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Supporting Information

Nature of selenium hydrogen bonding: Gas phase spectroscopy and quantum chemistry calculations

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1. Experimental and Computational Methods

Experimental Methods

Materials: Indole (Sigma-Aldrich, purity ≥ 99.0%), phenol (Sigma-Aldrich, purity ≥ 99.0%) and dimethyl selenide (Alfa Aesar, purity ≥ 90.0%) were used without any further purification.

The experiment was performed in a home-built jet-cooled Time of Flight mass spectrometer. The experimental setup was described elsewhere in details.[1] Only a brief description is presented here. The experimental techniques used in this work were two-color resonant 2-photon ionization (2C-R2PI) spectroscopy, resonant ion-dip infrared (RIDIR) spectroscopy, and IR-UV hole-burning spectroscopy.

Two-color resonant 2-photon ionization (2C-R2PI) spectroscopy: Mass selected electronic spectra of indole…dimethyl selenide (indmse) and phenol…dimethyl selenide (phdmse) dimeric complexes were measured using 2C-R2PI spectroscopy. To synthesize indmse/ phdmse complexes in a supersonic jet, mixed vapor of dimethyl selenide (maintained at -78^{0}C by keeping it in a dry ice bath) and indole (heated at 75 ^{0}C)/phenol (heated at 40 ^{0}C) is seeded in a carrier gas mixture of He/Ne (30:70) at 55 psig was expanded in high vacuum through a pulsed nozzle (General valve, series 9, 0.5 mm orifice diameter, 10 Hz rep. rate). The molecular complexes were ionized using 2-color resonant 2-photon ionization (2C-R2PI) technique. In this technique, the wavelength of the first photon obtained from frequency doubled output of a tunable dye laser (Continuum, ND6000, 10 Hz, 10 ns, 80 μJ/pulse) pumped by second harmonic output of a Nd:YAG laser (10 Hz, 10ns, Surelite II-10, Continuum) is scanned through the vibronic levels of the S_1 state. Subsequently another photon of fixed wavelength (355 nm) obtained from frequency doubled output of another tunable dye laser (Continuum, ND6000, 10 Hz, 10 ns, 800 μJ/pulse) pumped by second harmonic output of a Nd:YAG laser (10 Hz, 10 ns, Surelite II-10, Continuum) without any time delay from the first laser ionizes the molecules from the S_1 state. The ions were mass analyzed in the Time of Flight mass spectrometer and detected using a microchannel plate detector.

Resonant ion-dip infrared (RIDIR) spectroscopy: The IR spectra of the complexes were measured using RIDIR spectroscopy. In this technique, the excitation UV laser wavelength was fixed at one particular transition in the electronic spectrum and the ionization laser fired without any delay from the excitation laser was fixed at 355 nm. A tunable IR laser (resolution ~ 2 cm^{-1}, OPO/OPA, Laser Vision), pumped by a Nd:YAG laser (10 Hz, 10 ns, Surelite II-10, Continuum) preceded the UV lasers by 100 ns was scanned through the N-H/O-H stretching frequency region. Whenever the IR laser frequency is in resonance with any of the vibrational frequency of molecules or complexes, depletion in the UV signal appears as the IR spectrum.

IR-UV hole-burning spectroscopy: This technique is similar to the RIDIR spectroscopy. However the IR laser is fixed to a particular vibrational transition in the IR spectrum and the excitation UV laser is scanned through the whole region of the R2PI spectrum. Here, the ion signal for the electronic bands in the R2PI spectrum belonging to the same conformer is depleted while the IR laser is parked to specific vibration of the conformer. This spectroscopy was used to verify the presence of more than one conformer of indmse and phdmse complexes in the experiment.

Computational methods

We optimized the structures of different conformers of indole and phenol complexes at the B97-D level of theory using 6-311++g(d,p), cc-pVTZ and aug-cc-pVTZ basis sets. Vibrational frequencies of different conformers of the complexes were calculated using the same level of theory to ascertain that the optimized structures are true minima. Binding energies of the complexes were calculated considering basis set superposition error (BSSE) and zero point energy (ZPE) corerctions. Apart from the energy calculated at the B97-D level, we also calculated the energy of the monomers and complexes at the CCSD/6-311++g(d,p) level of theory (single point calculation), to check for the consistency of the DFT functional that was used. Thermal correction to the binding energy was done to calculate the Gibbs free energy (ΔG) at 10 K for the formation of the complexes using thermochemical analysis in Q-Chem. ΔG has been calculated at an average temperature of 10 K considering that translational (~ 1 K), rotational (<10 K) and vibrational temperatures (30-50 K) in supersonic jet are different.

