.002247000
6	3.469005000	0.934840000	1.075116000
1	3.058067000	1.918030000	0.852343000
1	3.063773000	0.571163000	2.017808000
1	4.558953000	0.967056000	1.106799000
6	3.468395000	0.464350000	-1.351319000
1	3.065394000	1.463448000	-1.507375000
1	3.055170000	-0.219228000	-2.091023000
1	4.558303000	0.473288000	-1.396364000
6	3.469718000	-1.401075000	0.268826000
1	4.559687000	-1.443239000	0.284025000
1	3.067992000	-2.035856000	-0.519026000
1	3.056885000	-1.701591000	1.230228000

3b/$^{+}$HPy(A) E=-849.709395422

6	-1.626125000	-1.803672000	1.157302000
6	-2.119568000	-1.081864000	0.030818000

6	-1.672575000	-1.757199000	-1.142581000
6	-0.916822000	-2.892489000	-0.745408000
6	-0.887533000	-2.920338000	0.684275000
1	-1.791356000	-1.548686000	2.195669000
1	-2.753648000	-0.206220000	0.061469000
1	-1.880872000	-1.461661000	-2.162292000
1	-0.454352000	-3.613235000	-1.405732000
1	-0.397840000	-3.665432000	1.296262000
74	0.248935000	-0.980562000	-0.016852000
1	0.106455000	1.631093000	-0.007723000
6	2.064554000	-1.719063000	-0.037499000
6	0.877324000	0.164272000	1.409488000
6	0.850713000	0.171937000	-1.448415000
8	3.132555000	-2.199414000	-0.050456000
8	1.190747000	0.862722000	2.321757000
8	1.147095000	0.875600000	-2.362348000
7	-0.089435000	2.680129000	-0.003362000
1	-0.030677000	2.686753000	2.052095000
6	-0.199864000	3.306278000	1.178735000
6	-0.478424000	4.662303000	1.211747000
1	-0.563446000	5.167427000	2.165958000
6	-0.634949000	5.347387000	0.008282000
1	-0.850903000	6.410644000	0.012906000
1	-0.611761000	5.176400000	-2.151175000
6	-0.505407000	4.667313000	-1.201222000
6	-0.226205000	3.311193000	-1.180065000
1	-0.076445000	2.695546000	-2.059635000

3b/$^{+}$HPy(B) E=-849.710816723

6	-1.357928000	1.539695000	0.957703000
6	-0.215999000	2.326167000	0.606803000
6	-0.267161000	2.570015000	-0.790020000
6	-1.437945000	1.946983000	-1.313439000
6	-2.104515000	1.305431000	-0.228390000
1	-1.613263000	1.196511000	1.950850000
1	0.548804000	2.675556000	1.286929000
1	0.458485000	3.133264000	-1.361556000
1	-1.765885000	1.966735000	-2.343482000
1	-3.026335000	0.743518000	-0.295905000
74	-0.025178000	0.227889000	-0.491068000
1	0.816456000	-3.135688000	-1.337794000
6	-0.597502000	-1.503599000	-1.055796000
6	1.049577000	-0.747286000	0.791528000
6	1.394980000	-0.038114000	-1.783006000
8	-0.835868000	-2.632276000	-1.406221000
8	1.682840000	-1.378640000	1.570309000
8	2.240977000	-0.233469000	-2.590338000
7	1.833599000	-3.308456000	-1.229147000
1	1.549903000	-3.799530000	0.756675000
6	2.286455000	-3.709104000	-0.029933000
6	3.637596000	-3.940199000	0.146776000
1	4.002535000	-4.251694000	1.117034000

6	4.500242000	-3.739058000	-0.929384000
1	5.564925000	-3.908312000	-0.809126000
1	4.649043000	-3.114082000	-2.999460000
6	3.998877000	-3.303405000	-2.154996000
6	2.639785000	-3.085896000	-2.280304000
1	2.168087000	-2.709351000	-3.177548000

3b/$^{+}$HPy(C) E=-849.713608506

6	-1.053120000	-2.787907000	1.157321000
6	-1.865767000	-1.851364000	0.442728000
6	-1.646607000	-2.054860000	-0.945560000
6	-0.708710000	-3.119187000	-1.102380000
6	-0.339414000	-3.560919000	0.203034000
1	-0.999251000	-2.893195000	2.232106000
1	-2.533628000	-1.123571000	0.882625000
1	-2.116770000	-1.502938000	-1.748335000
1	-0.352736000	-3.524736000	-2.039070000
1	0.359563000	-4.355445000	0.427403000
74	0.387711000	-1.337267000	-0.014249000
1	2.312626000	0.441972000	0.122607000
6	2.274897000	-1.810413000	-0.008176000
6	0.622744000	-0.025707000	1.392705000
6	0.726479000	-0.028338000	-1.413132000
8	3.419258000	-2.111893000	-0.031444000
8	0.734527000	0.764779000	2.273722000
8	0.936252000	0.744804000	-2.284503000
7	3.129939000	1.106307000	0.069122000
1	2.565974000	1.995010000	1.834817000
6	3.304056000	2.013619000	1.041029000
6	4.376908000	2.885922000	0.972185000
1	4.521343000	3.619943000	1.755084000
6	5.249216000	2.795345000	-0.111177000
1	6.095810000	3.469951000	-0.183520000
1	5.697674000	1.747140000	-1.953775000
6	5.035327000	1.838764000	-1.102187000
6	3.948098000	0.990925000	-0.985257000
1	3.694037000	0.216002000	-1.697156000

