

Supplementary Information:

A Colorimetric Sensor Array for Identification of Toxic Gases below Permissible Exposure Limits

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Experimental Section:

All reagents used were analytical-reagent grade, obtained from Sigma-Aldrich, and used without further purification unless otherwise specified. Certified, premixed gas tanks, including ammonia, methylamine, dimethylamine, trimethylamine, HCl, SO₂, fluorine, chlorine, phosphine, arsine, phosgene, hydrogen sulfide, hydrogen cyanide, and diborane were obtained from Matheson Tri-Gas Corp. through S. J. Smith, Co. (Urbana, IL).

The nanoporous pigment sensors are given in Table S1. For printing of the sensor array, we prepared sol-gel-colorant solutions by the simple hydrolysis of solutions containing commercially available silane precursors (e.g., tetraethoxysilane, methyltriethoxysilane, phenethyl-trimethoxysilane and octyltriethoxysilane) with a variety of chemically responsive indicators (Table S1). Final organically modified sol-gel formulations with the colorants were loaded into a 36-hole Teflon ink well. Sensor arrays (Fig. S1) were printed using an array of 36 floating slotted pins (which delivered approximately 130 nL each) by dipping into the ink well and transferring to a PET film. Once printed, the arrays were aged under a slow stream of N₂ for at least 3 days before sensing experiments were performed.

Gas streams containing the toxic industrial chemicals at their PEL or lower concentrations were prepared by mixing the prediluted analyte gas stream with dry and wet nitrogen gas. Importantly, gas stream concentrations and relative humidity were confirmed by in-line quantitative analysis using an FTIR multi-gas analyzer, MKS Instruments model 2030. MKS digital mass flow controllers were used to achieve the desired concentrations and relative

humidity (Figs. S2 and S5). The serial dilution apparatus (Fig. S5) could produce precise analyte concentrations to ~0.01% of the initial gas tank concentration. For nitric acid and HF, saturated vapors were generated from a diluted solution in a five gallon polyethylene carboy, which was further diluted to PEL concentration with nitrogen gas and confirmed by the multi-gas analyzer. Hydrazine (98%) was used directly to produce saturated hydrazine vapor, which was further diluted. Fluorine, chlorine, hydrazine, nitric acid and HF at their PEL concentrations were confirmed using Dräger detector tubes.

For all sensing experiments, the arrays were imaged on an ordinary flatbed scanner (Epson Perfection V200); the before-exposure image was acquired after 2 min. of 50% RH N₂ flow at 500 sccm. After-exposure images were acquired every minute with the same gas flow rates. Difference maps were obtained by taking the difference of the red, green, and blue (RGB) values from the center of every colorant spot (~300 pixels) from the “before” and “after” images; all difference maps shown here are averages of multiple trials. Digitization of the color differences can be performed using Adobe PhotoshopTM or with a customized software package, ChemEyeTM (ChemSensing, Inc., Champaign, IL). The chemometric analysis was carried out on the color difference vectors (provided as a database in Table S2) using the Multi-Variate Statistical PackageTM (MVSP v.3.1, Kovach Computing); in all cases, minimum variance (i.e., “Ward’s Method”) was used for HCA clustering.

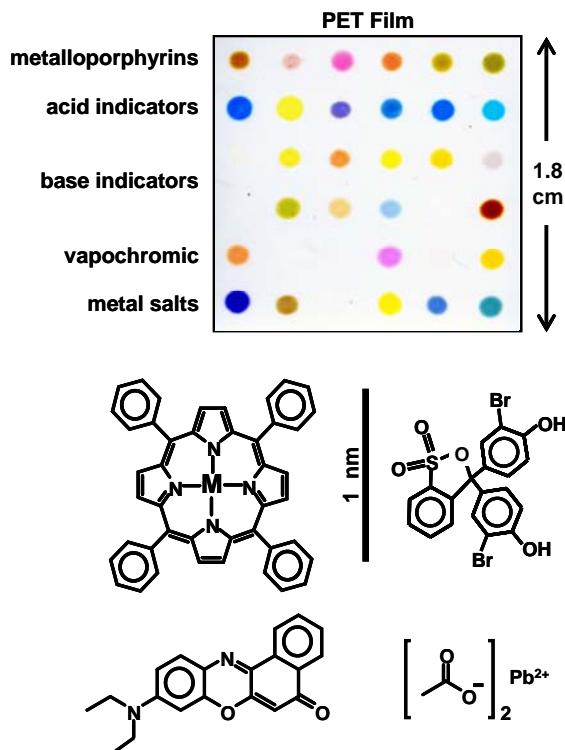


Fig. S1. The colorimetric sensor array consists of 36 different chemically responsive pigments that have been printed directly onto a non-permeable polyethylene terephthalate (PET) film. Examples of each dye class are shown. The 36 dyes (some of which appear transparent before exposure) were selected empirically based on the quality of their color response to a representative selection of different analytes.

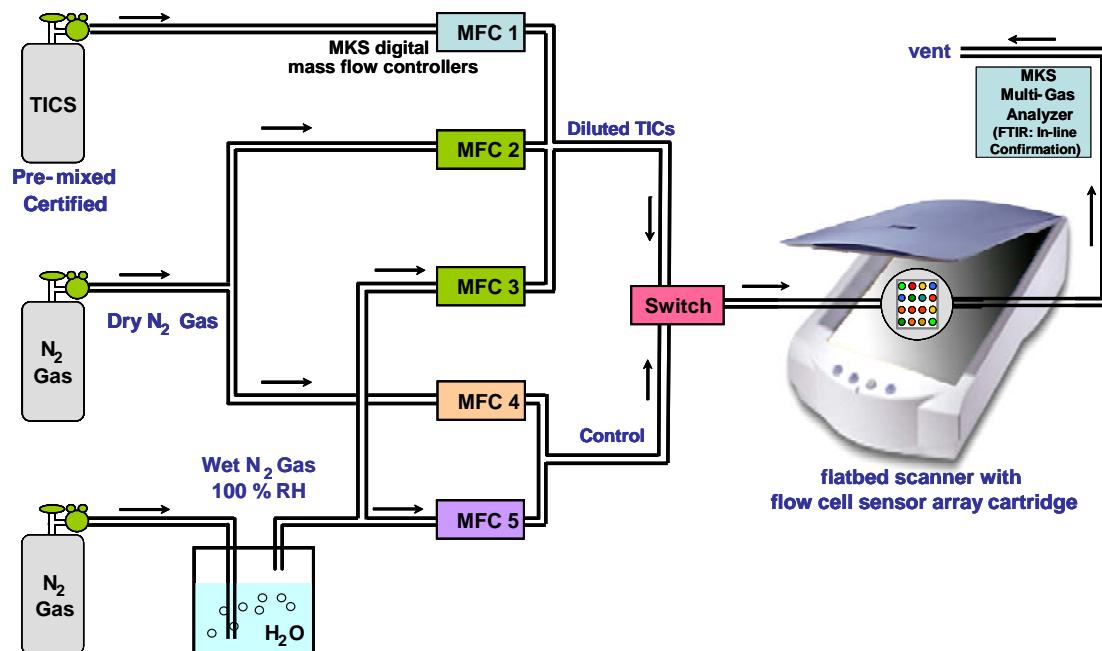


Fig. S2. Gas mixing rig used for exposure of colorimetric sensor arrays. The box labeled "switch" is actually a series of three three-way valves, which allows for venting and also diversion of analyte stream to the MKS multi-gas analyzer. MFC = mass flow controller.

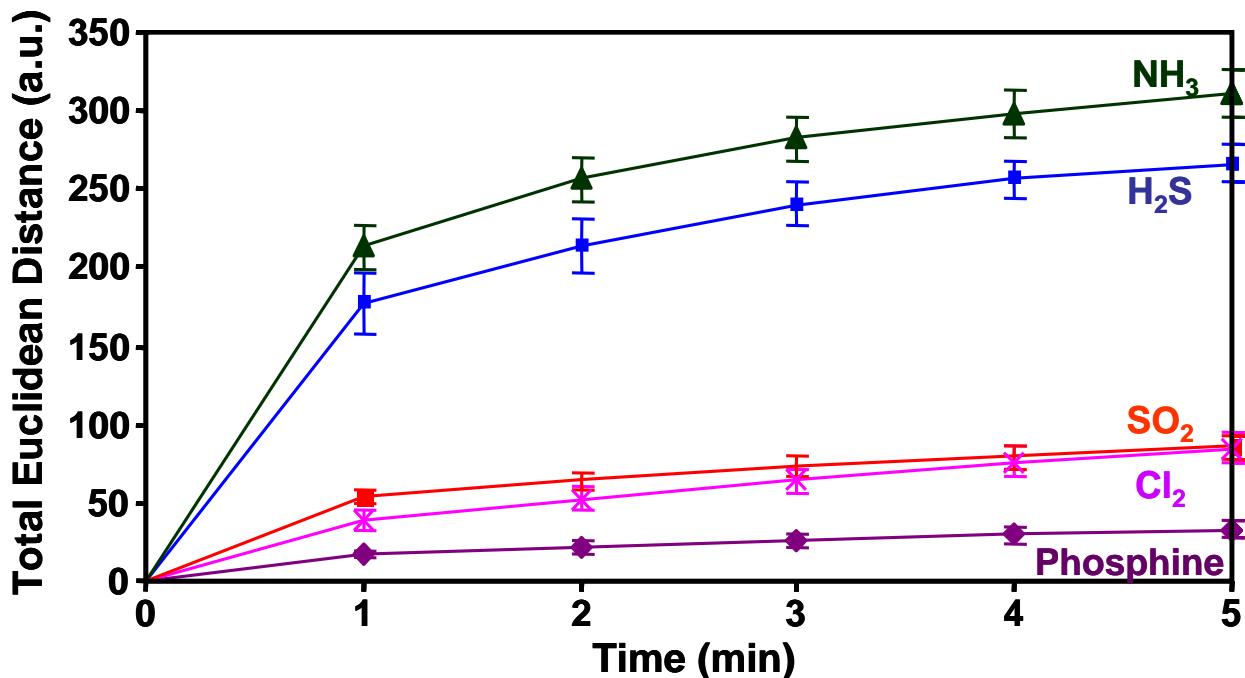


Fig. S3. Total Euclidean distance (i.e., total array response) versus time for five TICs at their PEL concentrations; the averages with the standard deviation of seven trials for each analyte are shown.

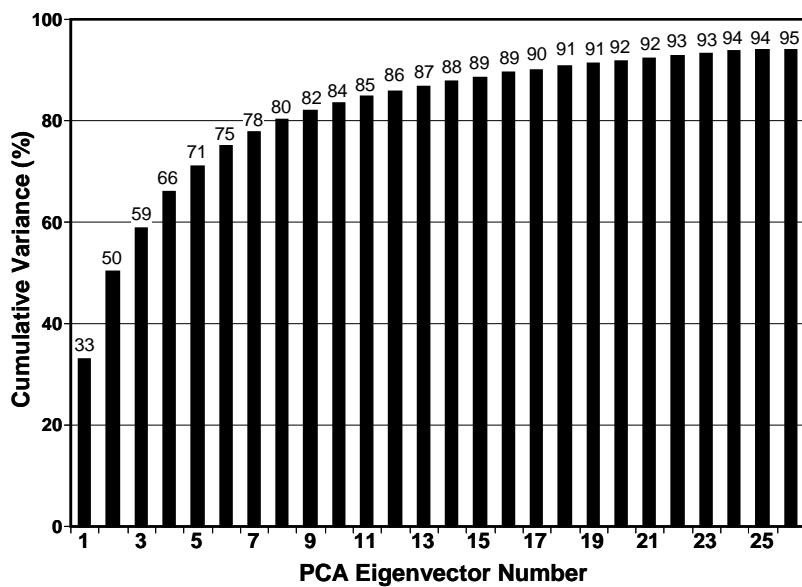


Fig. S4. Scree plot of the principal components from PCA of 147 trials using 20 TICs and a control. The colorimetric sensor array has an extremely high level of dispersion: 17 dimensions are required to define 90% of the total variance, 26 dimensions for 95% of the total variance, and 46 dimensions for 99%.

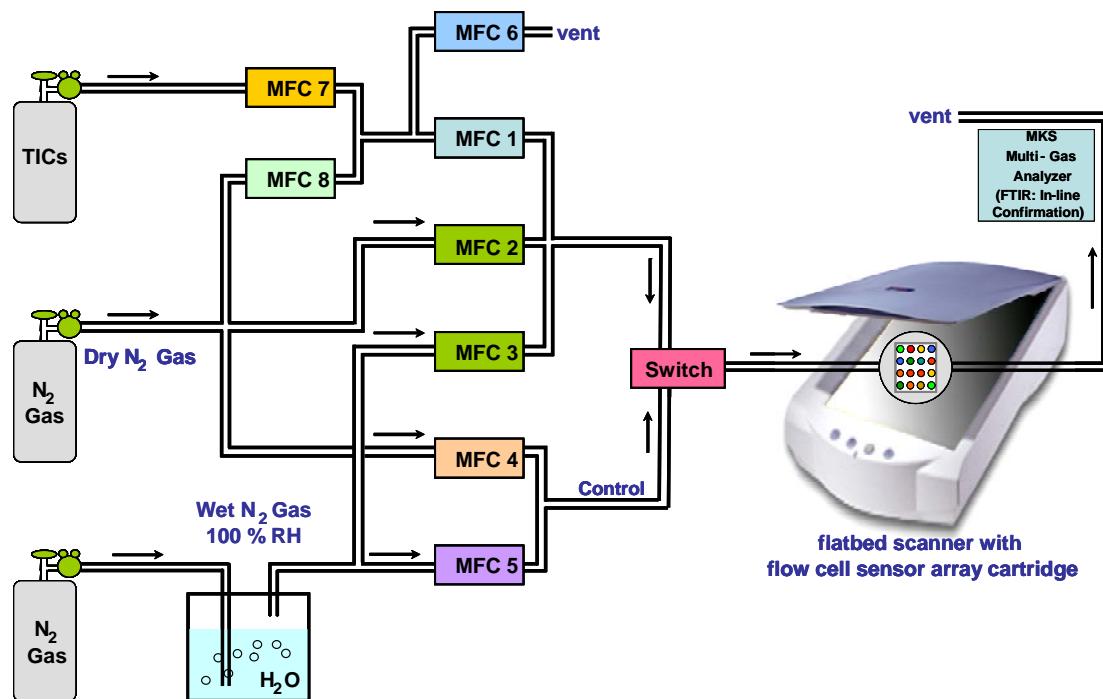


Fig. S5. Serial dilution gas mixing rig used for exposure of colorimetric sensor arrays. The box labeled "switch" is actually a series of three three-way valves, which allows for venting and also diversion of analyte stream to a MKS FTIR multi-gas analyzer model 2030. MFC = mass flow controller.

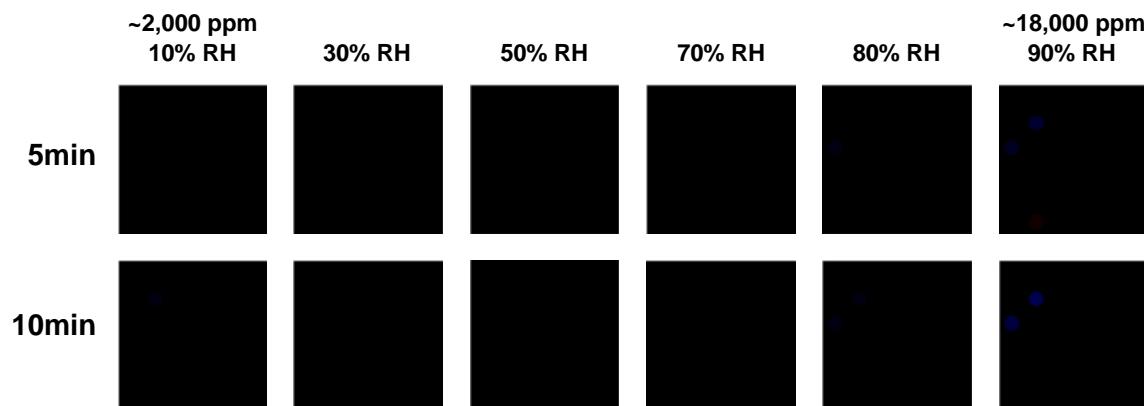


Fig. S6. The colorimetric sensor array is unaffected by humidity over a wide range. There is essentially no response to variations in humidity from 10% to 90% RH; average of three trials is shown. For display purposes, the color range of these difference maps is expanded from 4 to 8 bits per color (RGB range of 4-19 expanded to 0-255).

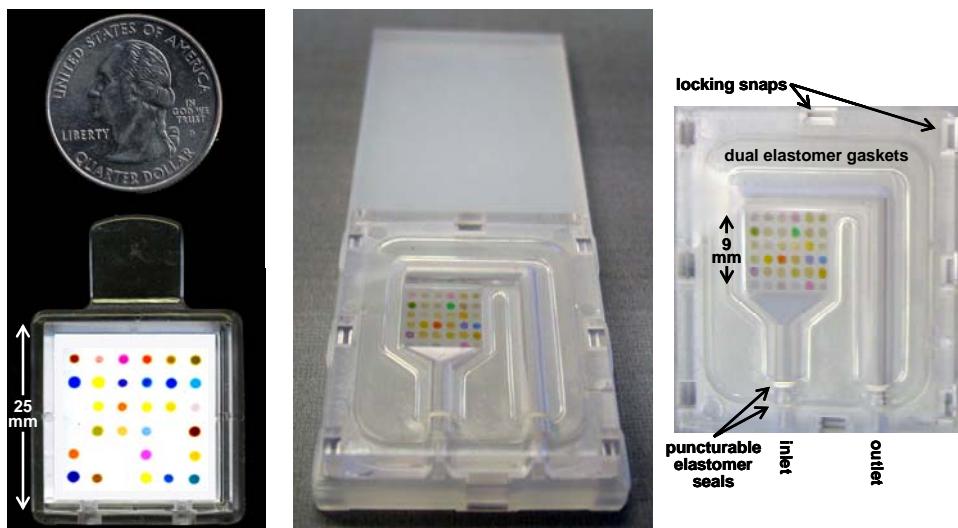


Fig. S7. Photographs of cartridged colorimetric sensor arrays, all on the same scale. Right: standard disposable cartridge used in these studies; the inside dimensions are 22x22x4 mm with a total dead volume ~2 mL. Middle: disposable low dead-volume self-sealing cartridge with the colorimetric sensor array printed directly on a PET (polyethylene terephthalate) flat. Right: close-up of the low dead-volume printed colorimetric sensor array and sealing system. The total head-space volume of the low dead-volume cartridge is ~150 μ L (i.e., >10-fold smaller volume). The cartridges are produced by standard injection molding.