To determine different components of the interaction energies in the S/Se hydrogen bonded complexes, Symmetry Adapted Perturbation Theory (SAPT) at the level of SAPT2/aug-cc-pVDZ and Absolutely Localized Molecular Orbital-Energy Decomposition Analysis (ALMO-

EDA) at the B97-D/6-31+G(d,p) level were performed. To determine the structures of the observed conformers of the complexes in the experiment, theoretical IR spectra of various conformers were compared with the experimental IR spectra of the complexes. As the vibrational frequencies were calculated according to harmonic approximation, the calculated frequencies (N-H and O-H) were corrected using a scaling factor. The scaling factor was obtained from the ratio of experimental N-H/O-H stretching frequency of monomer (indole/phenol) and calculated harmonic N-H/O-H stretching frequency of monomer (indole/monomer) obtained at a particular level of theory and basis set. The scaling factors obtained for N-H and O-H stretching frequencies at the B97-D/6-311++g(d,p) level of theory are 0.9588 and 0.9609, respectively while the same obtained for N-H and O-H stretching frequencies at the B97-D/aug-cc-pVTZ level of theory are 0.978 and 0.9795, respectively. All the calculations were performed using Gaussian09[2] and Q-Chem 4.0 software packages[3].

Detailed NBO calculations were performed using NBO6.0 program to determine charge transfer (CT) values in various conformers of indole and phenol with dmse, dms and dmo along with the change in the occupancy of lone pair orbitals ($\Delta\eta_s$and $\Delta\eta_p$) of the donor atoms (Se/S/O) and σ^* anti bonding orbital ($\Delta\sigma^*_{N\text{-}H/O\text{-}H}$) of the N-H/O-H bond upon complex formation. The NBO calculations were carried out at the B97-D level of theory using 6-31+G(d), 6-311++g(d,p) and cc-pVTZ basis sets. CT is defined as the difference between the sum of all the natural charges over individual atom in the complex and the sum of all the charges over individual atom in the monomers. In regard to the strength of the hydrogen bond, it is more important to look at the change in the occupancy of lone pair orbitals ($\Delta\eta_s$and $\Delta\eta_p$) of the hydrogen bond acceptor atoms (Se/S/O) and antibonding orbital ($\Delta\sigma^*_{N\text{-}H/O\text{-}H}$) of the N-H/O-H bond upon complex formation. The hydrogen bond acceptor atoms (Se/S/O) have s and p types of lone pair orbitals. However it has been found that the efficient charge transfer from the acceptor atoms to the hydrogen bond donor occur mostly from the p-type lone pair orbital for all the S and Se complexes. It is interesting to note that the charge transfer from both s and p type lone pair orbitals of oxygen atom in the case of indmo and phdmo complexes is negligible.

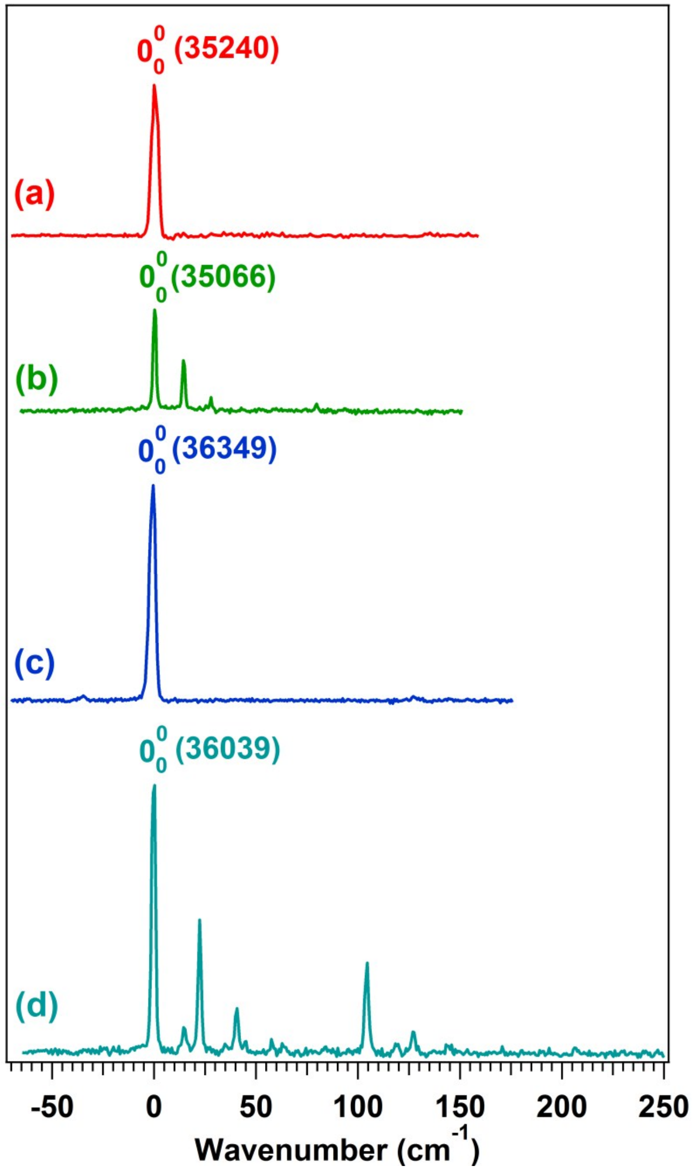

Figure S1. Electronic spectra of (a) indole, (b) indmse, (c) phenol, and (c) phdmse complexes measured using 2C-R2PI spectroscopy. The spectra have been presented in relative wavenumber scale with respect to the 0_0^0 bands of the complexes.