e. complexes with solvents

1b/THF E=-833.918643403

6	2.952660000	-1.109641000	-0.301023000
6	2.985050000	0.112351000	-1.027208000
6	2.912358000	1.184985000	-0.097336000
6	2.837305000	0.630035000	1.211949000
6	2.863112000	-0.796808000	1.086254000
1	2.996825000	-2.101796000	-0.729510000
1	3.040245000	0.208929000	-2.103000000
1	2.916636000	2.238163000	-0.344047000
1	2.798720000	1.188671000	2.137136000
1	2.851285000	-1.509645000	1.899384000
74	0.911458000	-0.030556000	0.102344000

1	0.228851000	0.071735000	-1.478331000
6	-0.239836000	-0.172894000	1.722125000
6	-0.220952000	-1.562067000	-0.408416000
6	-0.272831000	1.525330000	-0.205852000
8	-0.888892000	-0.277086000	2.678401000
8	-0.851769000	-2.480326000	-0.749042000
8	-0.907434000	2.469540000	-0.444505000
8	-3.311512000	0.545496000	0.773798000
6	-3.736352000	-0.798622000	0.646228000
6	-3.958641000	1.269140000	-0.249394000
6	-3.868661000	0.361296000	-1.468429000
6	-4.035709000	-1.033662000	-0.847990000
1	-3.445601000	2.225544000	-0.363427000
1	-5.011738000	1.462457000	0.017208000
1	-4.637287000	-0.966850000	1.255388000
1	-2.941964000	-1.438855000	1.037582000
1	-2.880193000	0.464949000	-1.925562000
1	-4.619097000	0.587665000	-2.229281000
1	-5.052626000	-1.410274000	-0.984705000
1	-3.352800000	-1.761319000	-1.289868000

1b/DCM E=-1561.28948569

6	6.513372000	5.125392000	-5.383246000
6	6.061295000	4.013839000	-6.145525000
6	4.753861000	3.672182000	-5.702849000
6	4.389542000	4.575831000	-4.663411000
6	5.484058000	5.478651000	-4.464577000
1	7.471145000	5.617125000	-5.487658000
1	6.620759000	3.507138000	-6.920105000
1	4.142404000	2.870346000	-6.094155000
1	3.442651000	4.595787000	-4.141411000
1	5.512967000	6.302226000	-3.764238000
74	6.192265000	3.350454000	-3.880378000
1	7.269631000	2.141384000	-4.473824000
6	5.746694000	3.496791000	-1.942914000
6	8.013926000	3.395567000	-3.116172000
6	5.647399000	1.487411000	-3.515829000
8	5.479071000	3.592978000	-0.818118000
8	9.107794000	3.404280000	-2.718225000
8	5.349046000	0.374054000	-3.352232000
6	8.463159000	0.037474000	-1.625594000
1	7.697611000	-0.308239000	-2.317145000
1	9.105378000	0.788884000	-2.080384000
17	9.470435000	-1.351351000	-1.181374000
17	7.644829000	0.789844000	-0.246587000

1b/AN E=-734.283540023

6	-2.729287000	1.152790000	-0.308269000
6	-2.797445000	0.003303000	-1.142349000
6	-2.729151000	-1.150871000	-0.314691000
6	-2.621456000	-0.718813000	1.038435000
6	-2.621463000	0.713225000	1.042367000

1	-2.760530000	2.180768000	-0.643509000
1	-2.874656000	0.006342000	-2.221127000
1	-2.760571000	-2.176961000	-0.655642000
1	-2.579464000	-1.359643000	1.908532000
1	-2.579327000	1.349233000	1.915996000
74	-0.702296000	-0.000111000	-0.045607000
1	-0.040548000	0.001603000	-1.638335000
6	0.502941000	-0.002404000	1.531642000
6	0.452581000	1.542066000	-0.484783000
6	0.452005000	-1.541446000	-0.488843000
8	1.222904000	-0.003765000	2.445718000
8	1.113491000	2.451840000	-0.782674000
8	1.112494000	-2.450730000	-0.789184000
1	3.582459000	-0.002351000	1.051875000
6	3.850625000	-0.000736000	-0.006879000
1	3.422274000	-0.888724000	-0.477238000
1	3.422659000	0.888925000	-0.474417000
6	5.296405000	-0.000813000	-0.160023000
7	6.454764000	-0.000920000	-0.283282000