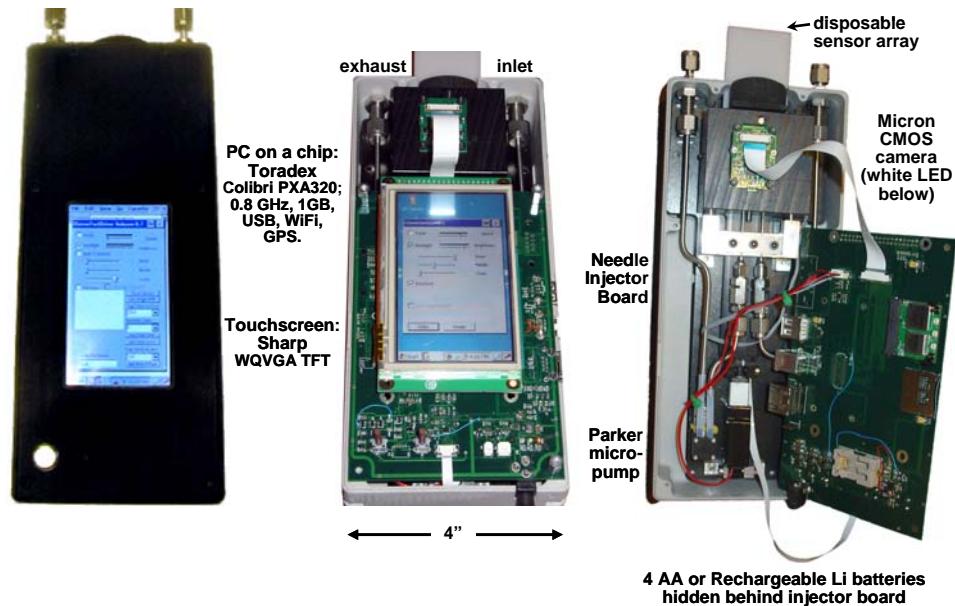


Fig. S8. Labeled photographs of a functional handheld prototype of the optoelectronic nose. Left: the fully assembled unit; center: with top cover removed; right: top electronics board and touchscreen display lifted vertically to the right. The disposable sensor array used with this prototype is shown in Fig. S1. The image quality of this prototype is considerably improved compared to the flat bed scanners used in this study (Epson Perfection V200); an improvement in S/N of a factor of 3 has been achieved even at this early stage of development.

Table S1. List of chemically responsive colorants.

Spot #	Name
1	5,10,15,20-tetraphenylporphyrinatozinc(II)
2	5,10,15,20-tetrakis(2,4,6-trimethylphenyl)porphyrinatozinc(II)
3	5,10,15,20-tetrakis(pentafluorophenyl)porphyrinatozinc(II)
4	5,10,15,20-tetrakis(2,4,6-trimethylphenyl)porphyrinatocobalt(II)
5	5,10,15,20-tetraphenylporphyrinatocadmium(II)
6	5,10,15,20-tetraphenylporphyrinatochromium(III) chloride
7	Bromophenol Blue + TBAH
8	Methyl Red + TBAH
9	Chlorophenol Red + TBAH
10	Nitrazine Yellow + TBAH
11	HgCl ₂ + Bromophenol Blue + TBAH
12	HgCl ₂ + Bromocresol Green + TBAH
13	Fluorescein
14	Bromocresol Green
15	Methyl Red
16	Bromocresol Purple
17	Bromophenol Red
18	Bromopyrogallol Red
19	4-amino-4-phenylbut-3-en-2-one + TsOH
20	H ₂ (P-COOHP)2(CF ₃) ₂
21	Ethanone, 1-[4-[4-(dimethylamino)phenyl]azo]phenyl]-2,2,2-trifluoro-
22	Pyrylium, 4-[2-[4-(dimethylamino)phenyl]ethenyl]-2,6-dimethyl-,tetrafluoroborate
23	4-(4-Nitrobenzyl)pyridine + N-Benzylaniline
24	Naphthal Red + TsOH
25	Disperse Red
26	Reichart's Dye
27	Reichart's Dye #3
28	Nile Red
29	Disperse Orange #25
30	Acridine Orange Base
31	Crystal Violet
32	Zn(OAc) ₂ + <i>m</i> -Cresol Purple + TBAH
33	Pb(OAc) ₂
34	LiNO ₃ + Cresol Red
35	AgNO ₃ + Bromophenol Blue
36	AgNO ₃ + Bromocresol Green

Spot numbering from left to right, top to bottom for 6x6 array shown in Fig. 1.

TBAH: 1.0 M tetrabutylammonium hydroxide in 2-methoxyethanol

TsOH: 1.0 M *p*-toluenesulfonic acid in 2-methoxyethanol

Table S2. Color difference database for 20 TICs and a control material (ESI) for Chemical Communications
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	R01	G01	B01	R02	G02	B02	R03	G03	B03	R04	G04	B04	R05	G05	B05	R06	G06	B06	R07	G07	B07	R08	G08	B08	R09	G09	B09
Control_1	-0.481155	0.234787	1.104349	-0.457977	-0.107246	0.431885	0.565216	0.571014	-0.910141	0.63768	0.226089	0.86377	-0.571014	0.031883	-0.263769	0.713043	-0.034782	-0.304348	0	-0.014492	1.214493	-0.342026	0.185516	0.41449	-0.556522	-0.144924	3.428986
Control_2	-0.13044	-0.301449	0.217392	0.292755	0.057968	0.350723	0.318848	-0.591309	-0.037674	-0.446381	0.805794	-0.205795	0.620285	-0.539124	-0.536232	0.455078	-0.040581	1.133331	0.182609	-0.182606	0.976807	0.03479	0.228989	0.47826	0.046377	0.052174	1.527542
Control_3	-0.965218	-0.559425	-0.243478	-0.220291	0.269562	-0.118835	-0.556519	-0.255066	-1.565216	-0.408707	0.284058	0.907249	-0.620285	0.762321	0.449275	0.573914	-0.005798	-0.124638	-0.107246	0.368114	-0.365219	-0.249283	0.486954	0.886955	-0.437679	-0.18261	-0.614487
Control_4	-0.284058	-0.13913	-0.089855	0.243469	0.168121	-0.628983	0.246368	0.237679	-1.457962	-0.289856	0.342033	-0.872459	0.423187	-0.023178	0.194202	-0.084061	-0.18261	-0.069565	0.101449	-0.11594	0.492752	0.573914	0.547821	-0.950726	-0.385504	-0.127537	1.533325
Control_5	0.055069	-0.09565	0.330435	0.536224	-0.54203	0.08696	0.46376	-0.150726	-0.037674	0.808701	-0.237686	-0.330437	0.518845	-0.286957	0.208695	0.582603	-0.707253	0.45797	0.069565	0.513042	0.446381	0.165222	-0.455063	0.440582	-0.211594	0.411594	4.788406
Control_6	-0.36232	-0.446381	0.481159	-0.078262	0.159424	0.539124	-0.402088	0.171013	0.466675	-0.156525	-0.243484	0.614494	-1.394196	-0.814491	-0.634783	0.289856	-0.00869	0.50145	0.101449	0.31884	0.588409	0.286957	0.118835	0.121738	-0.857971	-0.373913	2.594193
Control_7	-0.765213	0.23188	0.385508	0.284058	0.634789	-0.814484	0.53334	-0.168121	-0.843475	-0.124634	-0.115936	0.878265	-0.411606	-0.559425	-0.92174	-0.228981	0.173912	-0.284058	0.666667	1.197102	-0.530426	0.063766	0.089859	0.144928	-0.040577	-0.13623	2.431885
HCHO_1	0.626083	0.3121739	0.034782	-1.068067	0.078262	0.333328	0.159424	-0.060875	-0.228989	1.014496	1.105793	0.214493	0.313049	-0.086958	0.63768	0.831879	0.428986	-0.211594	-0.657967	0.028976	0.011597	0.41449	3.211594	-0.759415	-0.040581	1.988403	
HCHO_2	-0.008698	-0.63768	-0.397101	-0.171021	1.127533	0.297258	0.036766	-0.486961	-0.799988	-0.562317	-0.979713	-0.452171	-0.759415	-0.634781	-0.475363	0.303478	-0.434784	0.553623	0.002899	0.104347	-0.081146	0.255066	-0.330429	-0.124634	0.397102	0.040577	0.678268
HCHO_3	-0.124641	0.272465	0.121739	-0.979706	0.142029	-0.588402	0.069565	0.295654	-0.736237	-0.339994	0.36232	-0.107246	-0.304344	0.208694	0.489855	0.156526	-0.008698	0.27536	0.078261	0.043476	-0.101456	-0.55072	-0.026093	0.092754	-0.295652	0.046377	0.597092
HCHO_4	-1.113045	-0.605797	0.107245	-1.379715	0.002899	-1.814491	-0.301453	1.208694	-1.176819	-1.171005	0.481159	0.336231	-0.588402	-0.176811	0.962319	-0.147827	-1.165222	-0.611595	0.052174	-0.069565	0.115952	-0.72464	-0.278259	1.208694	-1.228985	-1.249275	-0.295654
HCHO_5	-1.750725	-1.950726	-1.484058	0.549422	0.368118	-2.959419	-0.55072	0.681156	-1.307251	0.350723	0.62318	0.631886	-0.063766	0.344925	0.008699	2.837677	0.233336	0.988407	0.110145	0.049274	0.486954	-0.298552	0.936234	-0.55072	-0.133335	0.060869	-0.515945
HCHO_6	0.26667	-0.089855	0.168116	0.272476	-0.144928	-0.324638	0.115936	-0.202904	-1.855501	-0.031891	0.049274	0.591305	0.028984	0.011589	0.901451	-0.588409	0.672462	1.130435	0.492752	0.339127	0.0850501	-0.428986	0.492752	0.185509	-0.069567	0.336227	
HCHO_7	0.86087	1.165218	0.889855	0.565216	-0.023186	0.182617	0.571014	0.186377	-0.252182	0.997101	0.208992	0.889852	0.77681	0.18261	0.918842	1.663768	0.255074	0.852173	-1.171014	-0.733334	0.150726	-0.046387	0.63768	0.2788406	0.544926	-0.072892	0.078292
Arsine_1	-0.591309	-0.295654	0.385508	0.281158	1.727539	1.936234	-0.513046	0.527534	-0.866669	0.576813	0.130432	0.115944	-0.055069	0.089859	-0.547826	1.730438	-0.176811	0.942028	-0.144928	0.18261	2.339127	-0.104355	0.692749	0.17971	0.115942	0.252174	0.10434
Arsine_2	-0.368118	-0.263767	-0.504348	-1.199997	0.794205	-1.324646	-1.663773	0.814491	-1.257965	-1.365219	0.133339	-0.281158	-0.826088	0.173912	-0.443479	0.005798	0.086952	0.069565	-0.234783	-0.162317	-0.481171	-0.1646378	0.084061	-0.130434	-0.49855	-0.086958	-0.020279
Arsine_3	-1.304344	-0.591305	-0.113043	-0.886948	-0.518837	-1.420288	-1.066666	-0.628983	-1.27536	0.402288	0.101448	0.263767	0.1026093	-0.084061	0.515943	-0.115936	0.249275	0.252174	-0.1545622	-0.127548	-0.42058	0.066667	-0.469574				
Arsine_4	0.539131	-0.127537	-0.707247	0.562317	0.710144	-0.043472	0.704346	-0.344927	-0.823181	0.718842	-0.645965	0.473565	-0.544926	0.260872	0.142029	0.469565	1.385500	0.942024	0.930431	0.124638	0.452179	0.704346	1.295639	1.13913	-0.211594	0.144926	1.582611
Arsine_5	-0.124634	0.6029	-0.150724	0.049271	0.549422	0.179718	-0.185501	0.762321	-1.571014	1.043488	0.182602	0.162315	0.089851	0.040581	0.350724	0.527534	-0.005798	0.478264	0.463768	0.304348	1.252182	1.199997	0.771027	0.886955	0.292753	0.652174	0.078262
Arsine_6	-0.246376	-0.066669	-0.223188	-1.197113	-0.463768	-0.197971	-0.420288	-0.194199	-1.359421	-1.005798	-0.034782	-0.089855	-1.246376	-0.5942	-0.194203	-0.333332	-0.991302	-0.29855	-0.095652	0.063768	0.171021	-0.521744	0.455078	1.084059	-0.249275	0.133333	-0.205795
Arsine_7	1.04348	0.721737	1.353622	0.643478	0.478264	0.524635	0.53624	0.440582	-1.228973	0.031891	0.194206	-0.217392	1.455078	0.191299	0.634783	0.901443	-0.794205	0.423189	0.388406	0.136232	0.713043	0.040573	0.898544	-0.356522	0.356522	0.151942	0.742035
Phosphine_1	-0.105217	0.199997	-0.472464	0.084061	0.643478	-0.36232	-0.423187	-1.249276	-1.802902	-0.197098	-0.182606	-0.072862	-0.73333	0.704348	0.127533	-0.773911	-0.217391	-0.056509	-0.58551	-0.20288	0.452179	0.125218	-0.736233	-0.055073	-0.176811	-0.049271	
Phosphine_2	-0.1046371	-0.559418	0.194204	-1.269567	-0.297097	-0.025973	0.102094	0.762321	-0.721741	-0.605804	0.043476	-0.142029	-0.475357	-0.228989	0.231884	-0.086989	-0.547825	-0.0452173	0.046377	0.597101	-0.910156	-1.179718	0.017391	-0.165217	-0.069565	-0.549437	
Phosphine_3	0.942024	0.301449	-0.063768	0.12175	0.68116	0.571014	0.214493	-6.565216	-4.582611	0.162323	0.701447	0.715942	0.017395	-0.600006	1.284058	-0.011597	-0.718838	0.956522	0.023188	0.394203	0.576813	-0.228989	0.020279	-0.82029	0.08116	0.208696	1.455078
Phosphine_4	1.115936	1.304348	1.185507	-0.049271	0.222091	-1.057968	-0.443481	-0.008694	-1.617386	-0.631882	0.059999	-0.014492	-0.623184	-1.31884	-0.431883	1.185504	0.460869	0.828987	0.046377	-0.124638	-1.017394	-0.388397	-0.110305	0.481159	-0.124638	-0.080461	
Phosphine_5	-0.715942	-0.356522	-0.46087	-0.834793	-0.507248	-0.881157	-1.562516	-0.715935	-0.08696	-0.171021	0.191303	-0.373912	-1.10144	-0.576813	-0.457972	-0.362519	-0.146956	-0.124638	-0.06087	-0.125737	-0.234783	-0.663373	0.275363	0.156522	-0.11884	0.321747	
Phosphine_6	-0.1260872	-1.353622	-0.863773	-0.634781	0.162323	-1.165222	-0.298553	-0.939133	-0.718842	-0.172141	0.301449	-1.379707	0.707245	0.263768	0.321739	-0.162323	-0.066676	0.037682	-0.840576	0.131944	0.198188	0.8116	-0.44928	0.154057	0.918833	0.205797	-0.101444
Phosphine_7	-0.533333	-0.031883	-0.194204	-0.973907	0.153625	-0.402088	0.115944	-1.936234	-0.12319	-0.1884	-0.324638	-0.22319	-0.782608	-0.072464	1.104347	-1.191299	-0.1037682	-0.614494	-0.217391	-0.489855	-0.704361	-0.388412	-0.330435	0.272464	-0.014492	-0.069565	
Diborane_1	-0.336227	0.156521	-0.107246	0.310135	0.110146	0.069565	0.750732	1.18261	-0.246384	0.773911	2.115936	0.852173	0.663765	0.50145	1.298553	-0.028984	1.350723	-0.211594	-0.385508	0.553619	0.382614	0.194199	-1.257973	0.73913	-0.0579	-0.823196	
Diborane_2	-0.843475	0.492752	-0.172157	0.431885	-0.031876	0.20294	-0.020294	-0.484045	-0.342026	0.579712	0.078262	-0.217392	0.333334	0.936234	0.036766	0.1046375	-0.226087	-0.344927	-0.866669	-0.446381	-0.072464	-0.472464	0.208696	-0.176811	-0.307674		
Diborane_3	-0.249275	0.4927																									