Table S1. Observed and calculated low frequency intermolecular vibrational modes of indmseA in the S_1 state. The S_1 state intermolecular vibrational modes are calculated at the TD-B3LYP/6-31G(d) level of theory

Observed (cm^{-1})	Calculated (cm^{-1})	Assignments
14	20	α
28		2α
	36	
	48	
	70	
79	85	σ
	110	

Table S2. Observed (S_1) and calculated (S_0)[a] low frequency intermolecular vibrational modes of phdmseA complex. The S_0 state low frequency vibrational modes are calculated at the B97-D/6-311++G(d,p) level of theory

Observed (cm^{-1})	Calculated (cm^{-1})	Assignments
14	17	α'
22	28	β'
34		α'+ β'
40		2β'
57	59	(α'+2β')/(γ')
62		3β'
	72	
104	86	σ'
119	113	(σ'+ α')/(δ')
127		σ'+ β'
145		σ'+2β'

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[a] Low frequency intermolecular vibrations of phdmse could not be calculated at the S_1 state as there was a problem in optimizing the geometry of the complex due to breaking of the Se-CH_3 bond. However the low frequency vibrations calculated at the S_0 level match pretty well with those observed in the experiment.

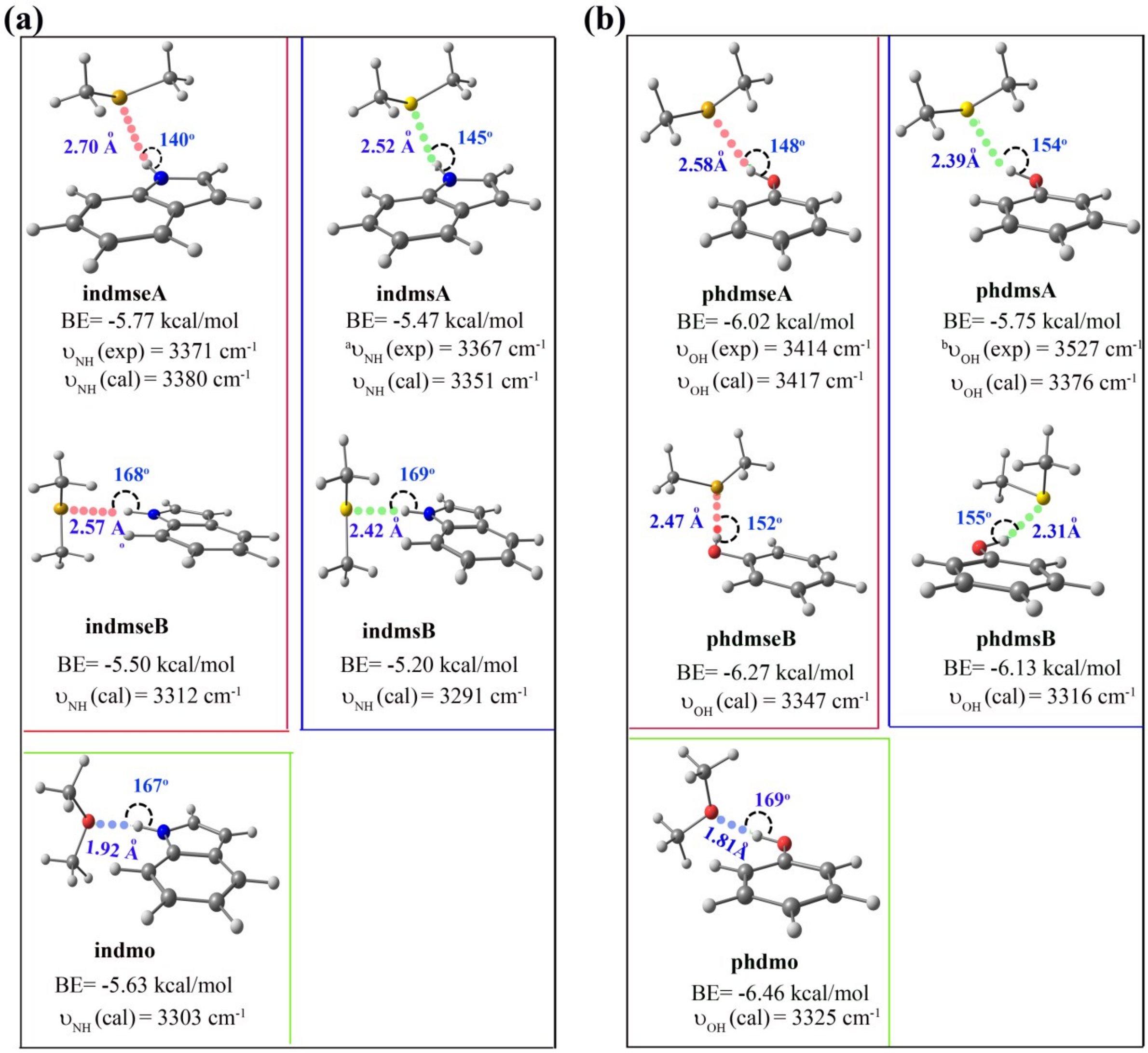

Figure S2. Structures of various conformers of (a) indole and (b) phenol complexes with dimethyl selenide (dmse), dimethyl sulfide (dms) and dimethyl ether (dmo) optimized at the B97-D/aug-cc-pVTZ level of theory. BE represents the BSSE and zero point energy corrected binding energies of the complexes. $^{a}\nu_{NH}$(exp) = 3367 cm^{-1} (Experimental N-H stretching frequency of indms) and $^{b}\nu_{OH}$(exp) = 3527 cm^{-1} (Experimental O-H stretching frequency of phdms) are taken from references 18 and 22 (in the manuscript), respectively. Theoretical harmonic N-H stretching frequencies [ν_{NH}(cal)] of the indole complexes and O-H stretching [ν_{OH}(cal)] frequencies of the phenol complexes provided with the structures in the figure are scaled using factors of 0.978 and 0.9795, respectively. It should be pointed out here that ν_{OH} (cal) of phdmsA is quite far away from ν_{OH} (exp). However this is a minimum energy structure and calculation at this level of theory shows two different structures of phenol...dimethyl sulphide complex.

Table S3. BSSE and zero point energy corrected binding energies (BE) in kcal/mol of various conformers of Se, S, and O centered hydrogen bonded complexes of indole as well as phenol calculated at various levels of theory. CCSD and B97-D/6-31+G(d,p) calculations are done at single point level

	Complexes	BE B97-D/6-311++G(d,p)	BE B97-D/6-31+G(d,p)	BE B97-D/cc-pVTZ	BE B97-D/aug-cc-pVTZ	BE CCSD/6-311++G(d,p)
Complexes of Indole	indmseA	-6.41	-6.83	-5.75	-5.77	-4.47
	indmseB	-6.11	-6.00	-5.53	-5.50	-4.26
	indmsA	-6.26	-5.77	-5.49	-5.47	-5.05
	indmsB	-5.75	-5.03	-5.27	-5.20	-4.23
	indmo	-6.78	-6.87	-5.51	-5.63	-5.70
Complexes of Phenol	phdmseA	-6.63	-7.02	-5.96	-6.02	-4.54
	phdmseB	-7.11	-7.40	-6.16	-6.27	-4.87
	phdmsA	-6.54	-5.52	-5.68	-5.75	-4.98
	phdmsB	-6.65	-6.36	-6.04	-6.13	-5.23
	phdmo	-7.70	-6.54	-6.29	-6.46	-6.51

Table S4. Comparison of BSSE and zero point corrected binding energies (BE, in kcal/mol) and Gibbs free energies (Δ*G*, in kcal/mol) of various conformers of hydrogen bonded complexes of indole and phenol calculated at the B97-D/6-311++G(d,p) level of theory. Δ*G* has been calculated at 10 K and 50 K

	Complexes	BE	Δ*G* (10 K)	Δ*G* (50 K)
Complexes of indole	indmseA	-6.41	-6.05	-5.58
	indmseB	-6.11	-5.81	-5.56
	indmsA	-6.26	-6.12	-5.92
	indmsB	-5.75	-5.48	-5.32
	indmo	-6.78	-6.51	-6.14
Complexes of phenol	phdmseA	-6.63	-6.44	-5.98
	phdmseB	-7.11	-6.72	-6.35
	phdmsA	-6.54	-6.16	-5.91
	phdmsB	-6.65	-6.29	-5.87
	phdmo	-7.70	-7.40	-7.23

Table S5. Different components of the total interaction energy (kcal/mol) of various conformers of hydrogen bonded complexes of indole and phenol calculated at the SAPT2/aug-cc-pVDZ level of theory. Theoretical red-shift ($\Delta\nu_{cal}$ in cm^{-1}) values in the N-H/O-H stretching frequency of the complexes with respect to indole/phenol monomer are also provided in the table

	Complexes	$\Delta\nu_{cal}$	ΔE_{Ele}	ΔE_{Pol}	ΔE_{Disp}	ΔE_{Rep}	ΔE_{Total}
Complexes of Indole	indmseA	151	-8.25	-2.96	-7.14	11.66	-6.69
	indmseB	181	-7.30	-3.32	-6.15	10.98	-5.79
	indmsA	163	-8.33	-4.78	-6.85	13.22	-6.74
	indmsB	219	-8.17	-3.75	-6.63	12.62	-5.93
	indmo	252	-10.70	-3.77	-4.88	12.42	-6.93
Complexes of Phenol	phdmseA	236	-9.23	-3.69	-7.08	12.69	-7.31
	phdmseB	322	-9.69	-4.34	-6.31	13.14	-7.20
	phdmsA	119	-9.41	-3.37	-7.42	12.84	-7.36
	phdmsB	326	-10.27	-4.64	-6.13	13.54	-7.50
	phdmo	218	-14.26	-5.16	-5.20	16.86	-7.76