	R01	G01	B01	R02	G02	B02	R03	G03	B03	Supplementary Material (ESI) for Chemical Communications This journal is © The Royal Society of Chemistry 2010	R04	G04	B04	R05	G05	B05	R06	G06	B06	R07	G07	B07	R08	G08	B08	R09	G09	B09		
Ammonia_1	-2.069565	-2.17977	-3.730434	-1.539139	1.084061	-7.237686	-1.634796	7.518837	-16.3595	S-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000		
Ammonia_2	-0.72464	-1.663769	-4.115943	-0.869553	0.031883	-6.855072	-0.802902	6.397102	-15.64928	-4.843491	-0.44928	12.51305	-0.98262	-2.898552	-0.608696	-12.65218	3.979706	0.301449	0.168116	-0.194206	-2.443466	-1.478271	-2.199997	-1.576813	-0.463768	-1.457972	2.666672			
Ammonia_3	-0.666664	-2.579708	-3.297254	-1.660873	-0.13044	-5.397095	-2.266663	4.924637	-12.83479	-8.011597	-1.298598	-11.22898	-1.565216	-2.492752	-0.884046	-9.99131	4.075363	1.286957	-0.086957	-0.846376	-1.39711	-1.272461	-1.918839	-1.97971	-1.730434	-1.756519	1.307236			
Ammonia_4	0.194199	0.353622	-1.585507	0.127533	0.240578	-3.39994	-0.643478	4.907242	-9.22319	-6.524628	-1.34203	11.65217	0.886963	-0.014494	-11.80869	4.492752	1.168118	-0.043478	0.249275	0.41449	-0.173904	0.295654	-0.22319	-1.344927	-1.640579	5.240585				
Ammonia_5	-0.666664	-0.913044	-3.76232	-1.579712	0.521736	-3.211594	-1.031891	5.226089	-13.80289	-6.747833	0.768112	13.19131	-0.478256	-1.301453	-0.463768	-12.33334	5.115944	1.118839	0.171014	-0.252174	-1.428986	-1.678268	-0.744934	-0.631882	-0.762319	-0.81739	2.86087			
Ammonia_6	-1.255074	-1.973911	-3.814493	-2.017395	-0.481163	-5.391304	-2.156525	1.918839	-7.701447	-7.286957	-0.588402	10.77971	-0.60289	-2.260864	-1.484058	-14.78841	4.37101	0.249275	-0.095652	-0.713043	-1.263779	-3.289856	-1.55072	-1.420288	-2.397102	-1.211594	2.484055			
Ammonia_7	-5.472466	-3.768116	-4.8	-0.788406	-0.165222	-4.336235	0.350723	5.750725	-9.953629	-2.89566	1.298546	11.2029	1.884048	-0.86377	-1.976812	-10.84638	7.081161	0.652176	-0.002899	-0.15942	-1.063766	0.594193	-1.095642	-2.869564	-0.933332	-1.913044	6.455078			
HCl_1	-5.736229	-0.675362	0.684058	-2.121735	-0.214493	-11.46957	-0.102024	-0.121742	-2.272461	-0.495667	-0.286957	-10.56233	0.124641	-3.597101	-0.802902	-0.057968	-0.002899	1.8	1.66087	-0.201159	-2.165652	25.71884	20.91884	-44.77681						
HCl_2	-5.573914	-0.188408	1.588406	-1.066666	0.426694	-12.50154	-0.481155	0.147827	1.098541	0.13623	0.466667	-1.533333	-3.805789	-0.382614	-2.478262	-0.605797	-0.446381	-0.228985	5.066667	9.652172	-52.51595	4.521744	-46.94202	25.79421	41.12464	34.7913	-44.95943			
HCl_3	-4.733337	0.29855	0.860869	-1.86087	-0.205803	-10.06377	0.028976	-0.202904	-1.269562	-0.147827	-0.831886	-2.197098	-8.89856	-0.782608	-1.950724	-2.507968	-1.768112	-1.76811	4.17971	6.243477	-50.30145	3.118851	-43.60291	23.69855	32.62899	27.35072	-44.37972			
HCl_4	-7.568115	-1.805801	1.747827	-3.376816	-0.092758	-14.11884	-1.979706	-1.898544	-0.002899	-1.886963	-0.005798	-2.539131	-11.88117	-2.084061	-2.828983	-2.973907	-1.695656	0.472462	4.628985	8.353622	-55.04057	2.828979	-49.83768	-2.95942	41.13623	36.05797	-40.06087			
HCl_5	-5.460869	-0.1046375	1.289855	-0.721741	-0.446381	-10.59421	-0.472473	-0.182602	-1.289856	-0.382616	1.753624	-2.869568	-9.704346	-0.849274	-1.742636	-1.086952	-0.460869	0.130432	3.8	3.74027	-45.37102	6.550755	-41.43189	21.86377	32.22319	25.87246	-42.46376			
HCl_6	-6.107246	0.455074	1.704349	-1.924637	0.278259	-10.84058	0.165207	0.188408	0.562317	-0.652176	1.330437	-3.281166	-9.495651	0.205795	-2.411594	-1.771011	-0.194206	-0.15942	3.976811	8.260872	-4.93768	3.211594	-47.74202	25.26667	35.71015	30.56522	-41.40458			
HCl_7	-12.28986	-2.915939	1.150724	-4.562332	-0.756523	-15.22029	-1.77681	-0.99131	-2.272461	-0.507248	0.686958	-3.304352	-13.29276	0.008698	-2.852175	-2.579704	-2.698555	-0.040577	4.02029	9.191307	-63.05797	1.330429	-53.44058	28.81739	41.05508	37.16812	-41.93333			
(CH3)NH2_1	-8.11592	0.26667	-2.550725	-0.979706	1.417389	-8.86087	-1.591309	0.455078	-18.16812	-0.404587	-2.344925	-0.696953	0.002899	-2.075363	0.730434	-9.571007	3.632974	-0.480458	-0.115942	-0.356522	-1.857971	-0.356522	2.397102	-3.055073	-1.637684	4.39711				
(CH3)NH2_2	6.843483	0.191307	-2.147826	-1.914993	2.591309	-8.924637	-1.066666	9.779709	-14.65508	-4.10144	-1.388409	6.953625	-1.756516	-0.857971	-0.991304	-2.72464	1.391304	-0.313048	0.115942	-0.193334	-0.542038	0.092758	0.568115	-1.014492	-0.333334	4.634781				
(CH3)NH2_3	-4.765221	-0.759422	-0.17971	-0.617386	1.371017	-6.799886	-1.289856	-3.478256	-1.97681	4.771015	-0.800003	-0.1846375	-0.1037682	-5.68115	3.762314	1.620289	0.185507	-0.397102	0.631882	-0.591293	-0.243484	2.811592	-3.36232	-2.127533	6.39711					
(CH3)NH2_4	-5.936234	0.49855	-1.527536	-1.652176	2.330437	-7.289856	-0.675354	7.142029	-10.91014	-4.095657	-1.504349	5.866666	0.066666	-2.008698	-1.855072	-3.288695	2.118843	0.391304	0.288986	0.417393	-0.765213	-1.344925	0.324646	2.460869	-1.568115	-0.614494	3.710144			
(CH3)NH2_5	-7.814491	1.371014	-1.571014	-1.525167	2.342026	-8.304145	-0.040573	0.125913	-19.35942	-4.234787	-3.034782	8.33913	-1.133331	-2.327686	-1.284058	-4.084061	3.776811	-0.208988	-0.0286087	0.165216	0.240585	-0.199997	0.762339	0.173912	-0.362318	0.124638	2.692764			
(CH3)NH2_6	-10.26956	-2.26667	-3.371014	-1.753616	2.571014	-9.91304	-0.60289	10.10145	-12.71724	-3.420288	-3.826207	5.997101	-2	-1.443481	-0.492754	-6.798457	2.147827	0.544926	-0.22029	-0.060871	-0.171015	-0.402976	-1.031883	0.454926	-0.324463	-0.571014	0.852173	0.4742458		
(CH3)NH2_7	-8.339127	-0.182606	-0.46376	-0.472466	-0.3742466	-10.4058	-0.324026	12.84638	-20.55072	-12.72464	-1.510147	12.73866	0.127533	0.286957	-0.243479	-2.74492	1.718842	0.101452	0.089859	-0.324463	-0.571014	0.852173	-0.457977	-0.113043	-0.542024	-0.669566	2.742458			
C12_1	-5.837685	0.863377	-0.92174	-3.057968	2.133331	-8.246368	-0.634781	0.121742	-0.47827	-0.985519	-1.118843	0.573914	-2.889862	0.284058	-3.194206	-1.869568	0.44928	-2.857971	2.692754	5.118839	-5.107254	0.301453	-4.330438	-0.193334	-0.542038	0.092758	0.568115	-1.014492	-0.333334	4.634781
C12_2	-4.547829	1.072464	-0.437681	-4.014496	1.953621	-3.550735	-0.3643781	-0.385508	-0.47827	-3.257965	0.678261	0.443478	-1.762329	-0.014488	-1.313044	-1.501442	-0.304344	-0.90435	3.176812	5.675362	-5.284058	-1.017395	-5.939133	18.24348	46.65507	40.69276	-18.42319			
C12_3	-2.689879	1.110146	-0.4	-4.028976	2.373909	-6.814499	-0.605804	-0.310340	-15.20726	-4.17392	-0.22319	-0.426086	-0.017395	0.739136	0.107246	-3.247382	-1.260872	-0.095654	5.50725	5.507248	-1.50725	-0.1726087								
C12_4	-4.901443	0.950722	-1.460869	-4.576813	1	-6.739136	-1.608688	-1.197098	-0.163473	-0.634781	-0.34263	-0.50724	0.843491	-3.631884	-3.628983	-0.712741	-0.405623	4.159215	0.535519	-3.535519	-0.333334	29.89565	26.292898							
C12_5	-3.562317	2.191307	0.092753	-2.777909	2.524635	-5.776817	0.391296	0.385506	0.075363	-3.194214	0.153625	-0.266666	-1.394203	0.588402	-0.008696	-1.205803	-0.101597	-0.686958	4.008698	-4.333328	1.231888	-4.628983	4.86087	35	27.75652	-27.88986				
C12_6	-4.730438	1.310304	-0.037682	-3.359421	2.263771	-5.22319	0.472458	0.092758	-0.10144	-3.263779	-0.168114	-1.866661	-1.744919	0.198839	-2.223188	-0.762314	0.104355	-2.594204	3.591304	6.36232	-6.159409	-0.373917	-3.939133	18.93623	51.02319	44.4174	-17.40869			
Phosgene_1	-3.44928	0.8111592	-0.953623	-3.544937	1.855072	-6.36232	-0.388412	-0.363211	-0.22319	-0.382895	0.026085	-0.915939	-1.695663	-1.208694	-1.805798	-1.446381	-0.481154	-0.008698	-0.866668	0.347839	-3.689865	-1.718842	10.33333	4.988403	-11.83479					
Phosgene_2	-0.400002	-0.162319	-0.104058	0.197024	-0.379707	-0.176819	0.510147	0.176811	-0.304342	0.211493	0.165211	0.162318	0.176811	0.084061	-0.16521	0.19711	0.102319	0.02028	0.156523	0.156815	0.310147	-0.356522	-0.715942	20.297	0.25507	-0.206093				
Phosgene_3	-0.263763	-0.289852	-0.165216	-0.686966	0.034782	-0.382614	0.675369	0.373913	-0.652176	-0.96521	1.217392	-1.568115	0.191299	0.13623	0.727535	0.144928	0.09565	0.463768	0.185507	-0.165215	-1.426086	0.046371	-0.440582	0.107391	6.176815	-8.246368				
Phosgene_4	-0.901443	-0.602894	-0.391304	-1.113052	-0.985504	-1.570372	-1.36232</																							

	R01	G01	B01	R02	G02	B02	R03	G03	B03	R04	G04	B04	R05	G05	B05	R06	G06	B06	R07	G07	B07	R08	G08	B08	R09	G09	B09
SO2_1	-0.049278	-0.02319	-0.336232	-1.037674	-0.084061	-0.953621	0.22319	-0.110146	-0.971009	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779	-0.970779
SO2_2	-0.075363	0.446377	0.344928	0.118835	-0.875366	-0.049271	0.043472	0.118843	-2.31015	-0.217392	-0.402901	-0.110146	0.086952	0.330429	0.655073	-0.226089	-0.182606	-0.730436	-0.226087	-0.544928	-0.2562317	3.10434	-26.32173	-9.582609	15.07826	6.797102	-51.30145
SO2_3	-0.910141	-0.373913	0.188406	-0.347824	-2.115936	0.391296	-2.631882	-0.559422	-0.979706	-1.144928	0.017391	-0.678261	-0.678261	-0.739128	0.991304	-0.324638	-0.472466	-0.330437	0.24058	-0.521738	-3.182602	2.713043	-28.14493	-7.573914	11.33044	4.799999	-52.31303
SO2_4	-0.023193	0.017391	-0.173913	1.507026	-0.22319	-0.478256	-0.376816	0.162315	-0.408691	-0.39711	-0.150723	-0.072464	0.243477	0.200005	0.347826	0.655075	0.159424	0.736229	0.536232	-0.144926	-3.156525	14.220291	-26.84638	-9.498552	14.25218	6.03768	-53.44927
SO2_5	-0.886955	-0.269566	0.127536	-1.173904	-0.762321	-0.124641	-1.466666	0.13913	-0.388397	-0.452164	0.411594	-0.127537	-0.620293	-0.663765	-0.31884	0.194199	-0.805794	-0.70145	0.510145	-0.127537	-0.279712	1.426086	-25.05217	-10.00869	11.06087	3.930435	-51.53334
SO2_6	-0.26667	0.626087	0.631884	-0.29274	-0.466667	0.686958	-1.142029	0.028988	-0.713043	-0.544922	0.284058	0.228985	-0.220291	0.130432	0.272465	-0.568115	-0.072464	-0.750725	0.263768	0.162319	-3.623184	2.579712	-28.03479	-5.611594	4.924639	1.2	-46.18262
SO2_7	-0.307243	0.484058	0.165217	-0.382614	0.055069	-0.886955	-0.881149	0.368118	-0.991302	-0.930435	0.4058	-0.29855	-0.797104	0.585503	0.695652	-0.82029	-0.011589	0.701447	0.315942	-0.031885	-1.628983	3.365219	-24.12465	-9.130436	12.26377	4.971016	-51.33913
HCN_1	-2.037682	0.028984	0.173913	-0.730438	0.028984	-4.446381	-0.026093	-0.788406	-0.130447	0.005798	-0.385506	-1.985508	-3.901451	1.00869	-0.939131	0.831879	0.521744	-0.672464	-16.65508	2.573914	-25.24059	-6.127537	3.686956	-0.739132	-41.88695		
HCN_2	-0.782608	-0.040581	0.07826	-1.263763	-0.623192	-4.45507	-0.373917	0.278267	0.171100	-0.055069	-0.588406	-5.063766	0.982613	-0.669565	-0.553627	-0.58551	-0.38261	0.278261	-1.220289	-2.63763	2.194199	-15.3942	-4.6029	5.191305	2.478262	-36.66667	
HCN_3	-1.391304	0.591305	0.455072	-0.162308	0.411591	-0.5028984	0.014496	0.144928	0.110138	0.73912	1.142029	-1.107246	-4.028984	1.692749	-1.744926	0.110146	-0.165222	0.150723	0.26087	-0.486956	-18.44348	4.234787	-36.88406	-7.556522	5.066668	1.889854	-28.08986
HCN_4	-1.840576	-0.046377	0.391304	-1.249268	0.011597	-3.5942	-0.904358	0.420292	-0.176804	-1.507248	-0.211597	0.510147	-0.544928	0.084057	-0.678261	0.313044	0.127536	-1.269568	-16.50433	2.846375	-25.79329	-1.715942	2.002897	-0.373913	-25.37972		
HCN_5	-1.17971	0.504349	0.298551	-0.333344	-0.31015	-4.159424	0.142029	0.202896	-0.124634	0.623184	0.133331	-0.692757	-1.368118	1.434784	0.142029	-0.234782	-2.608696	-0.950726	-0.243477	-12.29855	3.249283	-19.89566	4.257971	4.321739	1.402899		
HCN_6	-0.304344	1.057968	0.724638	-1.147827	-1.234787	-4.443474	-0.263763	0.388405	-1.278259	-0.727464	0.70145	-0.582611	-1.257965	1.031883	-1.01449	-0.599988	-1.084061	-0.13913	-0.215194	-1.371016	-14.24058	2.542023	-23.13623	-5.402898	3.701448	1	-25.40579
HCN_7	-0.939125	0.510145	-0.249275	-0.611588	-0.211601	0.311595	-0.50145	0.18261	-0.243484	0.524643	-0.02319	-0.669563	-0.388405	0.020899	0.208695	1.460869	1.26667	0.3049278	-0.478262	-4.524628	2.130432	-12.21449	-4.463769	3.959421	1.098551	-29.13335	
HF_1	-4.260864	-0.017391	1.220288	-2.110138	0.147827	-12.59421	0.527527	-0.649277	0.3060867	-1.504349	0.255074	-0.503434	-12.87246	-1.176811	-1.142029	-1.408691	-0.159416	-0.15942	-0.002899	-1.597101	-7.65217	4.220291	-40.06087	-7.278261	6.486956	2.049274	-33.56522
HF_2	-3.771019	0.275364	-0.084058	-3.989544	1.350723	-0.9855072	0.017395	-0.194206	-0.260864	-3.246368	-0.443474	-0.489857	-3.976814	1.736237	-0.799999	-0.553619	-0.121742	-0.49855	0.269565	0.127535	-3.936234	2.591293	-32.10146	-5.762318	7.269566	4.144928	-36.24059
HF_3	-1.875366	0.347824	0.597101	-3.307251	1.313049	-0.8043782	0.127533	0.411591	0.208696	-2.455063	-0.5034782	1.344933	-0.678261	-1.217681	-1.191307	-0.191307	-0.713043	0.869565	0.179771	-1.715940	5.208694	-30.53624	-3.4	12.39131	7.605797	-32.15942	
HF_4	-3.18261	0.602898	0.478261	-4.246368	1.556519	-7.852173	-0.226074	0.263767	1.492752	-4.028992	0.188404	-0.452175	-6.495651	0.875366	1.069565	-0.924637	-0.382614	0.623192	0.472464	-0.055073	-11.47826	3.460876	-37.48116	-2.231884	3.313044	2.113043	-22.8
HF_5	-4.631882	0.234783	0.962319	-7.173904	2.426094	-11.83189	-0.768112	-0.791298	0.057968	-4.991302	0.773914	-1.930431	-1.7594208	1.463768	-1.266667	-1.756523	-0.765221	-1.34203	0.539131	0.362318	-19.02608	5.182602	-48.98261	-9.402898	10.67247	6.949429	-27.21159
HF_6	-4.5942	0.556519	0.342029	-6.376801	2.313042	-12.22318	-0.408691	-0.327538	1.631882	-4.107254	1.527534	-0.8195653	-0.672464	0.81739	-0.956522	-1.185509	0.150726	-0.930435	0.733333	-0.782608	-16.56232	3.553619	-43.71594	-6.791305	6.640579	3.823189	-25.27827
HF_7	-2.579712	1.11594	1.298551	-4.27536	0.976814	-0.805569	-0.646378	0.568115	0.973907	-0.191299	0.686958	-0.307243	-2.849274	0.968117	0.481159	-1.211594	-0.504349	-0.460871	0.678261	0.449274	-13.05217	3.846376	-22.83479	12.39131	7.605797	-32.15942	
HNO3_1	-3.765213	-0.576813	0.295652	-2.194214	-0.478256	-8.628983	-0.750717	-0.440575	-0.884064	0.652176	-0.252171	-1.417393	-17.50145	2.701447	2.110145	0.002899	2.365219	0.66087	-0.026087	-1.243477	-4.710144	0.982605	-13.44638	-2.626087	2.052174	-0.710145	-19.15942
HNO3_2	-5.898552	-0.18261	1.753623	-1.08696	-0.026093	-7.933334	-0.228989	-0.550728	3.246368	1.721741	1.002891	-0.066673	-19.69276	-0.704353	2.21739	0.217392	0.901451	0.373913	0.846377	-0.144928	-1.130432	4.066666	-20.53044	-0.301449	2.197102	-0.359421	-13.57101
HNO3_3	-4.831886	-0.669563	1.507247	-1.014496	-0.023193	-8.034784	-1.292755	-0.330437	0.684052	0.394121	0.646378	-1.156525	-13.91594	-0.640579	1.188406	-0.744934	-0.228989	0.423187	0.115942	-0.713043	-3.26957	2.782608	-13.62608	0.921739	2.086956	0.84058	-16.58841
HNO3_4	-3.765213	-0.576813	0.295652	-2.194214	-0.478256	-8.628983	-0.750717	-0.440575	-0.884064	0.652176	-0.252171	-1.417393	-17.50145	2.701447	2.110145	0.002899	2.365219	0.66087	-0.026087	-1.243477	-4.710144	0.982605	-13.44638	-2.626087	2.052174	-0.710145	-19.15942
HNO3_5	-4.026085	-0.179707	1.437681	-0.350739	-0.18261	-7.223183	-0.495651	-0.791306	0.202079	2.031876	0.4058	-1.231888	-13.43478	-1.063774	1.249275	-0.597099	-0.411598	-0.008694	0.075362	-0.965218	-1.330429	2.226089	-7.736221	-0.026087	1.594204	-0.521739	-13.4087
HNO3_6	-2.852173	0.066666	1.321739	-1.069565	-0.194199	-7.168114	0.794205	-0.295647	1.373917	0.776825	0.733333	-0.005791	-13.28406	-0.910141	1.817391	0.475357	0.057968	0.089855	0.571014	-0.208694	-1	1.86087	-6.898544	-0.884058	2.211594	-0.550725	-12.95941
HNO3_7	-2.863762	-0.527538	0.4	-0.982605	-0.742027	-6.510139	-0.22319	-1.272461	0.869568	1.13623	0.881165	-0.298553	-11.08406	-0.742027	2.802608	2.426086	4.973915	0.211594	-0.336231	-2.052185	0.982605	-4.553619	-2.168116	1.585508	-0.211595	-9.388405	
Hydrazine_1	-6.336227	-1.037678	1.06087	-0.292755	0.620293	-1.611595	-0.469574	0.611595	-1.927536	-1.605789	1.289852	2.136234	-0.686958	0.1037682	0.518841	-0.089859	3.327538	-0.150726	0.162319	-0.046375	-0.13623	-0.715942	1.840576	1.657797	-2.753624	-1.214493	3.869568
Hydrazine_2	-5.800003	-0.66087	0.944927	-0.17392	0.14782	-0.101448	0.373917	0.962318	-2.10434	-0.631897	-0.7971	3.098549	-1.846382	-1.773911	0.611594	-0.747826	2.228989	0.043478	0.095652	0.156521	0.402893	0.301453	1.681168	1.965218	-2.542027	-1.13623	4.347824
Hydraz																											

	R10	G10	B10	R11	G11	B11	R12	G12	B13	B15	R16	G16	B16	R17	G17	B17	R18	G18	B18								
Control_1	-0.301449	-0.243477	0.507248	-0.289855	0.310143	0.037674	-0.324638	0.214493	-0.704791	0.000000	-0.000000	0.000000	-0.000000	0.000000	-0.000000	0.000000	0.000000	-0.000000	-0.272461	-2.356522							
Control_2	0.075362	-0.020579	-0.513046	-0.034783	-0.156521	0.60289	0	-0.104347	1.423187	0.078262	0.321732	1.495667	0.979706	-0.881149	-0.173914	0.202896	0.072464	0.330435	0.144928	-0.339142	0.17971	0.370170	-0.202896	0.672464	0.547821	0.043472	0.240585
Control_3	-0.142029	0.052174	-0.246384	-0.075362	0.68116	0.597017	0.014493	0.081161	-0.01738	-0.27536	-0.228989	1.594208	-0.32753	0.568115	-0.698551	-0.791306	0.333333	-0.292753	-1.263779	0.226074	0.275363	-0.222091	-0.118851	-0.023189	-0.336243	0.365204	-0.437683
Control_4	-0.107246	0.066669	0.194199	0.092754	0.011597	-0.020279	0.002899	-0.449272	-0.260868	0.820297	0.678268	0.217392	0.405792	-0.063782	0.373913	0.742035	-0.153624	0.153623	-0.127533	-0.58551	0.397101	1.63768	0.301453	0.026087	-0.399994	0.307236	-0.017395
Control_5	1.185507	0.385506	0.527542	0.501449	-0.098553	1.072464	0.086957	0.800003	1.142029	0.698547	0.124634	0.356522	0.342041	-0.089844	-0.426086	0.350723	-0.110145	0	0.55072	-1.08696	0.826088	1.081161	0.617386	0.431883	0.927536	0.002899	0.924637
Control_6	-0.304348	-0.347824	1.510147	-0.086957	-0.423187	0.371017	-0.049275	-0.075363	0.611588	-0.89856	-0.614502	3.298553	-0.153625	-0.026093	0.417393	-0.228989	0.237681	0.049275	-0.492767	-0.481171	1.089855	-0.698547	0.779709	2.623188	1.495651	0.884048	2.759415
Control_7	-0.014493	-0.246376	1.559418	0.208696	0.040581	-0.968109	0.028986	-0.13913	0.579712	-1.055069	0.484055	-0.333328	-0.066666	0.414449	-1.507246	-0.205795	-1.333332	-0.860861	-0.226074	-0.704361	0.76232	-0.298553	1.773911	0.976812	0.246384	1.278259	1.385513
HCHO_1	0.171015	0.243477	0.921738	0.298551	-0.023186	-0.527527	-0.014492	0.144928	-0.834778	0.79129	1.159424	-1.031891	0.255081	0.604579	0.997101	0.591309	0.049276	-0.197102	0.739136	0.263779	0.472462	0.852173	0.933334	1.205797	0.391296	0.510147	-0.8116
HCHO_2	-0.110142	-0.060867	0.98262	-0.078261	-0.231884	-0.481155	-0.228985	0.008698	1.252182	0.530441	0.031876	2.342041	0.785507	-0.660858	-1.243477	0.284058	0.185509	-0.620291	-0.376816	-0.600006	-0.09565	0.536224	-0.440582	0.597101	-0.956512	0.095642	0.826096
HCHO_3	-0.046377	0.240578	0.666672	-0.069565	-0.014492	-1.591308	0	-0.197098	-0.475357	-0.266663	0.2753	1.805786	-0.721747	0.179718	-0.811598	0.478256	0.139131	0.327533	-0.600006	0.243469	0.057971	-0.27536	0.075363	0.518841	-0.156528	-0.014488	0.298553
HCHO_4	-0.191304	0.252174	-0.10144	-0.26087	-0.037682	-0.168121	-0.408695	-2.250574	-1.72464	-0.281158	-0.426086	2.652176	-0.730423	-0.307236	0.678261	0.03479	0.481159	-0.092752	-1.376816	0.336227	0.65797	-0.194214	-0.718842	0.014492	-0.426086	0.559418	-0.026077
HCHO_5	-0.371014	0.318884	-0.411608	0.014493	0.101448	0.808685	0.014493	-0.075363	0.014496	-0.469574	0.339127	0.8116	-0.13913	0.559418	-0.489853	-0.028992	0.2	-0.12753	0.315948	-0.292755	0.243478	0.939133	0.127533	0.608696	0.823196	0.678268	1.414449
HCHO_6	0.04058	0.046375	-0.263779	0.15942	0.107246	-0.263779	0	-0.257973	2.243484	0.50145	0.58551	1.046371	1.359421	-0.144913	0.400002	1.208694	0.156522	-0.382609	-0.008698	0.005798	-0.113043	0.704346	-0.13913	-0.043478	0.460876	1.165222	1.17392
HCHO_7	0.942029	0.640587	1.394211	0.417391	0.310143	-0.959427	0.037681	0.426086	-0.828995	0.313049	1.03479	1.484055	0.678268	0.869553	2.898552	0.1017395	1.286957	0.979711	-0.278259	0.872452	1.620289	2.156525	1.46376	1.869564	0.243484	-0.031876	-0.106666
Arsine_1	0	-0.156523	0.426086	0.052174	0.127535	-0.773911	0	-0.104347	0.194214	0.428986	1.646378	0.2037689	0.159424	0.26088	0.747826	-0.017387	-0.591304	-0.330435	-0.084061	0.404348	-0.492767	0.910451	-0.017391	0.066666	0.376801	0.631889	
Arsine_2	0	0.118843	-0.202885	-0.101449	0.2029	-0.107395	-0.014493	-0.310143	-0.055069	-0.346666	-3.666672	-0.243484	-1.194214	-0.069563	-0.043478	-0.756523	0.005797	0.084058	0.843475	-0.489853	-0.289895	-1.382614	0.321739	0.011594	-1.391296	0.269562	-0.431885
Arsine_3	-0.011594	0.005798	0.257973	-0.211594	-0.143478	0.484055	0.86087	1.289856	-0.159424	-0.156525	-0.1092743	-0.147827	-0.463776	-0.600006	-0.171015	-0.324638	-0.002899	-0.084058	-0.956528	-0.263763	0	-0.657974	0.252174	0.014493	-0.072464	-0.965218	
Arsine_4	0.028986	0.330435	0.881157	0.121739	0.118839	0.20279	0.002899	-0.06377	-0.718842	1.698547	0.6203	1.36322	0.39711	0.840576	-0.33913	0.402893	0.046377	-0.46377	0.22319	0.518845	-0.24058	0.84639	-0.649269	-0.086957	-0.620293	-0.171013	-0.145507
Arsine_5	0.002899	0.313049	0.318832	0.2	-0.049274	1.408707	-0.057971	-0.281158	-0.105217	-0.84639	-1.889862	5.846375	0.663773	0.942032	0.536232	0.773918	0.057971	0.046377	0.100289	0.901443	0	0.402893	0.55072	0.049275	0.437683	0.669556	-0.205795
Arsine_6	0	-0.321739	1.240584	0.078261	-0.011593	-0.402893	0	-0.220291	-0.106207	0.428986	1.39131	2.423187	-0.837677	-0.424986	0.017391	-0.431885	0	0.002899	-0.936234	-0.469559	0	-0.678253	-0.681116	0	-1.45507	-0.717214	-0.785507
Arsine_7	0.069565	0.49855	1.405792	0.049275	-0.15942	0.046371	0	-0.463768	-0.324646	0.985504	-0.214493	0.802902	0.530426	0.362232	0.046377	1.118835	0.043478	-0.182609	0.437683	0.886963	0.756522	-0.313049	-0.382614	0.228985	-0.460876	-0.153625	-0.736221
Phosphine_1	0.011594	-0.028987	-0.547821	-0.307681	-0.643476	-1.431885	-0.026087	-1.147827	-2.924637	-0.773911	0.072464	-0.052174	-0.547821	-0.217392	-0.704348	0.008698	-0.052174	-0.234783	-0.255066	-0.156522	-0.257965	-0.579712	-1.515938				
Phosphine_2	-0.031884	-0.084045	-0.286957	-0.0975362	0.205797	-1.605789	0.075362	-0.304348	-0.588409	-0.255081	-0.122319	0.101456	-0.339142	-0.765228	-0.121739	-0.649277	0.434782	0.031884	-0.115583	-0.170103	0	-0.568115	-0.31884	0	0.13623	-0.359421	-0.524643
Phosphine_3	-0.002899	-0.139132	0.240584	0.286956	-0.263767	-1.127533	-0.014493	-0.191299	-1.924637	2.614502	3.385513	1.469559	0.350723	0.588409	0.234783	-2.194206	-1.214493	-1.110145	-0.565216	-0.330437	0.118841	-0.379715	-0.205795	-0.011594	-0.135622	-0.976814	0.110146
Phosphine_4	-0.002899	0.037682	-0.131594	0.072464	0.162319	-0.203769	-0.956562	-2.234779	-1.982605	-1.8116	-1.371017	1.942032	0.223175	-1.147812	-0.382609	0.547829	-0.014493	-0.005797	-0.1272461	-0.211594	-0.13913	-0.768112	-0.440582	-0.800003			
Phosphine_5	0.191304	-0.12174	0.107246	0.066667	-0.210435	-0.204946	-0.0514493	-0.750725	-2.800003	0.307674	-0.147827	-0.91304	-1.339147	-0.466675	-0.443478	-0.394203	0	0.055072	-0.178262	-0.707245	0.127536	-0.1455063	0.318383	0	-0.1217392	-1.424896	-0.515945
Phosphine_6	-0.023188	-0.881156	-0.075363	0.165506	-0.107246	-1.719321	-0.105726	-0.292755	-0.379715	-0.46376	-0.3030434	0.530434	0.084058	0.104347	0.860869	0.008696	0.115940	-0.069565	-1.5159409	0	-0.1542038	-0.469559	0	-0.137970	-0.553627	-0.37101	
Phiborane_1	-0.011594	-0.86087	-0.191299	0.307681	-0.333334	-5.953613	0	-0.90435	-5.385513	-1.765228	-0.727524	2.173904	-0.58551	-0.150711	-0.304348	0.585503	-0.008696	0.011594	-0.069565	-1.5159409	0	-0.1542038	-0.469559	0	-0.137970	-0.553627	-0.37101
Phiborane_2	-0.011594	-0.86087	-0.191299	0.307681	-0.333334	-5.953613	0	-0.90435	-5.385513	-1.765228	-0.727524	2.173904	-0.58551	-0.150711	-0.304348	0.585503	-0.008696	0.011594	-0.069565	-1.5159409	0	-0.1542038	-0.469559	0	-0.137970	-0.553627	-0.37101
Phiborane_3	-0.014493	0.704346	0.169274	0.298551	-0.104347	-0.243469	0.022899	-0.759422	-0.3466675	0.666715	0.568115	0.486377	0.826096	0.907242	0.727537	1.547821	0.602899	0.434783	0.050693	0.171000	0.002899	0.142029	0.388412	0.217393	0.1388412	0.023193	0.188416
H2S_1	0.066667	0.486958	-1.214493	0.2950725	0.034782	-69.82898	0.008696	2.50145	-27.15363	0.721725	0.834778	1.455078	0.686951	0.431885	0.142029	0.823196	0.507246	-0.037681	0.27536	0.44928	-0.197101	0.266663	0.623184	-0.286957	0.971008	0.600006	-0.452164