Table S6. Decomposition of interaction energies (kcal/mol) of different conformers of the complexes of indole and phenol obtained at the B97-D/6-31+G(d,p) method using ALMO-EDA method. Theoretical red-shift ($\Delta\nu_{cal}$ in cm^{-1}) values in the N-H/O-H stretching frequency of the complexes with respect to indole/phenol monomer are also provided in the table

	Complexes	$\Delta\nu_{cal}$	ΔE_{Frz}	ΔE_{Pol}	ΔE_{CT}	ΔE_{Total}
Complexes of Indole	indmseA	151	-2.94	-0.92	-3.05	-6.91
	indmseB	181	-1.71	-1.00	-3.69	-6.40
	indmsA	163	-2.50	-0.95	-3.09	-6.54
	indmsB	219	-0.87	-1.12	-4.09	-6.09
	indmo	252	-2.83	-1.58	-2.84	-7.25
Complexes of Phenol	phdmseA	236	-2.61	-1.10	-3.99	-7.69
	phdmseB	322	-1.83	-1.34	-4.54	-7.71
	phdmsA	119	-2.68	-1.06	-3.32	-7.05
	phdmsB	326	-1.33	-1.45	-4.68	-7.46
	phdmo	218	-2.40	-2.26	-3.88	-8.54

Table S7. NBO charge transfer values (CT) in various conformers of indmse, indms, and indmo complexes calculated at the B97-D/6-311++G(d,p) level of theory using various basis sets. Change in the occupancy of s and p-type lone pair orbitals ($\Delta\eta_s$ and $\Delta\eta_p$) of the hydrogen bond acceptor atoms (Se/S/O) and antibonding orbital ($\Delta\sigma^*_{N\text{-}H}$) of the N-H bond upon complex formation are also shown

Complexes	Methods	CT	$\Delta\eta_s{}^a$	$\Delta\eta_p{}^b$	$\Delta\sigma^*_{N\text{-}H}$
indmseA	B97-D/6-31+G(d)	0.0348	-0.0011	-0.0357	0.0331
	B97-D/6311++G(d,p)	0.0332	-0.0008	-0.0290	0.0279
	B97-D/cc-pVTZ	0.0304	-0.0010	-0.0262	0.0251
indmseB	B97-D/6-31+G(d)	0.0408	-0.0017	-0.0391	0.0368
	B97-D/6311++G(d,p)	0.0381	-0.0016	-0.0325	0.0322
	B97-D/cc-pVTZ	0.0358	-0.0017	-0.0301	0.0295
indmsA	B97-D/6-31+G(d)	0.0358	-0.0012	-0.0400	0.0306
	B97-D/6311++G(d,p)	0.0353	-0.0007	-0.0248	0.0288
	B97-D/cc-pVTZ	0.0296	-0.0007	-0.0201	0.0244
indmsB	B97-D/6-31+G(d)	0.0430	-0.0013	-0.0366	0.0391
	B97-D/6311++G(d,p)	0.0434	-0.0013	-0.0323	0.0368
	B97-D/cc-pVTZ	0.0376	-0.0014	-0.0266	0.0315
indmo	B97-D/6-31+G(d)	0.0363	-0.0084	-0.0074	0.0319
	B97-D/6311++G(d,p)	0.0308	-0.0066	-0.0011	0.0249
	B97-D/cc-pVTZ	0.0242	-0.0035	0.0038	0.0200

Table S8. NBO charge transfer values (CT) in all the possible conformers of phdmse, phdms, and phdmo complexes calculated at the B97-D/6-311++G(d,p) level of theory using various basis sets. Change in the occupancy of s and p-type lone pair orbitals ($\Delta\eta_s$ and $\Delta\eta_p$) of the hydrogen bond acceptor atoms (Se/S/O) and antibonding orbital ($\Delta\sigma^*_{N-H}$) of the N-H bond upon complex formation are also shown

Complexes	Methods	CT	$\Delta\eta_s$[a]	$\Delta\eta_p$[b]	$\Delta\sigma^*_{O-H}$
phdmseA	B97-D/6-31+G(d)	0.0422	-0.0012	-0.0388	0.0372
	B97-D/6-311++G(d,p)	0.0372	-0.0008	-0.0295	0.0305
	B97-D/cc-pVTZ	0.0362	-0.0012	-0.0284	0.0307
phdmseB	B97-D/6-31+G(d)	0.0528	-0.0004	-0.0490	0.0470
	B97-D/6-311++G(d,p)	0.0485	-0.0004	-0.0404	0.0415
	B97-D/cc-pVTZ	0.0467	-0.0006	-0.0390	0.0412
phdmsA	B97-D/6-31+G(d)	0.0329	-0.0018	-0.0260	0.0283
	B97-D/6-311++G(d,p)	0.0311	-0.0012	-0.0202	0.0233
	B97-D/cc-pVTZ	0.0267	-0.0013	-0.0164	0.0216
phdmsB	B97-D/6-31+G(d)	0.0543	-0.0012	-0.0450	0.0485
	B97-D/6-311++G(d,p)	0.0527	-0.0010	-0.0392	0.0449
	B97-D/cc-pVTZ	0.0465	-0.0012	-0.0346	0.0418
phdmo	B97-D/6-31+G(d)	0.0443	-0.0119	-0.0104	0.0417
	B97-D/6-311++G(d,p)	0.0400	-0.0092	-0.0039	0.0348
	B97-D/cc-pVTZ	0.0322	-0.0066	0.0020	0.0310