	R10	G10	B10	R11	G11	B11	R12	G12	B12	B15	R16	G16	B16	R17	G17	B17	R18	G18	B18								
Ammonia_1	-0.492754	-0.744926	0.15361	-0.136232	-0.991306	0.892761	-0.011594	-1.472466	-0.474705	0.506464	-0.010646	-0.010646	0.010646	1.597099	-0.9213624	-0.7509565	21.57681	-96.81739	38.82898	-21.1971	-40.14493	23.70435					
Ammonia_2	-0.005797	-1.095654	-0.579712	0.037681	-1.171013	0.095642	0.005797	-1.849281	-3.675354	6.292755	-11.39131	-125.8029	-153.9884	-98.23189	68.1884	-0.846375	3.49855	0.666668	-86.81158	-70.57682	18.84638	-127.7304	-90.03189	36.44348	-19.94202	-38.36812	20.14493
Ammonia_3	0.165217	-0.281158	-0.884064	-0.336232	-0.206089	2.304337	-0.133333	-1.530434	-0.48407	4.89856	-13.43768	-135.86383	-162.9913	-103.7739	69.14783	3.301437	5.782608	-0.942079	-77.29276	-60.52464	14.86087	-131.2232	-86.16522	31.27826	-19.14783	-28.11305	18.65956
Ammonia_4	-0.397101	-1.118483	0.194199	0.057971	-0.449276	1.208694	-0.008696	-0.504349	0.976822	6.420303	-0.068405	-0.1286145	-156.971	-97.44059	68.31594	-1.463776	4.385506	0.302094	-81.18261	-65.51884	16.76812	-130.1101	-89.24637	34.75362	-19.28116	-35.88406	22.26378
Ammonia_5	0.136232	0.165215	0.168121	-0.156522	-0.385509	2.13913	0.008696	-0.944923	-0.399999	5.295654	-0.68985	-127.7971	-155.5188	-97.45796	63.64348	-1.77681	4.765213	1.127537	-78.65218	-61.67536	16.43478	-123.2058	-82.52463	32.94203	-17.73624	-37.67825	23.41449
Ammonia_6	-0.788405	-0.907246	-1.634781	-0.315942	-2.330437	1.36232	-0.188406	-1.579712	-1.171005	4.182602	-11.53333	-123.8754	-153.6667	-95.55072	62.08986	-1.698547	7.005798	2.324638	-76.47537	-59.22028	15.02898	-125.6348	-85.48695	30.42609	-17.84638	-30.92464	14.88695
Ammonia_7	-1.136232	-0.376812	0.718842	-0.208986	-0.27536	4.17392	0	1.246376	2.165207	3.814499	-10.62898	-112.8116	-137.3507	-88.73332	59.98261	-0.918854	3.692757	1.921738	-76.46377	-60.67247	15.4	-112.069	-82.83478	31.27826	-13.95361	-29.34493	22.09566
HCl_1	2.76232	5.457973	-41.6058	5.046377	14.90435	-82.87825	0.594203	7.715942	-51.76521	0.13913	-0.315948	-22.1942	2.228989	1.886963	0.605799	-0.020294	-5.684059	1.266661	0.695648	-6.376816	3.336232	2.408707	-1.113052	0.852174	4.820297	5.826096	-5.79129
HCl_2	10.03188	11.63188	-41.85217	10.4058	25.24927	-83.52463	24.09275	14.18262	-52.55653	1.623199	0.765228	-23.43477	3.678253	1.956512	5.559422	0.144928	-5.257973	0.402901	-0.095657	-2.649277	3.307247	5.733337	-0.568115	4.681158	7.469574	5.814484	-6.228989
HCl_3	6.544927	8.791306	-47.05217	8.60687	18.77681	-80.44637	3.991304	9.626083	-50.50725	1.376816	0.634781	-23.23479	1.44928	1.814484	5.324638	1.779724	-3.475365	1.730434	0.704346	-3.936234	0.2037682	6.762314	0.373917	3.04058	7.701462	8.710144	-5.831879
HCl_4	13.9942	15.33913	-57.83188	14.25507	28.45218	-79.68115	12.73913	8.857971	-50.0145	-0.106376	-0.27536	-29.20869	-0.13913	0.298553	4.29565	0.157968	-8.159424	0.655075	-1.698563	-6.681152	4.530435	5.286957	4.385513	4.846375	-8.849274		
HCl_5	6.231884	8.631886	-40.51015	7.069565	16.74203	-75.46376	5.872464	7.846375	-52.95653	0.942032	1.431885	-14.74022	1.304337	0.7913106	3.878258	0.50145	-6.428986	1.649277	-0.702745	4.553635	0.788405	3.049271	0.991302	3.124638	5.147827	5.785507	-7.252167
HCl_6	14.78261	17.91304	-62.14204	9.275362	21.42609	-80.16812	36.2	17.24638	-57.94782	2.527542	-0.17392	-32.04927	3.095657	3.347824	3.823189	0.733337	-6.866669	1.571014	-0.342026	-4.907242	4.997101	4.455063	-1.457977	2.504347	5.828995	5.521729	-6.58551
HCl_7	5.57971	7.826092	-37.35075	6.823188	20.85797	-82.75653	6.828985	10.88406	-55.53334	-2.394211	-2.58551	-31.73044	-2.60289	-1.72464	3.515945	-0.208557	-11.18261	1.005798	-3.13015	-5.310135	2.866667	3.579712	-2.742035	3.133335	5.782608	7.31015	-8.994202
(CH3)NH2_1	-0.562319	-0.907242	1.060867	-0.481159	-3.884056	8.008698	-0.762319	-0.110597	-0.924637	8.44928	-0.344925	-9.43624	-7.765507	54.95653	-2.424384	5.515938	9.265218	-74.11015	-60.01449	18.4029	-112.1159	-74.31848	30.74493	-13.28406	-23.15363	11.31014	
(CH3)NH2_2	0.057971	0.031883	-0.272476	0.336232	-0.49855	1.86087	0	-0.782608	-0.178482	3.739136	-5.39711	-0.803447	-149.771	-88.35072	50.84348	0.77681	8.49276	0.600002	-78.51015	-55	15.06087	-111.487	-73.75073	28.53043	-9.304352	-13.15071	0.162323
(CH3)NH2_3	-0.695652	0.046379	0.318848	-0.756522	-3.971016	9.127533	-1.133333	-0.707245	2.713058	4.191299	-8.228989	-85.24928	-123.9623	-77.16811	64.61449	4.179703	11.73623	0.133333	-85.94202	-73.64059	25.13044	-98.50435	-71.81449	30.43478	-9.895645	-19.9971	11.85217
(CH3)NH2_4	-0.449276	-0.663765	-0.194214	-0.618159	-4.27536	9.107254	-0.333333	-0.794205	5.121735	9.434784	-10.646261	-145.0522	-89.29565	54.08696	0.203178	11.4087	2.513042	-71.49566	-55.84927	13.36323	-114.2493	-73.85217	28.50435	-12.04637	-23.8139	13.52173	
(CH3)NH2_5	0	0.176811	0.037689	0.176812	0.095654	0.904343	0.05797	-0.605797	0.072464	4.304352	-0.623184	-65.40869	-85.66087	39.82319	0.107239	5.266666	0.171013	-61.02898	-31.9855	4.008696	-101.8319	-57.15363	16.38551	-8.040581	-11.23478	2.359421	
(CH3)NH2_6	-0.173913	-0.571014	-0.63768	0.011594	-0.597099	0.2072464	-0.043478	-1.017395	-0.623184	3.739136	-6.72464	-8.659622	-153.1044	-89.45217	50.072426	1.49855	4.743477	0.307682	-85.96232	-65.028298	17.79421	-110.0783	-65.34493	21.08116	-8.62086	-10.02319	-0.840576
(CH3)NH2_7	-0.014493	-0.055073	0.513046	-0.037681	-0.463768	0.852173	0	-0.759422	-0.507248	3.075363	-5.695648	-74.44638	-154.7072	-90.62898	48.92464	1.481155	5.260886	-0.489855	-73.38841	-44.67536	8.623188	-113.5159	-62.44637	17.29275	-8.872467	-12.04927	-1.446365
C12_1	2.710145	3.307243	-8.417389	4.646377	9.310143	-7.805801	13.69855	6.727539	-7.344925	6.124634	-0.281158	0.846375	1.530441	0.579697	0.54203	4.220896	3.272859	2.110145	0.05217	-0.336227	0.649277	1.023193	-0.211594	0.376812	4.220291	6.565216	4.231888
C12_2	6.205799	4.288956	-9.104344	4.973913	13.0116	-6.084061	17.37971	9.020294	-7.214493	-0.092743	-0.481171	6.173681	-0.031876	0.715942	1.373917	2.312888	4.101448	1.860636	-0.565216	0.095657	0.791306	0.469559	-0.295654	0.252174	4.327545	6.13913	-0.194214
C12_3	4.237681	5.652176	-16.43189	2.814493	10.58261	-5.79129	8.153623	6.17392	-3.214493	-1.402893	-1.79129	-1.837677	0.681152	0.260864	-0.130432	-0.420288	4.771019	1.055077	-0.588409	-0.718842	1.455072	1.50145	-0.034775	0.621724	3.428986	7.782608	
C12_4	2.402899	3.2689569	-8.185516	5.217391	11.72754	-7.63768	12.41449	6.994202	-6.368118	-0.342026	-0.582611	-0.997101	-0.513046	-0.272461	0.686958	-0.875366	2.66086	-0.982605	-1.315948	-0.031883	0.102318	0.107316	0.32188	0.344925			
C12_5	3.269566	4.976807	-11.2058	4.991304	12.17681	-5.324631	8.852173	7.947983	-8.02902	1.56525	0.704346	0.1884	0.730423	1.715942	0.652172	0.623673	6.263763	3.513039	0.489853	0.220921	0.269566	0.791306	0.1008698	-0.228985	4.333328	6.663757	-0.866669
C12_6	3.057971	3.666664	-7.475357	13.58551	16.704035	-3.785507	18.69275	9.286957	-5.321744	-0.753616	-0.199997	0.718842	0.405792	0.985504	1.101448	0.747818	4.501545	1.626091	-0.194199	-0.762314	0.823189	2.115936	0.460861	-0.347826	5.234787	9.234772	-0.249268
Phosgene_1	0.234783	0.518841	-1.657974	0.489855	0.834785	-5.492752	0.336232	0.898552	-3.678253	-1.368118	-0.069565	-0.513031	0.649277	-0.057968	0.008696	0.655075	0.617391	0.130435	-0.573914	-0.481155	0.675217	0.579712	-0.484055	0.327536	0.371017	0.62899	1.13913
Phosgene_2	0.043478	0.578802	-1.93334	0.652174	1.211594	-0.582605	1.417391	0.793715	-0.005798	-0.855072	0.391296	-0.171021	-0.295853	1.098549	0.143472	-0.391306	-0.214493	-0.405807	0.820297	-1.527536	0.385513	-0.33913	0.168121	0.144928	-0.43187		
Phosgene_3	-0.442029	-0.226086	-1.469559	0.626087	0.140581	-4.617386	1.892754	0.226089	-0.353622	0.715942	0.837677	0.606867	-0.0452185	0.194499	-0.846375	0.307684	-0.052185	0.034782	-0.408697	0.353622	0.701462	-0.968124	-0.408697	0.620291	-1.171005	0.084061	-1.086945
Phosgene_4	-0.631885	-0.211594	-3.185501	0.397102	0.286957	-7.055069	1.257971	-0.852173	-7.408707	-0.965225	-0.739136	-1.028976															

	R10	G10	B10	R11	G11	B11	R12	G12	Supplementary Material (ESI) for Chemical Communications This journal is © The Royal Society of Chemistry 2010										B15	R16	G16	B16	R17	G17	B17	R18	G18	B18		
SO2_1	1.24058	6.211594	-27.24637	0.156522	0.200001	-6.744919	0.011594	-0.713043	-2.68957	0.008696	-0.634789	-3.579712	-0.118851	0.614502	-0.965225	0.750732	-0.446365	-0.171013	0.840591	-0.017391	-0.301449	-0.843475	0.32753	-0.62029	0.368118	-0.379715	0.15942	0.843491	1.655075	-1.68985
SO2_2	0.672464	4.947826	-22.3913	0.426087	-0.373913	-6.857971	-0.008696	-0.634789	-3.579712	-0.118851	0.614502	-0.965225	0.750732	-0.446365	-0.171013	0.840591	-0.017391	-0.301449	-0.843475	0.32753	-0.62029	0.368118	-0.379715	0.15942	0.843491	1.655075	-1.68985			
SO2_3	0.443478	4.168114	-24.22609	0.176811	-1.188408	-8.460861	-0.113043	-1.976814	-4.13913	-0.156525	-3.127545	-0.397095	0.478256	-1.10434	0.405796	-1.782608	0.034782	-0.005797	-0.095657	-1.113052	-0.631885	-0.576813	-1.568113	-1.055072	-0.750732	-0.069565	-3.373917	-1.971008		
SO2_4	3.75942	7.965218	-28.28407	0.35942	-0.533333	-7.171005	0.002899	-1.153625	-2.455078	0.159424	0.217392	0.194199	0.840576	-0.069565	0.675362	0.666656	0.373917	0.005798	-0.550773	-0.260864	-0.220291	0.805786	0.797104	0.762319	1.823181	0.576813	-1.971008	0.272323		
SO2_5	2.753623	5.579708	-24.52174	0.57971	-0.77681	-8.527527	0	-1.63768	-3.626083	-0.41449	-1.046387	0.75943	-0.75943	-1.573914	1.069565	-0.771011	-0.428986	-0.069565	-0.759415	-1.162323	-0.588406	-0.857971	-0.782608	-0.947826	0.037674	-0.153625	-3.081161			
SO2_6	0.017391	2.866667	-18.83188	-0.008696	-0.255072	-5.008698	0	-1.165222	-3.837677	-1.03479	-0.426086	0.515945	0.208694	-0.808701	0.373913	0.095657	0.107246	0.47826	-0.197098	-0.478271	0.42029	-0.255066	0.353622	0.501449	-0.446381	0.791298	-1.321732			
SO2_7	4.521739	8.324642	-28.61739	0.315942	0.075363	-7.756516	0.005797	-0.600006	-2.750717	-0.643478	0.571014	-0.852173	-0.46666	0.342026	0.266666	-0.872467	0.646378	0.22029	-0.527527	0.028992	0.385508	-0.399994	0.089844	0.15942	0.52185	2.600006	-2.008698			
HCN_1	0.028986	1.973913	-16.83479	0.2524638	1.776812	-56.20869	0	-0.643478	-30.11015	-0.736237	-0.455063	0.736237	0.127533	-0.339127	-1.643478	-0.057968	-0.246377	0.037681	-0.321747	0.582611	-0.336232	1.373917	-0.113045	-0.008696	0.944923	0.623192	-1.652176			
HCN_2	-0.005797	2.142027	-17.63768	0.915942	0.527534	-46.8203	0	-1.802895	-34.6174	1.399994	0.489853	7.669556	0.542023	0.057968	0.33913	-0.405792	-0.391304	-0.153623	1.142029	-0.176804	0	0.373917	0.031883	0.043478	1.075363	0.573914	-2.333336			
HCN_3	0.017391	1.695652	-17.26088	3.875362	1.605797	-55.27286	0.191304	-1.144928	-28.79998	1.040573	0.289856	1.930404	1.269562	0.681168	-0.947826	-0.25798	-0.231884	-0.266667	0.701447	0.385513	0.35942	1.050569	0.176811	0.008696	1.597107	1.136238	-0.727539			
HCN_4	0	1.069565	-15.74203	2.481159	0.733332	-46.30435	0.318841	-2.414494	-26.00578	-1.785507	-0.313034	0.86087	0.223175	0.040573	-0.118841	0.055084	0.081159	-0.098551	-0.597107	0.295639	0.028986	0.22899	0.249275	0.414494	0.924637	0.515945	-1.460869			
HCN_5	0.913043	2.240578	-15.55943	3.582609	1.750725	-56.76521	0.197101	-1.797104	-28.6145	0.831894	0.74202	1.24057	0.005798	-0.133331	0.168116	0.484055	-0.072464	0.226087	0.171378	0.466675	0.866667	1.110138	-0.197105	-0.292754	1.092751	0.686958	-1.147812			
HCN_6	0.008696	1.605799	-16.97102	3.234783	1.588406	-55.54492	0.005797	-2.156521	-25.83768	0.376801	0.950729	2.797104	0.681152	-0.185516	-0.64058	0.101456	-0.092753	0.026087	-0.77681	-0.084061	0.049275	0.220291	0.147827	0	0.333328	0.623184	-1.243484			
HCN_7	0.005797	1.466669	-13.75652	2.869565	0.968115	-58.87247	0	-1.692757	-31.91304	1.057968	1.640579	2.930433	0.376801	0.318848	-0.66666	0.681152	0.304348	-0.072464	0.631882	0.660858	-0.005797	0.573914	-0.689857	-0.014493	0.585503	0.339127	-0.162323			
HF_1	0.005797	4.034782	-27.30725	1.466667	0.788406	-32.36812	0	-2.388405	-19.1971	0.13623	0.779709	1.759415	1.602905	0.081161	-1.391304	0.255066	-0.365218	0.014493	-0.918839	-0.249274	0.321739	-0.646378	-2.791306	0.069565	0.208698	0.628983	-2.626099			
HF_2	2.594203	5.982609	-28.41738	1.808696	2.814491	-33.22609	0	0.840584	-18.79131	0.13913	-0.046371	-0.133331	0.684067	-0.420288	0.655075	0.179703	-0.284058	-0.573914	0.269562	-0.869568	0.568116	0.126957	-0.469566	0.005797	3.356522	2.460087	-2.41449			
HF_3	0.257971	5.715942	-25.51884	1.553623	2.805794	-32.93333	0	1.440582	-17.3884	0.985504	0.652176	-0.521729	2.58551	0.131891	0.701448	1.307251	0.533333	0.327538	2.402893	-0.1249268	0.255073	2.936234	0.614487	0.005797	3.408699	0.305798	0.217392			
HF_4	0.272464	3.785507	-23.88988	2.095652	1.710144	-34.24348	-0.142029	0.727539	-18.33913	-0.286957	-0.82608	0.13913	1.542023	0.17392	0.666667	0.771011	0.005797	0.313044	0.388397	-0.510147	0.049275	1.478271	0.292755	0.02029	0.924637	2.063766	-1.985504			
HF_5	0.231884	5.17971	-26.69855	2.188406	2.788406	-31.65797	0.005797	1.095657	-16.30145	-0.852173	0.744934	2.936234	1.304352	-0.475357	0.688954	-0.692749	-0.22319	-1.452175	-0.657974	-0.582611	0.84058	0.904343	0.518845	-0.043478	5.063766	4.886955	-3.898544			
HF_6	0.237681	4.65797	-25.30725	2.165217	2.226089	-32.41161	-0.002899	1.605797	-16.54782	-0.597092	0.086984	-0.043472	1.988403	0.823196	0.391304	0.123193	0.327538	0.765219	0.939133	-0.2388412	0.376812	2.318848	0.011597	-0.33913	2.94783	3.704346	-1.973907			
HF_7	0.388406	4.469566	-20.85217	3.623188	4.191303	-26.32175	0.052174	1.150726	-12.69565	0.101597	0.310135	0.588409	2.495651	0.553619	1.408695	-0.197098	0.031883	0.2029	0.756516	-0.252182	1.171014	1.675369	-0.504333	0.524638	3.881165	3.597099	-4.266663			
HNO3_1	0.005797	1.043478	-14.6029	1.269565	1.463768	-25.67825	-0.002899	-2.165215	-15.92174	-0.730438	0	-5.933334	-0.1052185	-0.496561	-1.284058	-1.153625	-0.568116	-1.85797	-2.50145	-0.086957	-1.611603	0.256811	-0.1255074	-2.582605	-0.608696	0.252174				
HNO3_2	0.510145	2.098549	-11.57681	2.246377	0.457972	-26.32175	0.002899	-0.86377	-14.58261	1.768112	2.231888	-14.0116	2.147827	0.72464	0.165217	0.559433	0.852174	0.594203	0.326088	2.118835	0.524638	4.081161	0.208984	0.028984	0.304344	0.304344				
HNO3_3	0.089855	0.985506	-12.14783	1.727536	-13.6232	-27.81448	-4.191305	-6.97971	-18.0058	-0.142029	0.171021	-10.23767	0.420288	-0.759415	-0.565217	-1.199997	-0.507246	0.107246	0.443481	0.252182	0.130435	0.118835	0.475362	1.602898	0.371017					
HNO3_4	0.005797	1.043478	-14.6029	1.269565	1.463768	-25.67825	-0.002899	-2.165215	-15.92174	-0.730438	0	-5.933334	-0.1052185	-0.496561	-1.284058	-1.153625	-0.568115	-1.857971	-2.50145	-0.086957	-1.611603	0.256811	-0.1255074	-2.582605	-0.608696					
HNO3_5	0.008696	0.707246	-6.765213	1.214493	-0.521738	-18.03188	0.127536	-0.802898	-12.65506	0.078262	-0.698547	-1.872467	0.892746	-0.744934	0.014493	0.228981	-0.228985	0.037681	-0.1031876	-0.408699	0.043478	0.817398	-0.434784	1.182606	1.159424	-1.623192				
HNO3_6	-0.002899	1.113045	-8.50145	1.098551	-0.104347	-16.52754	0	-1.310143	-10.25508	0.092758	0.588409	-2.124634	0.756531	-0.402893	-0.411594	0.933334	-0.046377	-0.031884	-0.333344	0.307236	0	2.315933	1.553627	0.371015	2.249275	0.202087	-0.768112			
HNO3_7	0.002899	0.846376	-8.252174	1	0.518841	-15.36232	0.156522	-0.898552	-11.21159	-0.620285	-1.078262	-1.226089	-0.428986	-0.530441	-1.269565	0.243484	0.315942	0.052174	-0.336227	1.400009	0.150725	-0.614502	-0.521736	-0.078261	1.36232	1.365219	-0.36232			
Hydrazine_1	-0.072621	-0.565216	1.220291	-0.211594	-0.455074	1.933334	-1.336232	-0.095657	1.727539	-0.005798	-0.681168	-12.47246	-21.8232	-8.704346	4.060871	-0.333344	0.5942	0.101448	-0.869568	-0.762329	0.686956	-13.93333	-5.031876	0.6	-2.020294	-2.521744	1.623184			
Hydrazine_2	-0.46087	-0.324638	1.782608	-0.510145	-0.460869	2.707245	-0.257971	1.237686	0.333328	-0.313049	-0.704346	-9.542038	-11.50435	-4.147827	3.411598	0.371017	0.62899	-0.492752	-0.553619	0.455063	0.385508	-11.54492	-4.53334	3.115942	-2.765228	-2.217392	1.176819			
Hydrazine_3	0.028986	-0.327538	0.573																											

	R19	G19	B19	R20	G20	B20	R21	G21	B24	R25	G25	B25	R26	G26	B26	R27	G27	B27									
Control_1	0.046387	0.124649	1.762314	-0.402908	0	0.675362	0.695663	0.785507	0.677926	0.695663	0.785507	-0.014493	0.234787	0.34203	0.527534	-0.072464	0.333344	0.605804	0.63768	-0.228989	0.930435						
Control_2	0.507248	-0.536224	-0.040588	0.715942	-0.544937	0.394203	0.44928	0.710144	0.353622	0.408691	0.715942	-0.08696	-0.075363	-0.669556	-0.092758	0.272469	0.327536	-0.211594	0.13913	-0.092754	0.084059	1.226089	0.597092	-0.014481	0.205795	-1.843475	
Control_3	-0.211594	-0.797104	0.066666	-0.423187	-0.043472	-0.156521	-0.150726	-0.162308	0.220291	-0.1037682	0.27536	0.388412	-0.614487	-0.057233	0.571014	-0.753624	-0.411594	-0.197102	-0.243636	0.237679	0.518841	-0.573914	0.046371	-0.759415	-0.779709	-0.423187	-0.286957
Control_4	1.666672	0.204927	2.144913	0.150726	0.417389	-0.400002	-0.234787	0.791306	-0.077681	0.376816	0.53334	0.05217	-0.68696	-0.031883	-0.246377	0.118841	0.150726	-0.066666	-0.10145	0.36232	0.602905	-0.171021	-0.107254	0.350723	0.779709		
Control_5	1.10434	0.246384	-0.017395	0.605804	-0.36232	0.255074	0.031876	-0.440567	0.2092758	1.081161	-0.568115	0.736237	0.371017	0.547821	0.742035	0.588402	-0.226087	-0.13913	1.255081	-0.017391	-0.110144	0.295654	-0.379715	2.028994	0.640579	-0.828995	3.478256
Control_6	0.359421	0.428986	0.939133	-0.263763	-0.739136	0.17971	-0.457977	-0.037689	0.895653	0.643478	-0.399994	0.289856	0.005798	-0.759415	0.823198	-0.089850	0.078261	0.318841	0.68985	0.666668	0.788406	0.953613	-0.597092	0.544922	-0.399994	-0.478256	2.313049
Control_7	-0.77681	0.353622	-0.915939	0.327538	0.197098	-0.15942	0.599991	-0.121735	0.588402	0.240585	-0.208694	1.278275	-0.733337	0.817383	-0.649277	-0.388412	-0.394203	0.104348	-0.321747	0.802898	0.826088	-0.142029	0.904343	-1.142029	0.715942	-0.686966	1.428986
HCHO_1	1.115952	1.356522	-4.779703	0.043472	0.214493	0.840576	0.936234	0.518845	1.31884	0.115944	0.142029	1.379715	1.084061	0.86377	1.130432	-1.515938	0.298551	0.026087	0.869568	1.072464	0.49858	0.773911	0.695663	-0.107254	1.211594		
HCHO_2	-0.063766	0.423187	-4.405792	-0.182602	0.069565	1.266666	-0.063766	-0.173904	0.805801	-0.020287	-0.281158	0.562317	-0.408691	-0.1037674	-0.049271	-2.026085	0.168116	0.11884	-0.147827	0.266663	0.124634	-0.344925	0.028976	-0.455078	0.026093	-0.576813	-0.124634
HCHO_3	0.040573	0.318832	-0.249855	-0.524643	-0.44928	-0.144928	0.107254	-0.342026	-1.127541	-0.257973	-0.115944	0.142029	-1.034775	0.307251	-0.1640579	0.318841	0.281510	-0.991302	0.953625	0.2040581	-0.489868	0.126952	0.211594	-0.475373	0.718842	-0.146381	
HCHO_4	-0.86377	-0.250566	-4.562317	-0.217377	0.289856	0.515945	-0.246368	0.434784	-0.930435	-0.402893	0.240578	0.637676	-0.98262	-0.657959	1.73912	-1.968117	0.286957	-0.249275	-0.828995	0.901451	0.609565	-0.605804	0.081161	0.944931	0.110153	0.544922	-0.892761
HCHO_5	0.324631	0.475357	-3.66665	-0.255068	0.701447	0.365215	0.924637	0.77681	0.223183	0.313042	0.486961	0.94783	0.591309	0.020294	0.802902	-1.101448	0.249275	0.208698	0.478271	0.466667	-0.22219	0.162308	0.179718	0.866669	-0.344925	0.081146	-0.8116
HCHO_6	-0.313049	0.507233	-3.988403	0.889847	0.26088	-1.321739	1.060883	0.102318	-0.014488	-0.040581	0.028984	0.872467	1.394196	-0.162323	-0.342026	-1.199997	0.078261	0.226087	0.55072	0.727539	0.205509	0.904343	0.234787	0.350723	1.759415	0.2057968	
HCHO_7	1.652176	1.39711	-3.376801	1.171021	0.315933	0.069565	1.507248	1.68985	0.414497	0.057976	0.339134	1.113052	-0.092758	0.023193	0.72464	-1.257973	0.457971	0.518841	1.788406	1.605797	1.857971	0.237671	1.214493	0.907257	1.510415	1.542023	
Arsine_1	-1.133331	-1.165222	-1.421837	0.121742	0.118843	0.463768	0.40009	0.466667	0.260872	-0.539131	0.22319	-0.942032	-0.208694	0.976822	0.130432	0.768116	0.37971	0.286957	0.075363	0.371016	0.637681	0.05217	0.237686	0.257965	0.333328	0.588394	0.179703
Arsine_2	2.704346	1.849274	-1.620285	-0.605797	0.434784	-0.02319	-1.249268	0.45507	-0.139137	-0.237679	-0.17971	-0.602905	-1.437683	0.22319	-0.765213	-0.628986	0.165217	-0.263768	0.475732	0.246376	-0.165276	-0.199997	0.075348	-1.944202	-1.327545	0.133331	-0.153625
Arsine_3	-0.605789	-1.118835	-0.991302	-0.626091	-0.440582	0.031885	-1.098557	-0.22319	0.240578	0.289856	0.243477	0.084061	-0.684052	0.678253	-0.063766	-0.055073	-0.121739	-0.197102	-0.556519	-0.275362	0.292753	-1.284058	-0.498555	0.521744	-0.971008	-1.347824	0.1081146
Arsine_4	1.031876	0.457962	0.292755	0.205795	0.428986	0.356522	0.002899	0.446373	0.350723	0.226088	0.281158	0.857971	0.985519	0.411591	0.055084	0.050571	0.176182	-0.060869	0.1915955	-0.153624	0.710144	0.782608	0.660873	0.942032	-0.405807	0.843491	0.318832
Arsine_5	0.956528	0.127192	1.495667	0.713043	0.794025	-0.356522	1.605789	0.939123	0.350723	0.191303	-0.118835	0.588409	-0.385513	0.401724	0.136521	0.208694	0.179718	0.617401	0.28116	-0.043478	0.179718	0.420288	1.657974	0.105657	0.205811	-0.1544922	
Arsine_6	1.542038	1.327545	1.32753	0.446381	0.118843	0.66087	0.092743	0.892754	0.13044	-0.084057	-0.205795	1.057968	-0.260864	-0.426086	-0.530441	-0.298555	0.098551	0.15942	0.863777	0.852174	0.724638	0.350723	-0.237686	0.92605	0.486954	0.58551	0.278259
Arsine_7	-0.153625	-0.950729	-2.576813	0.695648	0.779709	-0.34203	1.205795	0.79129	0.368118	-0.313042	0.973907	0.73912	-0.831894	0.805786	0.028984	0.243478	0.121739	0.318848	0.063768	0.130435	0.669556	0.095657	0.043472	0.107395	0.698547	-0.257965	
Phosphine_1	-3.571014	-2.982605	-0.288841	-0.782608	-0.037682	0.055073	-0.478256	-0.217392	-0.8223189	0.330433	0.17013	0.330429	-0.336227	-1.744919	0.301437	-0.055073	0.028899	-0.4	-0.002899	-0.255072	0.124639	-1.539139	-0.1884	-0.849274	0.211594	0.663375	-1.324646
Phosphine_2	-0.049271	0.011597	-0.295654	-0.950722	-1.118843	0.4	-1.597107	-1.089859	-0.924637	-0.301449	-0.559948	-0.907242	-0.1057968	-0.1023178	-1.582611	-0.26087	0.049275	0.472464	-0.376801	-0.684058	0.088955	-0.988419	-0.959412	-1.536224	-0.828979	-0.988403	-0.3797
Phosphine_3	0.197113	-0.521729	-2.008698	-0.226082	0.391304	-0.617392	0.031891	0.257973	-0.765221	-0.171017	-0.579712	-0.988403	-0.640579	-1.962326	-0.028992	0.142029	0.42029	0.765217	0.420288	-0.147825	-0.617392	-0.400009	-0.646378	1.460861	0.820282	0.63768	-1.252167
Phosphine_4	0.808685	0.127548	-1.043488	-0.144928	-0.272461	-0.533333	0.118851	-0.1002892	-0.837685	-0.072464	-0.739136	-0.556519	-1.13623	-0.44928	-3.150711	-0.211594	0.02029	-0.336227	0.130432	0.228985	0.318848	-0.704346	-1.571014	-0.301015			
Phosphine_5	-1.382614	-1.585511	-0.482896	-0.72464	-0.481155	0.057972	-1.530441	-0.223183	-0.17971	-0.811592	-1.310153	-1.721741	-0.204892	-0.002899	0.043478	0.289855	-1.006968	-0.13913	-0.4058	-1.747833	-0.971008	-1.840591	-0.681152	-1.426102	-1.118835		
Phosphine_6	-6.214493	-5.956512	-0.740458	-1.489275	-1.55072	-0.881161	-0.260006	0.157394	-0.146378	-0.501455	-0.163768	-0.463768	-0.240896	-0.246376	-1.22319	-0.313042	-0.072464	-0.146377	-0.718482	-0.173913	-0.166656	-0.263766	-0.834778	-1.794205	-1.753632	-1.605789	
Phosphine_7	0.110153	-1.608704	-1.930435	0.539131	-0.060867	-0.266666	-0.910141	-1.220291	-0.292753	-0.040577	-0.605804	-0.872467	-0.2147827	-0.295654	-0.379711	-0.226087	0.495652	-0.921738	-0.536232	-0.028986	-0.402908	-0.486954	-0.397095	-1.179718	-1.623233	0.750732	
Diborane_1	0.417389	0.513046	0.304352	0.333336	-0.101448	0.814493	1.197073	0.849281	-0.110146	0.715942	1.243477	0.260864	-0.098557	0.103479	-0.336227	0.518841	0.194206	0.10145	0.13913	0.171005	0.1576813	0.330444	0.344925	1.199997			
Diborane_2	0.098541	0.857971	1.417389	-0.31884	0.727539	1.327545	0.107395	0.217379	0.1327545	0.101735	0.208694	0.495651	1.524643	1.701462	0.634781	1.342026	0.585507	0.733337	0.614491	0.991304	-0.875366	0.085504	-0.278259	-0.084061	0.536519		
Diborane_3	0.405792	0.684067	1.982602	0.008698	-0.162315	0.504349	-0.6203	0.640579	0.13623	-0.020754	0.318754	-0.695648	0.872452	0.318823	-0.260958	-0.017391	-0.052174	0.130143	0.203188	-0.681152	-0.27536	-0.170015	0.474273	0.202688	0.707245	0.243188	
Diborane_4	0.230452	1.204058																									

	R19	G19	B19	R20	G20	B20	R21	G21	B24	R25	G25	B25	R26	G26	B26	R27	G27	B27
Ammonia_1	-1.979706	-1.75943	-0.86377	2.350723	-5.431885	4.005798	-4.388412	-2.846375	-0.277187	-0.777777	-0.120294	-0.120294	-0.120294	-0.120294	-0.120294	-0.120294	-0.120294	
Ammonia_2	-1.521744	-1.594208	-2.005798	3.060867	-6.182617	4.208698	-2.753632	-2.400009	-0.140582	6.831879	3.715942	-6.513045	-3.078247	-3.231888	-2.901459	44.10725	27.52753	-1.66087
Ammonia_3	-2.020294	-2.339127	-1.507248	3.750725	-7.040573	5.115944	-2.762314	-5.153046	-1.046379	6.918846	4.272461	-6.133331	-2.884048	-2.75943	-2.402893	40.9884	17.06087	-1.353623
Ammonia_4	-0.292755	-0.104342	3.933334	-4.211609	4.037682	-1.991302	-0.191299	1.057968	7.742027	6.36232	-4.6203	-1.150726	-1.031876	-1.513046	44.33333	30.76522	-3.686957	
Ammonia_5	-1.205795	-0.376816	-1.782603	3.736237	-5.597107	5.811592	-2.933334	-1.831879	-0.118843	7.156517	6.260872	-4.426086	-1.524643	-0.857971	-1.428986	48.50436	28.44638	-0.44058
Ammonia_6	-2.295654	-1.394211	-3.411591	3.246376	-6.762321	5.301453	-3.063782	-2.930435	-2.669571	7.144928	4.820297	-5.930435	-2.394211	-2.591293	-3.655075	45.61449	29.28116	-0.171014
Ammonia_7	-1.382614	-0.344925	0.002899	4.368111	-5.098549	4.408699	-2.440582	-2.104355	1.044928	6.104347	5.568115	-2.968124	0.663773	1.113037	2.686951	45.77681	22.35652	-0.927536
HCl_1	-0.118835	-1.211594	-1.260864	-0.617393	0.173912	-0.489857	2.324631	-17.31884	-2.49855	1.069565	-0.002899	-3.663575	11.77971	10.06668	5.907242	-17.53913	5.124638	0.475362
HCl_2	0.408691	-0.034775	1.666672	0.53334	0.678268	-0.678261	1.107254	-13.04927	-0.397095	0.434776	0.649277	-1.052185	11.92174	8.924637	5.399994	-23.09275	1.643477	1.411594
HCl_3	1.168106	1.031891	-1.368118	0.005783	-0.768112	0.255074	3.524643	-14.11304	0.107246	0.040581	-0.104355	-2.411591	1.897098	5.588409	3.971008	16.28985	4.156522	0.889859
HCl_4	-1.765213	-0.376816	-1.460861	-0.105217	-1.979706	-1.295654	-0.886963	-16.62608	-0.875366	0.41449	-1.617386	-3.427545	10.72464	9.234787	3.39711	-19.42603	3.631884	1.446377
HCl_5	0.773911	0.46376	0.226084	0.113052	0.284058	-1.481159	1.550735	-16.70435	-2.257973	-0.313049	-0.379715	-3.744934	13.51883	11.77101	8.272476	-19.13913	3.501449	1.681151
HCl_6	0.710144	0.434784	0.933334	-0.73912	0.649277	0.171017	2.142029	-17.78551	-1.144928	1.344925	0.542023	-2.579712	11.28696	7.089859	5.513046	-21.33913	2.466667	2.518841
HCl_7	-3.855075	-0.3794196	-0.5097243	-2.371017	-1.889862	-1.950726	-0.184416	-24.7942	-4.420288	0.301453	0.75943	-4.591293	13.15073	11.2	3.86377	-2.192568	1.510145	-1.519452
(CH3)NH2_1	-2.03479	-0.988403	-1.765213	-0.286957	-1.973907	-0.208694	-2.573914	-1.118835	0.31042	3.892754	1.199997	-3.310409	-0.040588	-3.307251	-1.942032	22.63769	25.44638	-0.02029
(CH3)NH2_2	-0.492752	-0.55072	-0.191315	0.486954	-2.35363	1.34203	-0.837677	-0.614487	-0.388405	4.507248	-8.730423	-1.179703	-2.744934	-0.46666	15.68116	3.107246	-0.6	-0.71014
(CH3)NH2_3	-1.110153	0.13623	0.730438	0.203479	-2.466675	2.220287	-0.843475	-0.43187	1.50145	6.072464	3.176819	-4.469559	-1.075363	-2.098557	0.008698	20.76522	20.24058	-0.226087
(CH3)NH2_4	-0.078262	0.281158	-0.469574	0.939125	-2.03479	0.11594	-1.046371	-0.588409	0.150726	7.655067	3.397095	-6.214934	-1.133331	-2.257965	-0.63768	23.08406	12.0058	-0.104348
(CH3)NH2_5	0.805786	0.072464	1.649277	0.020287	0.5942	0.565216	-0.518845	-0.744934	0.947823	8.469566	5.080461	-8.959412	1.24057	-1.423137	-0.394211	13.25507	0.455072	0.736232
(CH3)NH2_6	-2.655075	-2.814499	-3.947815	-0.002899	-0.475365	1.231884	-0.921738	-2.852173	-2.347785	9.936234	3.397095	-0.579712	-1.834778	-3.307236	-0.631882	12.49275	1.330435	-0.536232
(CH3)NH2_7	-1.243484	-1.234787	-0.686951	0.765221	-2.165215	0.568115	-0.553635	-0.576813	-0.4058	8.918846	4.5942	-7.8116	-0.828979	-2.25798	-0.614487	12.97971	0.214493	-0.721739
C12_1	0.002899	0.0	0.03479	0.191315	0.24057	0.156621	-0.333344	2.391312	1.522174	2.756516	0.272461	0.303444	5.095657	1.918839	1.942032	-17.51594	-3.304348	0.275362
C12_2	-0.515945	-0.359421	1.428986	0.084061	0.043488	0.852177	0.178262	1.927536	-0.27536	2.982613	1.379715	0.910156	0.286957	0.608704	1.127533	-22.66812	-5.739131	0.237913
C12_3	0.756516	0.295654	-0.072464	-0.185501	-0.530441	0.289854	0.008698	4.159409	-0.104927	2.599998	1.379715	1.41449	-0.202896	1.217392	0.771011	-16.62029	0.289855	0.4
C12_4	-0.255066	-0.0944202	0.63768	-0.933334	-0.431885	-0.005795	-0.336227	3.565216	-1.605797	1.747826	1.194199	-0.197113	-0.663773	-0.582611	-1.394211	-19.49275	0.710145	-0.185501
C12_5	1.144928	0.634781	0.915939	0.385513	0.205795	-0.147823	0.41449	2.510147	-0.397102	1.263219	1.573914	0.649277	1.605804	1.927536	1.834778	-19.45507	2.075363	0.104205
C12_6	-0.066666	0.68985	0.05217	-0.542023	0.628983	0.02029	2.324787	2.768127	-1.344925	3.192861	2.284058	-0.466666	-0.159409	0.519593	0.666656	-27.52464	-0.107246	0.771014
C12_7	-0.628983	0.344925	1.736221	-0.014486	0.608704	0.133331	0.782608	3.391312	-1.640579	4.402893	1.91304	-0.382599	-0.147827	0.77681	-0.026077	-21.32464	-6.081159	1.402899
Phosgene_1	-0.39711	1.330429	-1.107254	0.504349	0.130432	0.385508	-0.252182	0.284058	-0.469559	0.191307	0.539131	0.513046	0.881149	-0.085841	-2.930435	0.142029	0.220579	-0.17392
Phosgene_2	-0.249268	-0.350723	0.773911	-0.03479	0.701447	0.544926	1.330429	0.055069	0.475357	-0.521744	0.095657	-1.402908	-0.191299	0.67247	-1.594193	0.452171	-0.086956	-0.017391
Phosgene_3	0.756516	1.573914	1.455078	-0.200012	-0.365219	0.292755	-0.802902	0.05217	0.211601	0.59998	0.271392	-0.507248	-1.005798	-0.823181	-2.715942	-0.956218	0.318841	0.173913
Phosgene_4	-0.727539	-1.237686	-0.669556	-0.166666	-0.924637	-1.156521	-2.101456	-0.710144	-0.973915	-0.663765	-1.176819	0.362305	-1.202896	-4.475357	-0.744934	0.098551	-0.324638	-1.713043
Phosgene_5	-0.344925	-0.026077	0.321732	-0.791306	0.037689	-0.037682	0.405584	0.49855	-0.469559	-0.1057968	-0.657959	0.307326	-0.382686	-1.365219	-1.069563	0.110145	-0.089855	-0.156528
Phosgene_6	-1.657974	-2.289856	-0.643478	-0.559418	-1.710152	0.008698	-0.481155	-2.428986	0.133339	-1.037682	-0.2704264	-1.727539	-3.318848	-4.404058	-0.5942032	-1.530344	0.069565	-0.173913
Phosgene_7	1.243469	1.13913	1.950728	-0.391304	0.191299	-0.069565	-0.944931	0.605804	-0.469558	-0.985512	0.089859	-0.397111	0.36232	-0.600006	-3.368118	-0.434784	0.02029	-0.223188
F2_1	1.023193	0.391312	2.411591	0.24057	-0.663773	0.423187	1.124634	1.762314	1.628983	1.330429	0.539139	0.72464	-0.313034	-0.962326	-0.078262	-18.98551	-0.391304	-0.373913
F2_2	-0.05217	-0.347839	-0.037688	0.156525	-0.110345	-0.29568	0.234772	0.918839	2.200005	0.701447	0.127533	0.953629	0.696956	-0.249828	-0.159402	16.40863	2.507246	1.849275
F2_3	-0.060883	-0.237671	0.452177	-0.344925	0.368103	0.211594	-0.684052	1.533325	1.440575	0.402893	0.086898	-0.234844	0.417389	0.324646	-0.069565	15.63768	0.880458	1.478261
F2_4	0.41449	1.005798	0.634781	1.246384	0.169565	-0.570525	0.255081	1.521744	1.513046	1.914214	0.991302	-0.237688	0.284058	0.747818	-14.81874	14.96233	0.67247	0.67247
F2_5	-0.782608	0.060867	-0.1043472	-0.371017	-0.518829	1.31884	-0.588409	2.330429	1.428986	1.773911	0.075363	0.446381	0.084061	-0.353622	-0.475372	-22.91595	1.246377	-0.110138
F2_6	-0.614487	0.072464	0.347824	0.063768	-0.457962	0.988407	0.20294	1.411591	0.124641	0.353622	0.130432	-0.336227	-0.371017	-0.747818	-16.55652	0.727139	1.87261	0.353622
F2_7	1.27536	0.057968	1.36232	0.057958	-0.744934	0.176185	0.101456	1.342026	1.669571	0.823189	0.689865	0.289856	-0.44928	0.924637	-16.50145	0.77971	1.510343	0.994202
N02_1	1.67247	2.788406	0.765213	1.428986	0.608696	0.127536	0.284058	0.747826	7.771011	1.13044	1.028984	-2.56813	0.6286957	0.375945	-0.08696	-3.249275	0.368985	0.350725
N02_2	0.924637	1.376816	0.254643	0.353622	0.33913	0.313044	0.313034	0.718826	3.008698	0.1046376	0.185509	-3.536224	0.807262	5.886948	-3.553635	-3.846378	0.457942	0.457942
N02_3	-0.33344	-0.026093	-0.144															