Cartesian Co-ordinates of the optimized geometries of the complexes at the B97-D/6-311++G(d,p) level of theory:

indmseA

Atom	X	Y	Z
N	-0.4684236059	-0.8449167272	-0.8049382440
C	-3.7418590230	1.3439823226	0.4387728477
C	-3.6577554815	-0.0331977307	0.6132862671
C	-2.5057884078	-0.7092963995	0.1660260538
C	-2.0735225201	-2.0811677960	0.1844236081
C	-0.8321256422	-2.1154478855	-0.4035164617
C	-1.4655518207	0.0403313745	-0.4565862661
C	-1.5490321000	1.4276317938	-0.6393309154
C	-2.6974097263	2.0675811435	-0.1815212156
H	-4.6243947632	1.8773590158	0.7805102428
H	-4.4672856695	-0.5810160170	1.0884288101
H	-2.6152118889	-2.9312856564	0.5754277405
H	-2.7962188796	3.1420417695	-0.3083316599
H	-0.7502848471	1.9805820946	-1.1253988880
H	0.4561298406	-0.5815555063	-1.1286572340
H	-0.1706355712	-2.9521901528	-0.5817538317
C	2.3408038943	-1.1238944130	1.1968067836
H	1.2536515725	-1.2188811664	1.2712076675
H	2.7775786305	-2.0769316142	0.8849644751
H	2.7707180568	-0.8211843224	2.1552013824
C	1.8136378601	1.6946337058	0.6625605038
H	2.2903904554	1.9549193018	1.6114428771
H	1.8631949708	2.5482427728	-0.0191527043
H	0.7705870430	1.4074765077	0.8203001139
Se	2.7905568496	0.2082961311	-0.1829155336

indmseB

Atom	X	Y	Z
N	-0.6081194386	-1.1312939803	-0.3531905215
C	-3.7058279922	1.5551650119	0.1508806907
C	-3.8921324058	0.1787904584	0.2271072549
C	-2.7858904855	-0.6731671644	0.0444125557
C	-2.6022459997	-2.0994560389	0.0571529359
C	-1.2695426842	-2.3309752476	-0.1837382976
C	-1.5070278759	-0.0969365295	-0.2153679371
C	-1.3170124217	1.2897278417	-0.2929377560
C	-2.4299113581	2.1056750533	-0.1068768612

H	-4.5524323582	2.2214922657	0.2900117447
H	-4.8774505582	-0.2348602757	0.4254210210
H	-3.3589462835	-2.8540863510	0.2211117474
H	-2.3153222594	3.1845693341	-0.1628454757
H	-0.3393556459	1.7169953404	-0.4947300890
H	0.3921564544	-1.0291807109	-0.4965359976
H	-0.7273719318	-3.2640396317	-0.2541853939
C	1.9035678923	0.4371297741	1.5739876419
H	0.8668230437	0.6959837769	1.3451659772
H	1.9249644887	-0.3610418710	2.3209398354
H	2.4481121296	1.3071550546	1.9505254853
C	2.6957077295	1.3816380894	-1.1092362614
H	3.1613177559	2.2077609479	-0.5651410039
H	3.2473938120	1.1942423624	-2.0343658770
H	1.6545323092	1.6157005117	-1.3454611813
Se	2.8104804156	-0.2616331580	-0.0301998366

indmsA

I Atom	X	Y	Z
N	0.0559266969	-0.8590316057	-0.7689239741
C	-3.3468293584	1.1745559085	0.3869739911
C	-3.2033678624	-0.1971034003	0.5659705319
C	-2.0105902222	-0.8196397160	0.1484849064
C	-1.5147767980	-2.1694802454	0.1800787683
C	-0.2583781869	-2.1454308772	-0.3763795732
C	-0.9912593385	-0.0224880906	-0.4492604354
C	-1.1334441109	1.3595940292	-0.6346678293
C	-2.3215583276	1.9458049621	-0.2075035024
H	-4.2616312633	1.6664122148	0.7053664303
H	-3.9983197636	-0.7811760391	1.0222378183
H	-2.0246572917	-3.0440273633	0.5598233085
H	-2.4666530711	3.0145044734	-0.3382619646
H	-0.3489885212	1.9488807119	-1.1010501694
H	0.9690152531	-0.5520744694	-1.0880248391
H	0.4442643465	-2.9513508593	-0.5390406262
C	3.1330971327	-1.0347440026	0.8855459486
H	2.0980977648	-1.3173064855	1.1066002878
H	3.6575207057	-1.8834709412	0.4367435787
H	3.6484434142	-0.7396880180	1.8052982904
C	2.2352242924	1.5797776088	0.6376348142
H	2.7785222287	1.8344034164	1.5533995273
H	2.1434295057	2.4741247587	0.0145181271
H	1.2357529877	1.2048025592	0.8806617565
S	3.1730505563	0.3368220103	-0.3294624664