	R19	G19	B19	R20	G20	B20	R21	G21	B24	R25	G25	B25	R26	G26	B26	R27	G27	B27													
Supplementary Material (ESI) for Chemical Communications This journal is © The Royal Society of Chemistry 2010																															
DOI: 10.1039/C0000000000000000																															
S02_1	-0.376816	-0.695648	-0.382614	-0.388412	-0.00869	0.646378	-0.408070	-0.315948	-0.247174	-0.00869	0.646378	0.646378	0.666666	-0.232188	0.846375	0.234779	-0.06377	-0.205811	-0.353622	0.910156	-0.350723	0.373917	0.333328								
S02_2	0.440582	0.124649	0.353622	-0.594208	1.678262	-1.285509	0.530441	-0.249268	0.252174	-0.347824	-0.002899	-0.202896	0.234787	0.107254	-0.420288	-0.263771	0.22029	0.136223	-0.202911	0.298553	0.211594	0.497252	-0.295639	-1.185501	0.157098	0.626083	2.011597				
S02_3	0.556519	-1.423187	0.115936	1.663773	2.17971	4.005798	-2.385513	-0.510147	-0.568123	-0.440578	-1.034782	-0.678253	-1.686966	-2.991302	-1.713043	-1.124641	-0.982609	-2.173912	0.150711	-0.747826	-1.055073	0.350723	-1.582611	-1.005798	-2.107254	0.063766	1.89566				
S02_4	0.41449	0.08698	0.773911	0.49855	-1.431885	-2.463768	0.797104	0.2002899	0.492752	-0.220284	0.191299	-0.446365	0.808701	-0.162308	0.33912	0.063766	-0.350724	0.197101	0.1069566	-0.063766	-1.727535	0.988403	0.205795	1.611603	0.255081	0.866669	-0.26088				
S02_5	-0.698547	-1.144928	0.933334	-0.933334	-1.014448	0.837681	-1.289856	-0.321747	-0.481155	-0.460876	-0.692757	-0.108945	-0.449298	-0.779709	-0.239711	-0.568115	-0.359421	-0.431884	-0.962311	-1.336235	-1.507248	-0.944931	-2.281158	3.320429	-4.168121	3.13913	15.23189				
S02_6	-0.730423	-0.397095	0.1518845	-0.544922	-0.107242	0.382608	-0.185516	-0.31884	0.698551	-0.84058	-0.623192	0.901459	-0.026077	0.337674	0.542023	-0.591305	0.437681	-0.234782	-0.162323	0.046379	0.12464	-0.217392	0.078262	0.759451	-0.10434	0.043472	0.904343				
S02_7	-0.159424	0.63768	-0.414505	0.017395	1.005798	-0.162319	0.771011	1.985504	-0.295647	-0.023186	0.495651	-0.153625	0.124634	0.950729	0.231873	0.249275	0.857971	0.405797	0.94783	1.49855	0.655071	0.36232	1.568115	0.118851	-0.385513	1.295654	2.168121				
HCN_1	-0.556519	-0.333328	-1.936234	0.011597	0.336235	-0.449276	0.549492	-0.620293	0.092751	0.046375	-0.202896	-1.976822	10.9884	8.562332	2.762324	-9.130436	-0.063768	-2.113044	-0.107254	-0.542027	0.115942	0.069565	-0.121735	0.881165	0.211194	2.118835	2.968109				
HCN_2	1.130432	-0.594208	0.481171	0.330427	0.1178843	0.588408	0.052185	-0.226089	-0.220291	0.026093	-0.014488	-0.220291	4.44928	2.168106	1.040574	-6.828987	2.721739	1.924638	0.646378	-0.994202	0.150724	0.26088	-0.257965	0.951729	0.027029	1.588409	2.892746				
HCN_3	2.228989	2.344925	0.251282	0.321739	-0.127541	0.26087	1.562317	-0.791306	0.144928	0.246376	0.53334	0.753616	0.59131	6.36232	0.702745	-4.949247	4.785507	0.597101	0.704346	0.101452	0.597101	0.133622	0.457977	-0.330429	1.365219	0.1017395	4.365219				
HCN_4	0.028976	0.289856	-1.701447	-0.217392	0.27536	-0.18261	-0.252167	0.286957	0.347824	0.072464	-0.014488	-0.333328	5.681152	4.53624	3.231888	-6.463768	5.652174	2.898651	-0.350723	-0.278263	-0.162319	-0.266663	0.272461	-1.24057	0.257965	1.297275	3.055084				
HCN_5	-2.437683	-2.446365	0.901459	0.298546	-0.005798	0.371014	0.698547	-0.249275	0.408699	0.715942	0.791306	-0.608704	9.246384	6.434781	2.347826	-6.194202	3.388406	2.362319	0.449265	-0.266666	-0.200001	-0.12175	-0.800003	1.762314	0.455078	-0.686951	-0.321732				
HCN_6	-0.39711	-0.478256	-0.855072	-0.892754	-1.608696	-2.249275	-0.1081146	-0.046371	-0.333336	0.005795	1.768111	-0.324631	6.344925	3.214493	2.078261	-6.220287	3.078261	0.234787	0.449276	0.994202	0.165222	-0.828979	0.315948	-0.344925	2.339127	2.307251					
HCN_7	0.469574	0.414505	-0.394196	-0.060875	0.417398	-0.449298	0.040573	0.228989	-0.049278	0.171013	0.231888	-1.237671	7.91304	3.950714	2.13913	-7.614494	5.249275	3.484058	0.649277	-0.133913	0.513043	0.255081	0.703408	-0.1089844	0.185516	1.89856	2.486969				
HF_1	-0.817383	-0.805801	-1.614487	-0.701447	-0.391304	-0.968117	-0.53334	-2.744926	-0.463768	0.002899	-0.594208	-3.008698	7.237686	2.118851	-1.347824	-3.602898	8.797102	1.33913	-0.124649	-0.274246	-0.54203	-1.347839	-0.617401	-2.67247	-1.008698	0.979706	2.600006				
HF_2	-0.005798	-0.104344	-0.860855	-0.13623	0.121742	1.136232	0.843475	-0.973907	1.118835	0.159416	-0.397102	-0.484055	3.214493	2.747818	0.753632	-0.794205	10.8058	4.417392	-0.095642	-1.504345	-0.011593	-0.614487	-0.742035	0.513046	0.800003	1.455063	2.214493				
HF_3	1.582611	0.474273	2.513046	1.46666	0.750717	0.208694	2.011597	0.484055	1.956261	0.753624	0.73333	0.972536	1.202896	1.394211	0.31015	-6.133335	7.133333	2.2	2.359421	-0.54203	0.102884	1.954942	0.985504	2.286957	1.823181	2.521744	5.678253				
HF_4	-0.402893	-0.217392	0.684052	0.176811	0.063376	0.594202	0.756531	-0.142088	0.907246	0.110142	-0.307251	-0.185501	4.997101	3.206844	0.898403	-0.846378	8.4	1.376812	0.762327	-0.204347	1.34203	0.055063	-0.826088	0.359421	0.318848	2.168106	3.826086				
HF_5	-0.382614	0.440567	0.321732	-0.356522	-0.040581	0.066666	0.147827	-1.553627	0.823189	-0.081161	-0.014488	-1.228973	-0.101456	-0.092758	-3.657974	-4.197102	4.313043	-0.304348	0.220291	-0.260865	0.799999	-1.182617	0.104496	0.197098	0.040573	1.455078	3.228989				
HF_6	-0.765213	-1.236539	-0.342317	-0.078262	0.18261	0.484058	1.142029	-0.344933	1.133331	0.695656	-0.301453	-0.614487	4.423187	3.713043	-0.962326	-1.217971	4.488986	-0.185507	0.765213	-1.524639	0.71884	0.057983	-0.255066	0.185501	0.544922	1.107254	4.507248				
HF_7	0.620285	-0.878265	-0.837677	0.208694	0.055069	0.866667	0.368118	-0.246376	1.251217	0.443481	0.400002	-0.104355	4.426086	3.478271	1.527527	-1.371017	4.226087	0.02029	1.936234	-0.263771	0.666668	-0.10434	-0.130432	0.284058	-0.02899	1.982605	3.118851				
HNO3_1	-1.730438	-0.39711	-1.852173	-1.147827	-0.657967	-0.594202	-0.895645	-1.579424	-1.153618	-0.376812	-0.779709	0.176804	2.310135	-0.288862	0.940203	-0.298548	0.944942	0.414493	-0.613188	-1.965218	-0.655073	-0.869658	-0.133917	-0.128115	-1.086945	1.315948	0.747833				
HNO3_2	1.307251	2.281158	1.475357	1.402901	0.553627	0.072463	2.918854	-4.075363	1.365219	0.84058	1.527534	1.301453	6.072464	6.315933	4.431885	-6.124638	3.014493	2.495652	2.434784	-0.802898	1.284058	1.721741	1.028992	2.643478	1.817383	3.8116	7.446381				
HNO3_3	-0.402893	-0.753632	-0.359421	-0.365219	0.066666	-0.188406	-0.36232	-2.367368	0.263767	-0.194202	0.278259	1.318848	1.744919	1.042926	2.915933	-1.536234	4.486957	2.266666	0.626083	-1.6	0.614492	-0.559418	-0.785507	-0.008698	-0.269562	1.797104	4.817398				
HNO3_4	-1.730438	-0.39711	-1.852173	-1.147827	-0.657967	-0.594202	-0.895645	-1.579424	-1.153618	-0.376812	-0.779709	0.176804	2.310135	-0.288862	0.940203	-0.298546	0.944927	0.414493	-0.613188	-1.965218	-0.655073	-0.869568	-0.133917	-0.128115	-0.1086945	1.315948	0.747833				
HNO3_5	-0.13913	0.857971	1.939133	0.356522	0.510143	0.246376	0.296562	-0.168698	-0.17971	0.718838	0.31884	0.391296	4.843475	4.223119	0.584809	-0.325769	0.686956	0.93913	0.292755	-0.675362	0.455072	0.640579	0.202896	-0.852173	-0.692749	1.915955	3.315933				
HNO3_6	0.113037	0.63768	0.075363	0.1086952	0.339134	1.026087	1.481155	-2.246376	0.550724	0.17971	0.663765	1.559418	6.110138	4.199997	6.744919	-3.336231	-0.06087	1.150725	0.976822	-0.31884	0.472464	0.820297	-0.144928	1.298553	1.132005	1.240209	2.857971				
HNO3_7	-0.336227	-1.075363	0.104355	0.020287	0.13623	-0.704348	0.059567	-1.515945	0.805798	0.29565	0.54203	-1.162323	3.985504	3.011597	5.356522	-4.113041	1.313044	1.205797	-0.165207	-0.788406	0.97102	-0.756531	0.544937	-0.1055069	1.503625	1.200012	3.008698				
Hydrazine_1	-0.220291	0.594208	-2.092758	-0.373909	-0.281158	-0.257971	0.103674	1.62323	-0.104347	0.391304	-0.057363	-0.492752	-0.249283	-0.771011	-0.110153	0.585506	-0.947826	0.533333	-0.446365	0.421931	0.107240	0.339127	-0.482473	-0.008698	0.2028118	-0.027447	0.486666	0.579712	0.673534	-0.1359421	4.889862
Hydrazine_2	-0.208694	-0.362305	-0.182617	-0.417389	-0.428986	0.301449	0.423187	0.10153	0.168114	0.794205	0.556519	-0.126093	-0.733337	-0.246368	0.1095657	-0.881161	-0.102318	0.907247	-0.474273	-0.008698	0.2028118	-0.1362364	-0.466666	0.579712	0.673534	-0.1359421	4.889862				
Hydrazine_3	0.628983	-0.614487	1.478256	-0.092758	0.165218	0.144928	0.489853	0.286957	-0.846382	0.394203	-0.269562	0.205811	-0.304337	0.36232	1.886963	1.211594	-0.776812	0.486957	-0.13623	0.017391	0.826088	-0.127548	0.026077	-0.420303	0.768112	-1.698547	-3.50145				
Hydrazine_4	-0.431885	0.991302	-0.266663	-0.18261	-0.028984	0.156523	-0.194199	-0.144928	-0.730431	0.388405	0.327538	-0.692749																			