indmsB

N	-0.0175977772	-1.1318176100	0.0000112808
C	-3.1226929298	1.5983264959	0.0000628638
C	-3.3357838107	0.2237382286	0.0000047158
C	-2.2250160837	-0.6416364818	-0.0000084661
C	-2.0678950815	-2.0707712182	-0.0001548744
C	-0.7176634315	-2.3216020778	0.0001371697
C	-0.9118432943	-0.0824640432	0.0000463360
C	-0.6961867017	1.3035000157	0.0000963821
C	-1.8151135283	2.1327436842	0.0001078590
H	-3.9722981894	2.2753265175	0.0000465238
H	-4.3454730239	-0.1785413427	-0.0000625531
H	-2.8532858217	-2.8137692785	-0.0002967521
H	-1.6790925648	3.2105771525	0.0001336857
H	0.3038675689	1.7249997525	0.0001183235
H	0.9969768171	-1.0599739758	0.0000100243
H	-0.1851568277	-3.2628240624	0.0002216795
C	2.8193114707	0.7060765128	1.4063072382
H	1.7372346040	0.8650280180	1.4481039470
H	3.1398130173	0.1913846814	2.3166847707
H	3.3418974462	1.6654591408	1.3345261771
C	2.8193723606	0.7059518532	-1.4064040343
H	3.3419568224	1.6653392994	-1.3346833950
H	3.1399160365	0.1911793511	-2.3167209933
H	1.7372972953	0.8649013596	-1.4482662215
S	3.2843770478	-0.3756676947	0.0000100330

indmo

Atom	X	Y	Z
N	0.2807690619	-1.1044549475	-0.0001440719
C	-2.8900000052	1.5580769726	0.0000669645
C	-3.0767609703	0.1750669679	0.0000819658
C	-1.9464259490	-0.6704350036	0.0000069529
C	-1.7522929131	-2.0949249987	-0.0000020501
C	-0.3900309076	-2.3153659644	-0.0000920652
C	-0.6426239639	-0.0781619707	-0.0000820611
C	-0.4522059990	1.3126290341	-0.0001000625
C	-1.5906050194	2.1222510054	-0.0000230495
H	-3.7558110218	2.2192369508	0.0001249744
H	-4.0813389597	-0.2476550574	0.0001499766
H	-2.5205068939	-2.8599250180	0.0000499580
H	-1.4778340467	3.2057980082	-0.0000360501
H	0.5473239901	1.7460550592	-0.0001790732

H	1.2932060585	-0.9705869220	-0.0001750830
H	0.1658521159	-3.2461889504	-0.0001250718
C	3.3018670347	0.4928271280	1.1855088957
H	2.6388850129	1.3753031112	1.2246199035
H	3.0881640606	-0.1623878779	2.0374358977
H	4.3528140268	0.8275431544	1.2282178843
C	3.3021500086	0.4931171293	-1.1852881043
H	4.3531109997	0.8278311558	-1.2276721157
H	3.0886360157	-0.1618808756	-2.0374291023
H	2.6391909859	1.3756151126	-1.2243330965
O	3.0655620409	-0.2710068773	-0.0000131021

phdmseA

Atom	X	Y	Z
C	-2.0872052442	1.7865366529	0.0533786230
H	-2.6500952396	2.2017935489	-0.7901544312
H	-2.4794313095	2.1867146979	0.9954615767
H	-1.0208602566	2.0190267198	-0.0417293525
C	-1.3362550157	-0.5653774199	-1.5751241665
H	-0.3152870462	-0.1781563420	-1.4866961557
H	-1.3115369354	-1.6547314268	-1.6876530819
H	-1.8611280138	-0.1100875215	-2.4224022223
Se	-2.3288141089	-0.1847663601	0.1039397648
C	3.4619958198	1.1137510061	-0.3787221049
C	3.6519649237	-0.2621579963	-0.5825459917
C	2.7034919707	-1.1900710283	-0.1386819581
C	1.5475909132	-0.7422520578	0.5243509616
C	1.3586378085	0.6344889462	0.7482108484
C	2.3113657626	1.5538599773	0.2898068156
H	4.2022777839	1.8301180307	-0.7305661305
H	4.5446449689	-0.6175679736	-1.0964079289
H	2.8376600515	-2.2580310314	-0.3005838708
H	0.4723777639	0.9679409257	1.2857517876
H	2.1559766815	2.6178469802	0.4677347277
O	0.6430089622	-1.6823460890	0.9385909979
H	-0.2085120760	-1.2367101344	1.1205269298

phdmseB

Atom	X	Y	Z
C	-2.8904523393	1.3811501055	-0.4045518875
H	-3.5273332594	1.2594903379	-1.2878919771

H	-3.4566264333	1.8628718284	0.4006672123
H	-1.9971213533	1.9696122281	-0.6404036347
C	-1.3267001280	-0.9396045139	-1.3632954640
H	-0.5074981541	-0.2331434155	-1.5334561815
H	-0.9189960865	-1.9389085476	-1.1759167342
H	-2.0094360555	-0.9682202922	-2.2199195292
Se	-2.3361482928	-0.4075830664	0.2644526144
C	3.9016427675	-0.7694395652	-0.2155789802
C	3.8301037122	0.6048225149	-0.4925705682
C	2.6673436478	1.3315413643	-0.2148924432
C	1.5570296381	0.6806281290	0.3509282670
C	1.6236536926	-0.6951379551	0.6398468541
C	2.7925627572	-1.4116808009	0.3517687328
H	4.8090428175	-1.3292204467	-0.4354140754
H	4.6864177192	1.1170426968	-0.9303833416
H	2.6016406048	2.3969354255	-0.4284481247
H	0.7639026833	-1.1885371416	1.0920656330
H	2.8350287990	-2.4764668679	0.5797734125
O	0.4400615744	1.4320409884	0.6039664033
H	-0.3015744117	0.8363648725	0.8462801608

phdmsA

Atom	X	Y	Z
C	2.1951226843	0.8233208304	-0.3334323402
H	1.1367952540	1.0044280637	-0.5462058117
H	2.4291196613	1.1951841524	0.6676452948
H	2.8288909213	1.3246867513	-1.0715752517
C	1.9160148022	-1.3678353702	-2.0143876815
H	2.5578406726	-0.8973213906	-2.7661713648
H	1.9556102776	-2.4541137548	-2.1379527224
H	0.8840932877	-1.0202764111	-2.1335160651
S	2.5247236225	-0.9800027061	-0.3317895672
C	-2.8537864074	0.9341635331	-0.6339070831
C	-2.6030384454	1.5689544076	0.5886443656
C	-1.6017604779	1.1046244278	1.4431826785
C	-0.8395131298	-0.0130682106	1.0770146569
C	-1.0958649348	-0.6653054537	-0.1386051089
C	-2.0947859775	-0.1848220629	-0.9894470076
H	-3.6313384918	1.3036565091	-1.2953537252
H	-3.1881604179	2.4373069478	0.8793399993
H	-1.3929461577	1.5955948286	2.3888671582
H	-0.5100069831	-1.5408556876	-0.4042763316
H	-2.2858815370	-0.6957394954	-1.9296791825
O	0.1347013745	-0.4308794150	1.9316492788

H	0.7367857386	-1.0202527587	1.4513655919

phdmsB

Atom	X	Y	Z
C	3.504994	0.988539	0.174007
H	4.239215	0.782819	0.963383
H	4.016968	1.421887	-0.693225
H	2.741356	1.688790	0.535209
C	1.909669	-1.068002	1.186088
H	1.196387	-0.298723	1.506567
H	1.367142	-2.000220	0.992648
H	2.664868	-1.239920	1.963622
S	2.718343	-0.573388	-0.386376
C	-3.456934	-0.690690	0.192127
C	-3.305476	0.664041	0.527063
C	-2.101549	1.332363	0.279889
C	-1.029775	0.642187	-0.313229
C	-1.176455	-0.714044	-0.659972
C	-2.386144	-1.372253	-0.402273
H	-4.396058	-1.205101	0.388326
H	-4.131307	1.206685	0.986310
H	-1.974111	2.382189	0.538030
H	-0.348269	-1.237474	-1.136646
H	-2.490654	-2.421954	-0.675732
O	0.129271	1.336703	-0.536006
H	0.836811	0.708769	-0.800627

phdmo

Atom	X	Y	Z
C	-3.7266325746	0.3417907673	0.2206281891
H	-4.4279351047	-0.4925393207	0.3732005717
H	-3.6438491403	0.9221611832	1.1433089121
H	-4.1034904641	0.9867706298	-0.5882210849
C	-2.3987050985	-0.8974145526	-1.2944915769
H	-2.7371748411	-0.2838841326	-2.1432844138
H	-1.3609912458	-1.2024195517	-1.4546138832
H	-3.0393505086	-1.7880008544	-1.2114844542
O	-2.4298184487	-0.1474623852	-0.0866386056
C	3.2316995966	-0.7525934324	0.2435151319
C	3.2863419545	0.5728752430	-0.2056349809
C	2.1217821410	1.3271942408	-0.3514338187
C	0.8770559763	0.7574044100	-0.0432836978

C	0.8151456939	-0.5694787931	0.4150632778
C	1.9899274165	-1.3145543075	0.5531468712
H	4.1419518390	-1.3341900168	0.3533071647
H	4.2452142210	1.0243290311	-0.4467686238
H	2.1551013368	2.3546572251	-0.7012141834
H	-0.1492577965	-0.997716605	0.6745201091
H	1.9293477879	-2.3394608727	0.9103022401
O	-0.2311944835	1.5263614281	-0.2009212424
H	-1.0287031322	0.9838822979	-0.0543780480

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