	R28	G28	B28	R29	G29	B29	R30	G30	B30	B33	R34	G34	B34	R35	G35	B35	R36	G36	B36								
Control_1	-0.507248	-0.342026	-0.069565	0.339127	0.443481	-0.005798	-0.768112	0.217392	0.519816	-0.000000	-0.000000	-0.000000	0	1.371014	1.385513	-0.663757	0.342028	0.54203	-2.110138								
Control_2	-0.272476	-0.144928	0.953629	-0.327545	0.675369	-0.652176	-0.240585	-0.208694	0.208696	0.536232	0.023188	0.817398	-0.45507	-0.892754	1.200001	-1.034775	-0.440567	-0.005798	0.220291	0.536224	0.014493	-0.110144					
Control_3	-1.115936	0.336235	-0.173904	-0.530426	-0.017793	0.205795	-0.626083	0.881165	0.594203	-0.110145	0.368116	0.849274	-1.098459	-0.5675213	0.547825	-0.550735	-0.933334	-0.744934	-0.773911	-0.301453	-0.292754	-0.057968					
Control_4	-0.73912	-0.371017	-0.049271	0.118851	0.571014	-0.524643	0.252182	0.449265	0.005797	0.139131	0.223188	0.284058	-1.217392	-0.777907	-0.452171	-0.185501	-0.576813	-1.233331	-0.147827	-0.246368	0.002897	0.289852	0.594204	-0.171005			
Control_5	0.402893	-0.376816	0.371017	1.25798	0.208694	1.220291	0.921738	0.072464	-1.301449	0.481159	-0.066667	0.304352	-1.09565	-1.524643	1.286957	0.32753	-0.744919	1.907242	0.028976	-1.191299	0.640579	0.971016	0.408699	-0.020294			
Control_6	-0.214493	-0.898552	0.002894	0.046387	-0.594208	1.878263	0.118835	0.142029	0.026087	0.060869	0.185507	0.643478	-1.266663	-1.968124	1.171005	-0.634781	-0.710144	0.228998	-0.753616	-1.460876	-0.895652	-0.084061	-0.09565	0.17392	0.771013	0.159424	-0.110138
Control_7	-0.281174	0.153625	0.571014	-0.168106	0.956512	-1.579712	-0.405792	-0.768127	-0.42029	0.162318	0.124638	-0.194199	-0.397102	-0.034782	1.298546	0.884064	-0.489853	1.565216	0.417389	-0.046387	0.205797	1.455072	1.486954	-0.846375	0.185509	0.26667	-0.553619
HCHO_1	0.649277	0.802895	1.307238	-0.220291	0.559433	-0.347824	0.089844	0.759415	-0.262087	0.101449	-0.127536	0.124634	-0.368118	-0.402893	0.904343	0.997101	0.037674	1.594208	1.185501	0.046377	0.376808	0.260872	0.950714	0.25507	0.365219	-2.257965	
HCHO_2	-0.359421	0.217392	-0.260864	0.118835	-0.41449	-0.527542	-0.715942	0.188416	0.034783	-0.055072	0.168116	0.043472	-0.217392	0.228989	1.356522	-0.428986	-0.44928	-0.368118	-0.513031	-0.379715	0.707247	0.530434	0.710144	-0.197098	0.394203	0.715942	0.107395
HCHO_3	-0.86087	0.020294	0.269562	-1.484055	0.363223	-0.423187	-0.402893	-0.176819	0.005797	-0.014493	0.147826	0.03479	0.489853	0.568115	1.336227	-0.286957	0.744934	-0.469559	-0.211594	0.281158	0.420293	0.527534	-1.484055	0.272465	0.295654	-0.878265	
HCHO_4	-0.791306	0.788406	-1.495651	-0.791306	-0.269562	0.495651	-0.078262	-0.005798	0.260807	-0.208695	-0.095652	0.1043472	-1.368118	-0.889854	1.002892	-0.356552	-0.052185	-1.336227	-0.60289	0.736237	-0.481159	0.101597	0.568115	-0.046371	0.736233	0.437683	-0.631882
HCHO_5	-0.008682	0.742035	0.281174	0.49855	0.333344	0.159424	0.347839	0.286957	0	-0.034783	0.066667	0.1072464	0.037682	0.321739	0.727531	0.718842	0.295654	-0.971024	-0.147827	0.342026	-0.011594	0.475365	0.385506	-1.547821	0.162319	0.050569	-0.747826
HCHO_6	0.104355	0.515945	1.173904	1.428986	0.333328	-0.371017	0.031876	0.055069	0	0.24058	-0.078261	1.10144	0.466667	0.260864	0.04348	0.504349	0.58551	-1.12175	0.205795	0.568115	-0.002899	0.315941	-0.310143	-2.495651	0.550726	0.394203	0.13623
HCHO_7	0.733322	0.875366	-0.481155	0.382614	0.956512	1.460661	0.594208	0.692749	0.011594	-0.031884	0.028899	1.344925	-0.54203	-0.194199	1.576813	1.284058	1.452164	1.753632	0.939133	0.657974	1.086957	0.513046	0.675362	0.550735	0.327536	-0.97536	
Arsine_1	-0.118835	0.756523	-0.721741	-0.562317	0.611603	0.608704	0.97104	0.811159	0	0.13043	0.034783	1.118835	-0.373917	-0.359421	0.142608	0.481171	1.121735	0.985451	-0.234787	0.173904	0.063768	0.315942	1.147827	-0.727469	0.000000		
Arsine_2	-0.252182	0.049278	-0.1524628	-0.208694	-0.1649277	-0.2175735	0.226089	0	-0.020899	0.078261	-0.591301	-0.017391	-0.475365	-0.591293	-0.297255	0.41448	-0.623184	-0.478256	0.171014	0.531333	1.562231	-0.1073044	2.026087	1.771011	-0.889854		
Arsine_3	-0.284058	-0.069569	0.118851	-1.171021	-0.202896	-1.695648	-0.1072464	0.08696	0	0.049275	0.04058	-0.446373	-1.608696	-0.927536	-0.034782	-1.020294	-0.939133	-0.686951	-0.457962	-0.857971	0	0.504348	0.284058	-0.737101	0.217391	0.88406	-0.605217
Arsine_4	0.446365	0.313042	-0.014496	1.107239	0.866669	-0.727539	0.394211	0.620293	0.011594	0.031884	0.350724	0.249275	-0.411598	-0.397102	0.524635	0.869568	1.359421	0.203676	0.75943	0.431835	0	0.330435	0.220291	-0.515938	-0.107246	0.02029	-0.031883
Arsine_5	0.762329	0.727539	0.115797	0.150726	0.550722	0.570372	0.440582	0	0.008696	0.165622	0.118843	-0.205795	0.310146	0.402899	0.202079	0.107246	0.351362	0.576813	1.278259	0.985159	0.068069	1.281159	1.513042	0.865217	0.1098551	0.1559422	-7.750725
Arsine_6	-0.194199	-0.17971	1.266674	0.234787	0.515945	0.907242	-1.191315	-0.234779	0	-0.014492	0.098851	0.976814	-0.568115	-0.208694	0.220288	0.350723	0.310437	0.098541	0.078262	0.063766	0	1.034782	0.698851	-7.428986	0.573913	0.1060867	-0.579706
Arsine_7	0.437683	0.486954	0.249283	0.324631	-0.988403	-1.107254	0.269562	-0.597107	0	0.234782	-0.136232	1.127533	-0.327538	-0.481159	0.553623	0.513046	0.22319	-0.933334	0.037674	0.626083	-0.121739	2.971014	0.294208	-11.61449	0.194208	1.756516	-8.646378
Phosphine_1	-0.944931	-1.144928	-1.179703	-0.078262	-0.988403	0.623199	-1.243469	-0.507248	-0.174826	-1.872464	-1.953623	-0.646378	0.414497	0.107159	0.976814	-0.255068	-0.923334	-3.434782	0.815562	6.713043	-31.0116	5.301449	2.765217	-21.16522	0.000000		
Phosphine_2	-0.665507	0.31884	-0.82608	-0.571014	-0.600006	-1.1884	-0.110138	-0.057968	0.034783	-0.559421	-0.121739	-0.176811	-0.199987	-0.826088	-0.026089	-1.86087	-0.298553	-0.1739136	-0.397111	-1.784806	-0.849274	2.82029	0.220889	-22.8	0.681159	-0.237679	-17.54203
Phosphine_3	-0.191299	1.797104	-0.324631	-0.373917	-0.104926	-2.36232	-2.753616	-1.443481	0.156522	0.185508	-0.098551	-0.188408	3.782608	4.353622	5.759422	0.747818	0.565619	-0.513046	-0.192743	-0.971024	2.90145	4.994204	3.356522	-24.54783	3.284058	1.65797	-16.4116
Phosphine_4	-0.597107	0.121738	-0.217377	-0.443481	-0.817383	-0.205798	-0.688985	-0.655067	0.014493	0.440582	-0.084058	0.689857	-0.272469	-0.799999	0.466667	0.127548	-0.1669571	-0.750717	0.1884	-0.266663	-0.069565	0.2785507	0.2072464	-25.08406	0.344928	-0.0550724	-17.28986
Phosphine_5	-1.142029	0.443478	-1.347824	-1.440582	-2.144928	-1.820282	-1.8116	-1.147827	-0.260807	-0.222089	-0.168116	-1.194206	-1.901443	-1.017391	-0.194204	-1.231888	-0.202280	0.350723	0.310433	-0.455069	-0.808696	0.62029	2.105797	-23.36521	-0.417391	-15.7942	
Phosphine_6	-0.197108	-1.162319	-1.968109	-0.305798	-0.455072	-0.301745	-0.237686	-1.263768	0.0126371	-0.047464	0.0424058	-0.595419	-1.31015	-0.0840576	0.707245	-0.2020012	-0.272464	-0.217397	-0.2950797	0.005797	3.171014	2.712015	4.73913	1.272461	-17.3913		
Phosphine_7	-0.982605	-0.698551	-0.179703	-1.515945	-0.211594	-0.2072464	0.202896	0.005797	-0.031884	-0.318841	-0.486961	-1.086952	-0.971012	-0.602898	-1.915939	-1.657974	-0.014481	-1.779709	-1.457977	0	0.62029	0.124638	-17.01739	0.765217	-0.194202	-15.48985	
Diborane_1	1.084061	0.118843	0.136246	0.576813	1.228989	1.437683	1.356522	0.86087	0.031884	-0.208695	-0.031884	0	0.026085	-0.176811	-0.440578	0.950729	1.249283	0.50145	-0.026093	0.108161	-0.069565	0.043478	0.411594	-0.8116	-2.147826	-2.571014	-2.614494
Diborane_2	1.028976	0.133331	0.63768	1.127533	0.715942	1.884064	0.684067	0.151045	0.121739	0.423189	0.95652	0.301453	0.1057972	0.675362	0.228989	0.237268	0.7297113	0	0.284058	0.072464	-1.344925	-0.113043	-0.130436	-1.91304			
Diborane_3	-0.568115	0.121738	-0.334775	0.402893	0.210735	-0.310135	-0.388948	0.321739	0	-0.556521	-0.2	-0.382614	0.302291	0.307247	-0.344927	-1.173331	0.60289	0.026093	0.304352	0	0.063768	0.02029	-0.2857971	0	-0.073563	0.884056	
Diborane_4	0.260864	0.686954	0.060687	0.017395	0.217392	0.263779	0.113037	0	0.440579	0.115942	0.399994	0.742027	0.081161	-0.68116	-0.08696	-1.231888	0.318848	0									

	R28	G28	B28	R29	G29	B29	R30	G30	B30	R31	G31	B31	R32	G32	B32	R33	G33	B33	R34	G34	B34	R35	G35	B35	R36	G36	B36	
SO2_1	0.510132	-0.710144	-0.084061	0.634781	0.179703	-0.971024	-0.60289	0.191299	-0.483956	0.010499	-0.000499	0.000499	-0.000499	0.000499	-0.000499	0.000499	-0.000499	0.000499	1.597107	-1.371017	-1.669571	-0.02029	21.41449	17.34493	-26.74783	18.10145	16.32174	-22.51595
SO2_2	-0.350723	-1.173912	-0.663757	0.217392	0.057968	-0.597092	-0.142028	0.49276	-0.063768	0.226087	-0.11884	-0.518829	17.96812	19.32174	-5.028992	0.915939	-0.576813	0.405792	0.828979	-1.44928	0.008696	20.58261	16.51014	-26.39421	16.55652	15.03768	-22.74203	
SO2_3	-1.962311	-1.147827	-2.446381	-2.782608	-0.417395	-3.371017	-2.542038	-1.852173	-1.324638	-0.217391	-0.611594	-0.495667	18.32463	18.97681	-5.915939	-0.53334	0.800003	1.713043	-1.110138	-3.101456	0	14.88406	13.09275	-24.85797	9.855073	10.89565	-20.50725	
SO2_4	0.89856	0.971016	0.455063	0.817398	0.373917	0.736237	-0.089858	0.234787	0.617391	0.344928	0.249275	0.559418	18.76232	20.53623	-5.515945	0.36232	0.220291	-0.011597	0.089859	-1.049271	-0.405797	20.72174	16.23188	-23.27246	17.13044	14.75942	-20.54202	
SO2_5	-0.956528	-0.426086	-1.77681	-0.828979	-0.405807	-2.411591	-0.82608	-0.886955	0.286956	-0.139131	0.011594	0.342026	16.94782	18.24058	-4.47826	-1.368118	-0.58551	-0.371017	-1.101456	-3.968109	0.049275	19.44348	15.37101	-25.67535	14.85217	13.15653	-21.35073	
SO2_6	0.240585	-0.318844	0.130432	0.310135	-0.292755	-0.750732	-0.391296	-0.356522	-0.005797	0.037681	0.089855	-0.27536	15.92754	16.29565	-3.82026	-0.405792	-1.194214	0.814484	0.295654	-2.394211	0.037681	6.881159	8.66087	-18.48116	4.663768	7.747826	-12.55942	
SO2_7	0.492752	0.901451	0.907242	0.927536	1.25798	0.333328	-0.371017	0.953613	-0.136232	0.376812	0.231884	0.405792	21.59421	23.68406	-5.292755	1.515945	2.594208	1.394196	1.889862	0.359421	0.492754	19.78841	16.51884	-24.33623	18.46377	16.47247	-20.11594	
HCN_1	-1.423187	-0.333336	-0.881165	1.301452	-1.13913	-3.191315	-0.933334	-0.165215	0	-0.185507	0.008696	-0.478256	39.46957	40.98261	-6.150723	-0.226089	0.017395	-0.298553	8.205795	-97.2058	0.991304	162.3449	116.8203	-75.06087	115.6087	79.85797	-79.11015	
HCN_2	-0.252167	-0.22319	1.072464	1.115936	-2.431885	-5.426086	0.002899	0.124634	0	-0.455073	-0.527536	-0.084061	47.01739	48.85798	-5.434784	1.049271	-0.547836	0.133331	9.336227	-105.9159	5.724638	157.3884	116.7391	-57.44637	183.0783	99.87537	-89.68696	
HCN_3	-0.237688	0.005798	0.127533	0.944916	-1.22319	-2.611603	1.492752	0.643478	0	-0.008696	0.095662	1.121733	47.97911	52.13913	-6.959423	2.565216	1.044928	0.286979	7.394196	-87.31305	12.22029	162.4986	119.3478	-64.06377	154.5971	87.45797	-77.89565	
HCN_4	0.443474	0.15942	-0.304775	-0.336243	-0.263763	-3.60289	-0.956562	0.110146	0	-0.22029	-0.017391	0.460869	33.84058	33.7826	-4.52174	0.521744	-0.226074	-0.365204	7.292755	-84.16232	0.530435	160.5246	112.8493	-78.08406	153.6319	84.91016	-75.0218	
HCN_5	0.434784	-0.06377	-0.666656	1.475357	0.594193	-2.379715	0.376801	0.217392	-0.063768	-0.153623	0.026087	-0.22219	45.6174	47.72754	-4.950726	0.573914	-0.043472	0.081161	8.095657	-73.2058	10.76522	165.9102	121.9681	-63.52754	158.8667	88.15653	-78.14203	
HCN_6	-0.86087	-0.115944	-1.1884	0.805801	-0.017395	-2.962311	-0.113052	0.078255	0	-0.336232	-0.243478	0.994202	45.97681	49.86667	-5.144928	-0.576813	-0.113052	-1.565216	7.063766	-84.14494	2.133333	157.6841	110.258	-67.82898	147.3768	77.6	-56.91304	
HCN_7	0.304352	0.310146	-0.078262	0.03479	-0.486954	-0.17392	-0.095657	0.142029	0	-0.034783	0.130435	0.524635	47.64349	54.95652	-5.394199	1.814499	2.194199	3.321732	7.918839	-74.46378	0.75942	173.9971	126.5362	-75.05218	160.2087	93.31305	-85.9864	
HF_1	-2.243469	-0.231884	-1.289856	-0.634781	-3.304352	-4.226089	-0.1788406	-0.092751	0	-0.315942	-0.069565	-0.400002	6.002899	6.878258	-0.349492	0.434844	-0.828979	-0.217392	5.959412	-115.4435	2.191304	32.85797	30.29276	-52.37972	24.42899	21.46956	-39.36232	
HF_2	-0.478271	-0.417389	0.107254	-0.028992	-0.620282	-0.886965	0.101456	-0.194206	0	0.130435	0.182609	-0.107254	7.449274	7.524635	-0.278263	-1.907242	-2.269577	-2.898544	8.513046	-99.22138	8.785857	23.24638	24.61739	-45.72173	14.95362	16.69565	-31.91884	
HF_3	1.217392	0.484058	1.388397	1.36232	1.568115	0.472473	0.814499	0.533333	0	0.176812	0.075362	1.782608	8.608696	7.327538	0.191303	4.779709	4.368118	5.394211	8.252182	-74.9884	4.64058	15.26087	16.50435	-34.93043	16.23768	17.77391	-28.92754	
HF_4	-1.391304	0.255072	-0.68984	1.026093	-1.078262	-2.568115	-0.881149	1.028984	0	0.281159	0.286957	-0.681168	5.663765	4.704346	0.44058	2.336227	0.582611	0.634781	5.831894	-129.9275	9.736232	21.89275	22.56232	-37.61739	15.67246	18.89855	-30.89276	
HF_5	-2.162323	0.365215	-0.037689	-0.182617	-2.721725	-5.96521	-0.997101	-0.486961	0	-0.153624	0.017391	-1.237686	5.536232	5.823189	-1.591305	0.469574	-0.211594	-0.205795	6.86377	-119.4754	7.918839	19.4202	46.85507	39.86667	49.67246	13.91884	15.65217	-26.27826
HF_6	-0.388412	0.350727	-0.184061	0.979706	1.834778	-0.060687	-0.333328	0.440575	-0.084058	0.142029	0.202899	-1.150726	4.991302	5.759415	-0.18261	1.321732	-0.539139	1.147827	7.707245	-111.4638	8.64058	39.24058	32.62318	-45.98261	15.68116	16.25507	-26.22609	
HF_7	-0.133331	0.721737	1.356522	0.944916	-0.571014	-3.510147	0.286957	0.344925	-0.014493	0.142029	0.081159	0.046387	4.840576	4.857971	-0.313042	0.631882	-0.040573	1.704346	8.31015	-100.4812	4.443478	24.53043	22.6116	-38.73043	13.16232	14.29565	-20.83768	
HNO3_1	-2.376816	-0.118841	-1.194199	-1.278275	-1.17392	-2.046371	-2.597107	-0.014496	0	0.089855	0.156522	-0.484055	-3.944916	-7.118843	-10.51303	-0.918839	-2.110153	-3.330429	3.565216	-53.12463	16.99104	-15.42319	7.165216	11.65216	1.208696	1.805798	-9.333336	
HNO3_2	-2.159424	0.785507	0.108696	1.286957	-1.866669	-5.686951	0.1043472	1.828987	0	0.124638	0.046377	0.138506	3.440582	3.631886	0.8464376	4.301437	0.4095657	0.6260864	6.272852	-62.06667	0.002899	11.2058	11.64928	-12.62029	2.626087	4.463768	-7.736229	
HNO3_3	-1.652176	0.457972	0.110138	-0.657974	-1.023178	-3.321732	-1.040573	-0.599998	0	0.121739	-0.02029	-0.472466	1.950722	2.568115	0.489857	-0.837677	-0.933319	-0.423187	4.286957	-57.55363	0.002899	7.973913	9.008696	-15.03768	0.953623	2.991304	-9.028984	
HNO3_4	-2.376816	-0.118841	-1.194199	-1.278275	-1.17392	-2.046371	-2.597107	-0.014496	0	0.089855	0.156522	-0.484055	-3.944916	-7.118843	-10.51304	-0.918839	-2.110153	-3.330429	3.565216	-53.12463	0.002899	7.973913	9.008696	-15.03768	0.953623	2.991304	-9.028984	
HNO3_5	-0.62899	0.133333	-0.631882	1.313034	-1.023193	-1.457962	-0.472458	0.62899	-0.04058	-0.156522	0.150725	1.460869	2.13044	1.710144	-0.707247	-0.150711	0.228989	0.652176	4.113037	-50.46087	0.014493	2.672463	3.686957	-8.336231	1.443478	2.797102	-6.559422	
HNO3_6	0.072464	0.107246	0.834778	1.371017	0.53334	1.420288	1.185501	0.521744	0	0.150725	0.107246	0.785507	3.823189	2.791306	-1.072464	1.733337	-0.284058	1.281158	3.968109	-46.58261	0.226087	3.73913	5.168116	-10.47826	1.327536	2.489857	-5.875362	
HNO3_7	-0.86087	0.486956	-0.628983	-0.069565	-0.733337	-1.289856	-1.05217	-0.333336	0	-0.023188	-0.014493	0.794205	2.617386	2.289856	-1.486956	0.933334	0.678268	-0.026093	3.286957	-41.15072	0	3.055072	3.197102	-6.715942	0.24058	0.362318	-3.011593	
Hydrazine_1	-0.72464	0.4058	-0.228989	-0.628998	-0.681168	0.759415	-0.315948	1.005798	0	-0.165217	0.150725	-0.3797	-0.913048	-1.034782	0.191305	-0.263779	1.260864	1.307251	-1.055084	-2.127533	-0.005797	-1.530434	-2.768116	-3.194214	-1.362319	-4.385506	-5.026093	
Hydrazine_2	-0.373917	0.057976	0.136246	-0.634781	0.037689	0.779724	-0.295654	0.50145	0.034783	0.823189	-0.15942	0.976822	-1.834778	-2.162319	0.571014	0.25798	0.982605	-0.89566	-1.298553	-0.823196	0.585507	-1.71594	-4.97681	-7.31884</td				